Collection of Simulated XRD Powder Patterns for Zeolites

Editors:

M.M.J. Treacy
and
J.B. Higgins

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PREFACE

The synthesis and characterization of new zeolite materials continues unabated. The IZA Structure Commission has recognized thirty-five new topologies since the 3rd edition of this *Collection* was prepared in 1995. The total number of zeolite structure refinements has surpassed 3000 with over 1000 new refinements since 1995. Not surprisingly, the most scrutinized framework topology is that of faujasite, **FAU**, with about 600 structural studies. Probably no other inorganic host structure has received such attention. With these numbers it is apparent that this *Collection* is not comprehensive. The scope of the *Collection* has been broadly defined to include materials of interest to zeolite scientists, following the policies established at recent IZA conferences. We have attempted to be as inclusive as possible to give the users of this publication the maximum information. The structures of the porous solids that we considered comprise corner-sharing tetrahedra, and are not limited to a specific chemical composition. Materials such as metal phosphates and silica polymorphs are included.

The present *Collection* serves as a source of reference patterns for pure zeolite phases. The data will be helpful in establishing the structural purity of experimental phases and in indexing their diffraction patterns. The data will also aid in the determination of changes in the lattice parameters with changing composition, assessing preferred orientation effects, background evaluation, and line broadening. We have also included diffraction patterns of several common dense silicate phases to facilitate their detection in mixed phase syntheses.

The numerical data comprises 2θ values for CuKα radiation ($\lambda = 1.5418$ Å), d-spacings, relative intensities, hkl Miller indices and multiplicity, M_{hkl}. Data representing 133 framework topologies have been included in this *Collection*. In most cases, X-ray or neutron refinements of hydrated or as-synthesized forms are used.

This edition differs significantly from the 1996 3rd edition which included atomic coordinates. Because of space constraints coordinate data has not been included in this edition, but are available in electronic form, along with the complete contents of this edition, at:

http://www.iza-structure.org/databases/

This web site also contains an interactive powder pattern calculator that allows the user to change the input and variables for a powder pattern calculation.

This book was typeset using LaTeX with the standard computer modern typeface. The LaTeX file, and associated postscript plots, were generated using a C program written by M. M. J. Treacy.

We wish to acknowledge the assistance and collaboration of the members of the IZA Structure Commission in proofreading the manuscript and for providing additional information. We are indebted to our companies (NEC Research Institute, Inc., and Air Products and Chemicals, Inc.) for support of this project. We are grateful to Peggy Bisher for keeping the reference data files impeccably organized. Finally, we acknowledge the patience and support of our wives Laura and Carol.

Michael M. J. Treacy, Princeton, NJ
John B. Higgins, Bad Dog Ridge, PA
January 2001

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Additional IZA publications:

Atlas of Zeolite Framework Types, 5th revised edition (2001),
Ch. Baerlocher, W. M. Meier and D. H. Olson.

Compilation of Extra Framework Sites in Zeolites (1982),
W. J. Mortier. (out of print)

Verified Syntheses of Zeolitic Materials, 2nd revised edition (2001),
H. Robson, editor; and K. P. Lillerud, XRD patterns.

See also: http://www.iza-online.org/

EXPLANATORY NOTES

The numerical data and the simulated powder patterns presented in this *Collection* are to a great extent self-explanatory. In order to facilitate the use of these reference patterns some pertinent remarks regarding the keywords used in the data section are summarized below. The input structural data have been deposited on the worldwide web at:

http://www.iza-structure.org/databases/

This *Collection*, including updates, will be accessible at the above address.

ZEOLITE FRAMEWORK TYPES

The three-letter framework type codes, recognized by the IUPAC Commission on Zeolite Nomenclature, have been used to organize the entries in this publication. The powder diffraction data and simulated patterns for the reference structures are listed alphabetically according to the respective framework type code. An index of material names, and associated three-letter codes, is included in the companion volume, the *Atlas of Zeolite Framework Types* (Baerlocher, Meier and Olson (2001)).

COMPOSITION

Compositions are expressed in terms of the full unit cell content. Two compositions are provided. The CHEMICAL COMPOSITION is the nominal material composition provided in the original reference, and is usually obtained from chemical analysis. The REFINED COMPOSITION is derived from the structure refinement. Because of the complexities of structure refinements, the chemical and refined compositions do not always concur. When available, refinements of hydrated zeolites were used to calculate the patterns. For synthetic zeolites, if the zeolite had been synthesized in the presence of organic material, those refinements of the uncalcined products that contained the occluded organic molecules were chosen. The sample locality is given in the case of natural zeolites.

CRYSTAL DATA

Crystal data includes lattice parameters and space group information from the International Tables for Crystallography, 4th revised edition 1995, and incorporates the new *e* 'double-glide' plane. Consequently, some space group symbols will differ from those listed in the original references. Two entries in this *Collection* are affected by this change; EU-1 (**EUO**) which has space group symbol *Cmme* (formerly *Cmma*), and gottardiite (**NES**) which has space group symbol *Cmce* (formerly *Cmca*). The type of refinement, along with the final *R*-values, is listed with the unit cell parameters.

REFERENCE

Reference cites the literature from which the crystal data, atomic coordinates, and temperature factors were obtained. In many cases there are multiple refinements of the same zeolitic material, but because of space limitations not all refinements could be included. We would be appreciative if

authors and users would inform us of any errors or omissions. A listing of the references for isotypic species can be found in the *Atlas of Zeolite Framework Types* (Baerlocher, Meier and Olson (2001)). A list of references to structure analyses of zeolites with different cations, up to 1982, is given in the *Compilation of Extra Framework Sites in Zeolites*, W. J. Mortier (1982).

POWDER PATTERN IDENTIFICATION TABLE

A table is provided to assist in the identification of powder patterns of unknown materials. The 2θ (°) values of the three most pronounced low-angle reflections are listed. Usually, these reflections are simply the three strongest peaks. In many instances, a pronounced low-angle reflection will be included, even if it is not among the most intense. In the 3rd edition (1996) of the *Collection* this table was assembled by visual inspection of the computed powder patterns. For this fourth edition (2001) of the *Collection*, the table was generated automatically from the computed diffraction patterns. To achieve good correspondence with the hand-generated table of the 3rd (1996) edition of the *Collection*, a peak intensity weighting function $W(2\theta)$ was used

$$W(2\theta) = 1 + A \exp\left[-(2\theta)^2/2\sigma^2\right]. \quad (1)$$

The parameters were set to $A = 10$, and $\sigma = 7°$. This function is strongly weighted towards the low angle peaks, particularly those below about 10°, which, even if relatively weak, tend to offer a more characteristic fingerprint of a material compared to the abundance of strong peaks that tend to cluster around 25° in most zeolitic materials.

The data for all the materials presented in this work are sorted by increasing 2θ value in the table. To identify an unknown material, measure the 2θ values of the three most pronounced peaks (assigning strong weighting to any pronounced low-angle peaks, particularly those below about 10°) and find those materials with corresponding reflections at those values. This provides a starting point for a more detailed comparison of the experimental and calculated patterns.

CALCULATED POWDER DIFFRACTION DATA

The powder diffraction data include the 2θ-values for CuKα radiation, d-spacings, relative intensities $I_{\rm rel}$, Miller indices hkl and multiplicity M_{hkl}, for the strongest 135 reflections with an integrated intensity $I_{\rm rel}$ greater than 0.1. The strongest reflection is set to $I_{\rm rel} = 100$. The scattering factors used for the framework T- and O-atoms in the structure factor computations were those selected by the authors of the original work. If none had been specified, we chose atomic (neutral) scattering factors. No adsorption corrections were applied to the data, and anisotropic temperature factors were converted to isotropic temperature factors $B_{\rm iso}$ (Å^2) using equations reported by W. C. Hamilton, *Acta Cryst.*, **12** 609–610 (1959).

Materials with the same framework type code (i.e. framework topology) may have very different diffraction patterns, so for some framework type codes several different reference materials have been included. Examples listed under **FAU**, **GIS**, **MFI** and **NAT** illustrate the extent of the differences observed in the diffraction patterns of materials with identical framework topologies but

variations in composition and/or symmetry.

SIMULATED POWDER PATTERNS

The powder patterns for CuKα radiation are reproduced from 0° to 50° 2θ. The patterns, and associated tables, were calculated using a custom C program written by M. M. J. Treacy. The intensity scale is kept variable to accommodate extreme situations. The intensity range is usually plotted between 0 and $I_{\max} = 100$. If only one or a few peaks are very intense, and the rest of the pattern consists of low-intensity reflections, $I_{\max}$ is set at a lower value (see ordinate) to show sufficient detail in the low-intensity region of the pattern. The scale of the ordinate is always calibrated in percent relative intensity of the maximum peak height. Frequently, the peak intensities in the plots will not be identical to the integrated intensities listed in the corresponding tables, because of the possibility of overlapping diffraction peaks. A Lorentzian profile was assumed for the calculation of the pattern. The full width at half maximum (FWHM) of all peaks was set to be 0.08° 2θ. Many real samples will in general give diffraction patterns with broader lines due to instrumental broadening, disorder, or small crystallite size. However, synchrotron powder diffraction data of some zeolite materials exhibit FWHM of less than 0.04° 2θ.

Because hydrated forms of natural zeolites or as-synthesized forms were used whenever refined atomic parameters were available, the plots should be easily comparable to experimental patterns. In some cases, only structure refinements of dehydrated or calcined forms were available. Significant differences in the intensities of low-angle peaks may be found when comparing the calculated pattern to experimental patterns of hydrated or as-synthesized materials.

Finally, a note of caution. The patterns are useful in helping to establish the structural purity of a zeolite phase, yet they may not always allow one to readily and unambiguously determine the framework type of the sample. This assignment is often not straightforward and may require more sophisticated analyses. W. J. Rohrbaugh and E. W. Wu review the factors affecting the diffraction characteristics of zeolite materials (ACS Symposium Series **411** 279–302 (1989)).

POWDER PATTERN SIMULATIONS OF DISORDERED INTERGROWTHS

A number of zeolitic materials crystallize as disordered planar intergrowths of "end-member" frameworks. Two of the better-studied series are the **FAU**/**EMT** intergrowths (such as ZSM-2, ZSM-3, ZSM-20, ECR-30, CSZ-1 and CSZ-3) and the intergrown zeolite beta and its natural analog tschernichite. Powder patterns for five of the more commonly observed coherently intergrown series were calculated using the DIFFaX computer program (M. M. J. Treacy, J. M. Newsam and M. W. Deem, *Proc. R. Soc. Lond.* A **433** 499–520 (1991)). Random stacking faults are assumed. The five series are; the beta family; SSZ-33/SSZ-26; **FAU**/**EMT**; **MFI**/**MEL**; and **OFF**/**ERI**. The stacking fault probability is incremented from 0 to 1 in steps of 0.1. Stacking fault probabilities of 0 and 1 represent the unfaulted end-members.

Additional information on disordered intergrowths can be found in the *Catalog of Disordered Zeolite Structures*, which is available electronically at http://www.iza-structure.org/databases/.

CHANGES SINCE THE THIRD REVISED EDITION

- 35 new framework types have been approved since the third revised edition, and are included in this fourth revised edition. The new framework types are:

ACO	**AEN**	**AFN**	**ASV**	**AWO**	**CFI**	**CGF**
CGS	**CZP**	**DFT**	**DON**	**ESV**	**FRA**	**GON**
IFR	**ISV**	**ITE**	**MSO**	**MTF**	**MWW**	**OSI**
OSO	**SAO**	**SAS**	**SAT**	**SAV**	**SBE**	**SBS**
SBT	**SFE**	**SFF**	**STF**	**STT**	**TER**	**TSC**

- Due to space constraints, the refined structure coordinates are not listed in the printed version of this *Collection*. An electronic PDF version of this *Collection*, complete with coordinates, can be found at:

http://www.iza-structure.org/databases/

- Errors in the space group settings of Maricopaite (**MOR**) and chiavennite (**-CHI**) have been fixed. These corrections change the diffraction patterns and the listed peak intensities.

- The distance least squares refinement of liottite (**LIO**), given in the third revised edition, has been replaced by a single crystal x-ray refinement.

- The entry for Na-exchanged K-F (**EDI**) has been removed due to inconsistencies in the refinement.

- A typographic error in the published coordinates for perlialite (**LTL**) has been corrected. This correction has changed the diffraction pattern noticeably.

- An error in the cation occupancies for the mineral faujasite (**FAU**) has been corrected. This correction has changed the diffraction pattern noticeably.

- The refinements of MAPO–39 (**ATN**) and offretite (**OFF**) have been replaced.

- A refinement for low silica zeolite-X (**FAU**) has been added.

- A small number of typographic errors in atom coordinates have been corrected.

POWDER PATTERN IDENTIFICATION TABLE

Powder Pattern Identification Table

$2\theta^\circ$	Material	Code
3.33	Franzinite	**FRA**
3.42	Cloverite	**-CLO**
3.56	Paulingite	**PAU**
4.14	NaZ-21	**LTN**
4.56	Decamethonium DAF-1	**DFO**
4.80	VPI-9	**VNI**
4.83	Cloverite	**-CLO**
4.84	Tschörtnerite	**TSC**
5.04	Paulingite	**PAU**
5.31	AlPO–8	**AET**
5.38	VPI-5	**VFI**
5.50	Perlialite	**LTL**
5.55	Linde Type L	**LTL**
5.55	Mazzite	**MAZ**
5.59	Tschörtnerite	**TSC**
5.63	UCSB–8Co	**SBE**
5.64	Chiavennite	**-CHI**
5.72	UCSB–6GaCo	**SBS**
5.76	MCM-35	**MTF**
5.87	EMC-2, Calcined	**EMT**
5.87	EMC-2, Partially Dehydrated	**EMT**
5.92	Cloverite	**-CLO**
5.96	Li-LSX	**FAU**
6.02	UCSB–10GaZn	**SBT**
6.04	UTD-1	**DON**
6.10	Na-X, Dehydrated	**FAU**
6.12	Na-X, Hydrated	**FAU**
6.19	Faujasite	**FAU**
6.23	EMC-2, Partially Dehydrated	**EMT**
6.24	EMC-2, Calcined	**EMT**
6.31	Na-Y, Siliceous	**FAU**
6.32	UCSB–10GaZn	**SBT**
6.33	Ultrastable Y, Dehydrated Dealuminated	**FAU**
6.39	Maricopaite	**MOR**
6.41	UCSB–8Co	**SBE**
6.48	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
6.50	UCSB–6GaCo	**SBS**
6.51	Mordenite	**MOR**
6.57	AlPO–8	**AET**
6.57	Di-n-propylamine MAPSO–46	**AFS**
6.58	UCSB–6GaCo	**SBS**
6.58	SSZ–48, Calcined	**SFE**
6.65	EMC-2, Calcined	**EMT**
6.65	EMC-2, Partially Dehydrated	**EMT**
6.69	(Cs,K) ZK5, Dehydrated	**KFI**
6.77	NaZ-21	**LTN**
6.78	VPI-8	**VET**
6.82	UiO-6, Calcined	**OSI**
6.82	Roggianite	**-RON**
6.85	AlPO–41, Calcined	**AFO**
6.88	ITQ–7, Siliceous, Calcined	**ISV**
6.93	CIT-5	**CFI**
6.96	GUS-1	**GON**
6.98	Beta, Polymorph A SiO_2 Framework	***BEA**
7.01	ITQ–7, Siliceous, Calcined	**ISV**
7.04	UCSB–10GaZn	**SBT**
7.05	NU-87	**NES**
7.09	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**
7.10	Beryllophosphate-H	**BPH**
7.18	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**

$2\theta^\circ$	Material	Code
7.18	Linde Type A, Hydrated	**LTA**
7.20	Linde Type A, Dehydrated	**LTA**
7.33	CIT-5	**CFI**
7.40	Terranovaite	**TER**
7.41	N_2, Piperidine Dodecasil 1H	**DOH**
7.42	SAPO–56	**AFX**
7.42	Gmelinite	**GME**
7.43	Boggsite	**BOG**
7.43	Tetrapropylammonium Fluoride AlPO-5	**AFI**
7.47	ZSM-12, Calcined	**MTW**
7.49	MCM-61	**MSO**
7.55	UTD-1	**DON**
7.61	Tetrapropylammonium SAPO–40	**AFR**
7.63	ZSM-12, Calcined	**MTW**
7.66	Offretite	**OFF**
7.66	CIT-1	**CON**
7.67	STA-1, Magnesium Aluminophosphate	**SAO**
7.68	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
7.69	Erionite	**ERI**
7.71	Bellbergite	**EAB**
7.71	Piperidine AlPO–17	**ERI**
7.72	ITQ–7, Siliceous, Calcined	**ISV**
7.72	Di-n-propylamine MAPSO–46	**AFS**
7.72	SSZ-44, Calcined	**SFF**
7.73	ERS-7 Framework	**ESV**
7.74	Beta, Polymorph A SiO_2 Framework	***BEA**
7.75	ZSM-18, SiO_2 Framework	**MEI**
7.78	Ferrierite	**FER**
7.80	Gottardiite	**NES**
7.82	ZSM-57, SiO_2 Framework	**MFS**
7.84	Boggsite	**BOG**
7.84	CIT-1	**CON**
7.88	MAPO–36, Calcined	**ATS**
7.89	Dodecasil 3C	**MTN**
7.90	NU-87	**NES**
7.91	Decamethonium DAF-1	**DFO**
7.92	EU-1, Calcined, Rehydrated	**EUO**
7.93	ZSM-11, Calcined	**MEL**
7.94	NaZ-21	**LTN**
7.94	ZSM-5, Calcined	**MFI**
7.94	Ammonium Fluoride ZSM-23	**MTT**
7.95	Tetrapropylammonium ZSM-5	**MFI**
7.95	2-aminopentane Nonasil	**NON**
7.99	SSZ-35, Calcined	**STF**
8.01	ZSM-5, Calcined	**MFI**
8.01	Di-n-propylamine CoAPO–50	**AFY**
8.01	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**
8.02	AlPO–52, Calcined, Rehydrated	**AFT**
8.06	Tetrapropylammonium SAPO–40	**AFR**
8.06	SSZ-44, Calcined	**SFF**
8.07	SSZ–48, Calcined	**SFE**
8.09	SSZ-35, Calcined	**STF**
8.09	Di-isopropylamine MnAPO–11	**AEL**
8.10	AlPO–11, Calcined	**AEL**
8.11	ERS-7 Framework	**ESV**
8.11	SSZ-23	**STT**
8.11	Beryllophosphate-H	**BPH**
8.15	Decamethonium DAF-1	**DFO**
8.15	ITQ-4, Calcined	**IFR**
8.15	Diethylamine Theta-1 (Silica ZSM-22)	**TON**

Powder Pattern Identification Table *continued*

$2\theta^\circ$	Material	Code
8.17	STA-1, Magnesium Aluminophosphate	**SAO**
8.20	Cobalt Gallium Phosphate-6	**CGS**
8.20	MAPO–36, Calcined	**ATS**
8.21	Partheite	**-PAR**
8.22	Ammonium Fluoride ZSM-23	**MTT**
8.32	Gottardiite	**NES**
8.32	Rho, Hydrated	**RHO**
8.37	NU-87	**NES**
8.49	Di-n-propylamine SAPO–31	**ATO**
8.56	Levyne	**LEV**
8.58	ITQ–3, Calcined	**ITE**
8.62	Terranovaite	**TER**
8.64	SAPO–56	**AFX**
8.64	RUB-13	**RTH**
8.68	1-aminoadamantane NU-3	**LEV**
8.71	SSZ-44, Calcined	**SFF**
8.72	RUB-17	**RSN**
8.73	STA-6	**SAS**
8.75	EU-1, Calcined, Rehydrated	**EUO**
8.81	Terranovaite	**TER**
8.81	ZSM-11, Calcined	**MEL**
8.82	GUS-1	**GON**
8.84	Tetrapropylammonium ZSM-5	**MFI**
8.87	VPI-7	**VSV**
8.88	Tetrapropylammonium ZSM-5	**MFI**
8.90	ZSM-5, Calcined	**MFI**
8.91	ZSM-12, Calcined	**MTW**
8.93	Rho, Deuterated Berylloarsenate	**RHO**
8.94	Lovdarite	**LOV**
8.95	Ammonium Fluoride ZSM-23	**MTT**
8.98	Maricopaite	**MOR**
9.01	ITQ–3, Calcined	**ITE**
9.01	1-aminoadamantane Sigma-2	**SGT**
9.05	RUB-13	**RTH**
9.07	Pahasapaite	**RHO**
9.08	AlPO–14, Calcined	**AFN**
9.10	CIT-1	**CON**
9.14	AlPO–C, Hydrated	**APC**
9.16	RUB-3	**RTE**
9.18	Quinuclidine AlPO–22	**AWW**
9.23	Ferrierite	**FER**
9.23	Cobalt Gallophosphate	**LAU**
9.24	Laumontite	**LAU**
9.28	UCSB–8Co	**SBE**
9.30	Tetramethylammonium OH AlPO–12	**ATT**
9.36	Magnesium STA-7	**SAV**
9.36	AlPO–25	**ATV**
9.38	Leonhardite	**LAU**
9.40	Chabazite	**CHA**
9.42	ZSM-57, SiO_2 Framework	**MFS**
9.42	Magnesium STA-7	**SAV**
9.43	SSZ–48, Calcined	**SFE**
9.45	Ferrierite, Siliceous	**FER**
9.45	Di-isopropylamine MnAPO–11	**AEL**
9.47	MAPO–39	**ATN**
9.47	(Cs,K) ZK5, Dehydrated	**KFI**
9.48	Methylbutylamine SAPO–47	**CHA**
9.49	AlPO–18, Calcined	**AEI**
9.49	Bellbergite	**EAB**
9.50	SSZ-23	**STT**

$2\theta^\circ$	Material	Code
9.54	AlPO–52, Calcined, Rehydrated	**AFT**
9.54	Perlialite	**LTL**
9.55	ZSM-18, SiO_2 Framework	**MEI**
9.57	AlPO–11, Calcined	**AEL**
9.59	VPI-8	**VET**
9.61	2-aminopentane Nonasil	**NON**
9.62	Mazzite	**MAZ**
9.64	(Na, Tetramethylammonium)-E	**EAB**
9.65	UiO-6, Calcined	**OSI**
9.65	Roggianite	**-RON**
9.68	Erionite	**ERI**
9.68	Beta, Polymorph A SiO_2 Framework	***BEA**
9.69	Tschörtnerite	**TSC**
9.69	ITQ-4, Calcined	**IFR**
9.70	Stilbite	**STI**
9.71	Stellerite	**STI**
9.72	Barrerite	**STI**
9.72	AlPO–41, Calcined	**AFO**
9.73	SSZ-35, Calcined	**STF**
9.74	Li-LSX	**FAU**
9.75	MCM-35	**MTF**
9.75	Chiral Sodium Zincophosphate, $P6_122$	**CZP**
9.77	Mordenite	**MOR**
9.77	Piperidine AlPO–17	**ERI**
9.81	Chiral Sodium Zincophosphate, $P6_522$	**CZP**
9.81	Di-n-propylamine CoAPO–50	**AFY**
9.82	ERS-7 Framework	**ESV**
9.85	Heulandite	**HEU**
9.88	Clinoptilolite	**HEU**
9.90	Stellerite	**STI**
9.91	Barrerite	**STI**
9.95	Dachiardite	**DAC**
9.96	Stilbite	**STI**
9.97	Epistilbite	**EPI**
9.97	Na-X, Dehydrated	**FAU**
9.99	AlPO–8	**AET**
10.00	Cobalt Gallium Phosphate-5	**CGF**
10.00	Na-X, Hydrated	**FAU**
10.06	RUB-10, SiO_2 Framework	**RUT**
10.06	ITQ–3, Calcined	**ITE**
10.07	ASU-7	**ASV**
10.08	Tetramethylammonium ZAPO-M1	**ZON**
10.10	AlPO–21	**AWO**
10.12	OSB-1	**OSO**
10.14	AlPO-EN3	**AEN**
10.16	VPI-9	**VNI**
10.16	Diethylamine Theta-1 (Silica ZSM-22)	**TON**
10.17	Linde Type A, Hydrated	**LTA**
10.18	RUB-13	**RTH**
10.19	Linde Type A, Dehydrated	**LTA**
10.27	MCM-61	**MSO**
10.31	Na-Y, Siliceous	**FAU**
10.34	Ultrastable Y, Dehydrated Dealuminated	**FAU**
10.47	AlPO – H2	**AHT**
10.48	Magnesium STA-7	**SAV**
10.50	STA-6	**SAS**
10.58	SSZ-23	**STT**
10.61	AlPO–18, Calcined	**AEI**
10.70	Paulingite	**PAU**
10.75	Nepheline Hydrate	**JBW**

Powder Pattern Identification Table *continued*

$2\theta°$	Material	Code
10.77	RUB-10, SiO_2 Framework	**RUT**
10.77	VPI-5	**VFI**
10.85	Levyne	**LEV**
10.90	Harmotome	**PHI**
10.90	Partheite	**-PAR**
11.07	Heulandite	**HEU**
11.08	1-aminoadamantane NU-3	**LEV**
11.11	Mazzite	**MAZ**
11.17	ZSM-18, SiO_2 Framework	**MEI**
11.19	Clinoptilolite	**HEU**
11.29	Bikitaite	**BIK**
11.30	Chiavennite	**-CHI**
11.33	Cobalt Gallium Phosphate-5	**CGF**
11.38	Chiral Sodium Zincophosphate, $P6_122$	**CZP**
11.41	Chiral Sodium Zincophosphate, $P6_522$	**CZP**
11.42	Li-LSX	**FAU**
11.43	Barium Chloroaluminosilicate	**MER**
11.45	Quinuclidine AlPO–16	**AST**
11.49	Cobalt Gallium Phosphate-6	**CGS**
11.52	Gmelinite	**GME**
11.53	Levyne	**LEV**
11.54	Losod	**LOS**
11.57	AlPO–14, Calcined	**AFN**
11.57	SAPO–56	**AFX**
11.64	AlPO–52, Calcined, Rehydrated	**AFT**
11.65	Offretite	**OFF**
11.67	Quinuclidinium fluoride octadecasil	**AST**
11.69	Na-X, Dehydrated	**FAU**
11.73	Na-X, Hydrated	**FAU**
11.77	Linde Type L	**LTL**
11.79	Nepheline Hydrate	**JBW**
11.86	Faujasite	**FAU**
11.86	Wenkite	**-WEN**
11.95	Magnesium Phosphate UiO-20	**DFT**
12.10	Na-Y, Siliceous	**FAU**
12.13	Amicite	**GIS**
12.14	Ultrastable Y, Dehydrated Dealuminated	**FAU**
12.15	Gismondine	**GIS**
12.22	AlPO–21	**AWO**
12.22	ACP-1	**ACO**
12.32	Cobalt Gallium Phosphate-6	**CGS**
12.35	Gobbinsite	**GIS**
12.36	Phillipsite	**PHI**
12.38	Garronite	**GIS**
12.38	Di-n-propylamine MAPO–43	**GIS**
12.40	Harmotome	**PHI**
12.41	Goosecreekite	**GOO**
12.42	Tetrapropylammonium SAPO–40	**AFR**
12.44	Merlinoite	**MER**
12.44	Tetramethylammonium ZAPO-M1	**ZON**
12.46	Na-P1	**GIS**
12.46	Linde Type A, Hydrated	**LTA**
12.48	Phillipsite	**PHI**
12.49	Linde Type A, Dehydrated	**LTA**
12.54	Merlinoite	**MER**
12.55	AlPO–C, Dehydrated	**APC**
12.57	Gobbinsite	**GIS**
12.58	Ferrierite, Siliceous	**FER**
12.59	Goosecreekite	**GOO**
12.60	ACP-1	**ACO**

$2\theta°$	Material	Code
12.65	Tetramethylammonium OH AlPO–12	**ATT**
12.71	Laumontite	**LAU**
12.73	MCM-61	**MSO**
12.76	Franzinite	**FRA**
12.78	ZSM-57, SiO_2 Framework	**MFS**
12.78	Dachiardite	**DAC**
12.80	Maricopaite	**MOR**
12.83	Ferrierite, Siliceous	**FER**
12.84	Epistilbite	**EPI**
12.88	RUB-17	**RSN**
12.89	Methylbutylamine SAPO–47	**CHA**
12.90	AlPO–C, Hydrated	**APC**
12.91	Dodecasil 3C	**MTN**
12.91	AlPO–D	**APD**
12.91	AlPO–18, Calcined	**AEI**
12.99	AlPO-EN3	**AEN**
13.00	Leonhardite	**LAU**
13.07	Brewsterite	**BRE**
13.15	AlPO–14, Calcined	**AFN**
13.16	Lovdarite	**LOV**
13.17	Di-n-propylamine MAPSO–46	**AFS**
13.33	(Na, Tetramethylammonium)-E	**EAB**
13.34	Erionite	**ERI**
13.37	Scolecite	**NAT**
13.38	Piperidine AlPO–17	**ERI**
13.39	Thomsonite	**THO**
13.41	Montesommaite	**MON**
13.41	MAPO–39	**ATN**
13.41	Gonnardite	**NAT**
13.44	Mesolite	**NAT**
13.45	Mordenite	**MOR**
13.50	Bellbergite	**EAB**
13.56	Natrolite	**NAT**
13.60	Edingtonite	**EDI**
13.64	AlPO–C, Hydrated	**APC**
13.72	ITQ-4, Calcined	**IFR**
13.72	Losod	**LOS**
13.73	AlPO–41, Calcined	**AFO**
13.76	Tetramethylammonium ZAPO-M1	**ZON**
13.80	Li-ABW	**ABW**
13.88	RUB-17	**RSN**
13.89	STA-1, Magnesium Aluminophosphate	**SAO**
13.89	VPI-7	**VSV**
13.90	Harmotome	**PHI**
14.00	AlPO–C, Dehydrated	**APC**
14.02	Cancrinite	**CAN**
14.02	Brewsterite	**BRE**
14.14	RUB-3	**RTE**
14.16	Sodalite Octahydrate	**SOD**
14.31	Tugtupite	**SOD**
14.41	RUB-10, SiO_2 Framework	**RUT**
14.50	Roggianite	**-RON**
14.56	Partheite	**-PAR**
14.71	Linde Type L	**LTL**
14.74	Melanophlogite	**MEP**
14.80	AlPO–21	**AWO**
14.96	Gonnardite	**NAT**
14.96	AlPO–25	**ATV**
14.97	Weinebeneite	**WEI**
15.00	(Cs,K) ZK5, Dehydrated	**KFI**

Powder Pattern Identification Table *continued*

$2\theta^\circ$	Material	Code
15.04	Natrolite	**NAT**
15.10	Scolecite	**NAT**
15.10	N_2, Piperidine Dodecasil 1H	**DOH**
15.11	Mesolite	**NAT**
15.14	Dodecasil 3C	**MTN**
15.20	Chiavennite	**-CHI**
15.23	Ferrierite	**FER**
15.26	Chiral Sodium Zincophosphate, $P6_522$	**CZP**
15.27	Chiral Sodium Zincophosphate, $P6_122$	**CZP**
15.30	Yugawaralite	**YUG**
15.42	OSB-1	**OSO**
15.45	Weinebeneite	**WEI**
15.61	Faujasite	**FAU**
15.81	Analcime	**ANA**
16.16	Melanophlogite	**MEP**
16.24	STA-6	**SAS**
16.34	STA-2	**SAT**
16.42	STA-2	**SAT**
16.57	Merlinoite	**MER**
16.84	N_2, Piperidine Dodecasil 1H	**DOH**
17.13	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
17.35	Amicite	**GIS**
17.65	Gmelinite	**GME**
17.82	Lovdarite	**LOV**
17.87	RUB-3	**RTE**
17.87	Garronite	**GIS**
17.90	AlPO–C, Dehydrated	**APC**
18.04	Gismondine	**GIS**
18.35	Liottite	**LIO**
18.40	Afghanite	**AFG**
18.54	Quinuclidine AlPO–22	**AWW**
18.61	Losod	**LOS**
18.67	Rho, Hydrated	**RHO**
18.75	Quinuclidine AlPO–16	**AST**
18.89	Edingtonite	**EDI**
19.06	MAPO–36, Calcined	**ATS**
19.15	Cancrinite	**CAN**
19.16	Yugawaralite	**YUG**
19.21	Thomsonite	**THO**
19.56	1-aminoadamantane Sigma-2	**SGT**
19.76	1-aminoadamantane Sigma-2	**SGT**
19.82	Goosecreekite	**GOO**
20.01	Moganite	–
20.08	CIT-5	**CFI**
20.09	VPI-8	**VET**
20.18	Di-n-propylamine SAPO–31	**ATO**
20.34	Gottardiite	**NES**
20.36	Diethylamine Theta-1 (Silica ZSM-22)	**TON**
20.45	Chabazite	**CHA**
20.52	Tridymite	–
20.53	EU-1, Calcined, Rehydrated	**EUO**
20.58	Tridymite	–
20.61	Quinuclidine AlPO–22	**AWW**
20.62	2-aminopentane Nonasil	**NON**
20.62	AlPO–D	**APD**
20.62	Methylbutylamine SAPO–47	**CHA**
20.64	UiO-6, Calcined	**OSI**
20.66	GUS-1	**GON**
20.71	AlPO–D	**APD**
20.82	Gismondine	**GIS**

$2\theta^\circ$	Material	Code
20.86	Alpha Quartz	–
20.96	UTD-1	**DON**
20.97	Tetrapropylammonium Fluoride AlPO-5	**AFI**
21.03	Amicite	**GIS**
21.04	Di-isopropylamine MnAPO–11	**AEL**
21.10	Barium Chloroaluminosilicate	**MER**
21.13	AlPO–25	**ATV**
21.18	Cobalt Gallophosphate	**LAU**
21.22	Bikitaite	**BIK**
21.23	AlPO–11, Calcined	**AEL**
21.52	Di-n-propylamine MAPO–43	**GIS**
21.52	STA-2	**SAT**
21.57	Gobbinsite	**GIS**
21.60	Cs-Aluminosilicate	**CAS**
21.67	Na-P1	**GIS**
21.68	Tridymite	–
21.87	AlPO – H2	**AHT**
21.89	Stilbite	**STI**
21.90	Stellerite	**STI**
21.92	Barrerite	**STI**
22.00	Alpha Cristobalite	–
22.03	1-aminoadamantane NU-3	**LEV**
22.03	Quinuclidine AlPO–16	**AST**
22.13	Quinuclidinium fluoride octadecasil	**AST**
22.22	Heulandite	**HEU**
22.38	Tetrapropylammonium Fluoride AlPO-5	**AFI**
22.49	Clinoptilolite	**HEU**
22.52	Perlialite	**LTL**
22.58	Di-n-propylamine SAPO–31	**ATO**
22.59	MAPO–39	**ATN**
22.60	VPI-5	**VFI**
22.62	Quinuclidinium fluoride octadecasil	**AST**
22.65	ASU-7	**ASV**
22.96	Epistilbite	**EPI**
23.05	Boggsite	**BOG**
23.11	Cobalt Gallium Phosphate-5	**CGF**
23.13	ZSM-11, Calcined	**MEL**
23.24	Magnesium Phosphate UiO-20	**DFT**
23.48	ASU-7	**ASV**
23.53	Offretite	**OFF**
23.57	(Na, Tetramethylammonium)-E	**EAB**
23.78	Rho, Deuterated Berylloarsenate	**RHO**
23.86	Keatite	–
23.86	Franzinite	**FRA**
23.95	Liottite	**LIO**
23.96	AlPO-EN3	**AEN**
24.08	Afghanite	**AFG**
24.16	Pahasapaite	**RHO**
24.18	Di-n-propylamine CoAPO–50	**AFY**
24.65	Sodalite Octahydrate	**SOD**
24.68	Cs-Aluminosilicate	**CAS**
24.71	Bicchulite	**SOD**
24.79	Edingtonite	**EDI**
24.79	Melanophlogite	**MEP**
24.80	Tugtupite	**SOD**
24.83	Cs-Aluminosilicate	**CAS**
25.14	Tugtupite	**SOD**
25.14	Rho, Hydrated	**RHO**
25.18	Laumontite	**LAU**
25.19	Cobalt Gallophosphate	**LAU**

Powder Pattern Identification Table *continued*

$2\theta^\circ$	Material	Code
25.37	Leonhardite	**LAU**
25.42	Thomsonite	**THO**
25.59	MCM-35	**MTF**
25.73	Dachiardite	**DAC**
25.76	Bikitaite	**BIK**
25.77	Wenkite	**-WEN**
25.96	Analcime	**ANA**
26.03	Keatite	–
26.07	Magnesium Phosphate UiO-20	**DFT**
26.10	Nepheline Hydrate	**JBW**
26.29	Moganite	–
26.49	Tiptopite	**CAN**
26.65	Alpha Quartz	–
26.73	Moganite	–
26.73	Keatite	–
26.91	Liottite	**LIO**
27.01	Montesommaite	**MON**
27.02	Afghanite	**AFG**
27.02	Rho, Deuterated Berylloarsenate	**RHO**
27.43	VPI-7	**VSV**
27.46	Pahasapaite	**RHO**
27.54	Tetramethylammonium OH AlPO–12	**ATT**
27.66	Di-n-propylamine MAPO–43	**GIS**
27.72	ACP-1	**ACO**
27.74	Cancrinite	**CAN**
27.89	Phillipsite	**PHI**
28.10	Na-P1	**GIS**

$2\theta^\circ$	Material	Code
28.15	Li-ABW	**ABW**
28.33	Garronite	**GIS**
28.37	Wenkite	**-WEN**
28.42	Montesommaite	**MON**
29.03	AlPO – H2	**AHT**
29.10	VPI-9	**VNI**
29.29	Yugawaralite	**YUG**
29.36	OSB-1	**OSO**
29.50	Li-ABW	**ABW**
30.19	Tiptopite	**CAN**
30.40	Chabazite	**CHA**
30.50	Brewsterite	**BRE**
30.54	Analcime	**ANA**
30.96	Scolecite	**NAT**
30.98	Mesolite	**NAT**
31.01	Gonnardite	**NAT**
31.22	Natrolite	**NAT**
31.44	Alpha Cristobalite	–
31.99	Sodalite Octahydrate	**SOD**
32.07	Bicchulite	**SOD**
32.08	Beryllophosphate-H	**BPH**
32.32	Barium Chloroaluminosilicate	**MER**
35.58	Tiptopite	**CAN**
35.73	Weinebeneite	**WEI**
36.15	Alpha Cristobalite	–
39.49	Alpha Quartz	–
43.51	Bicchulite	**SOD**

POWDER PATTERNS

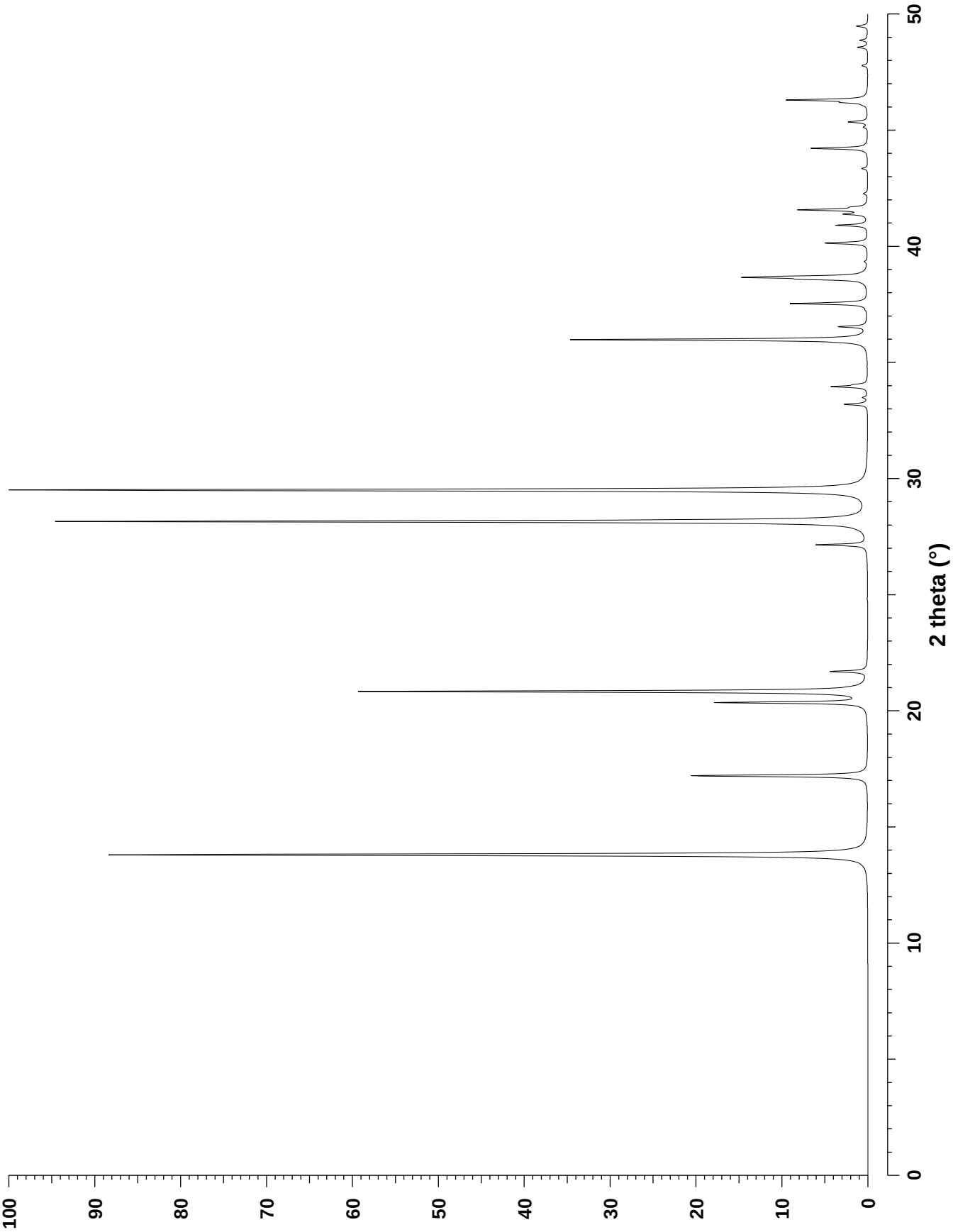
CHEMICAL COMPOSITION: $|Li_4(H_2O)_4|\ [Si_4Al_4O_{16}]$

REFINED COMPOSITION: $|Li_4(H_2O)_4|\ [Si_4Al_4O_{16}]$

CRYSTAL DATA: $Pna2_1$ (No. 33)
$a = 10.313$ Å $b = 8.194$ Å $c = 4.993$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.081$

REFERENCE: E. Krogh Andersen and G. Ploug-Sørensen,
Z. Kristallogr. **176** 67–73 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	13.80	6.416	4	88.5	0	0	2	35.97	2.497	2	34.7	3	3	0	42.26	2.139	4	0.5
2	0	0	17.20	5.156	2	20.6	4	1	0	36.53	2.459	4	3.3	1	2	2	43.34	2.088	8	0.7
2	1	0	20.35	4.364	4	17.5	2	3	0	37.25	2.414	4	0.1	0	4	0	44.21	2.049	2	6.6
0	1	1	20.83	4.264	4	59.3	0	3	1	37.53	2.396	4	9.0	1	4	0	45.12	2.009	4	0.4
0	2	0	21.69	4.097	2	4.3	1	3	1	38.57	2.334	8	5.5	5	1	0	45.34	2.000	4	1.9
2	1	1	27.14	3.286	8	5.9	3	2	1	38.65	2.329	8	11.3	4	2	1	45.36	2.000	8	0.4
2	2	0	27.81	3.208	4	0.1	1	1	2	38.70	2.327	8	6.0	2	2	2	46.07	1.970	8	0.2
3	1	0	28.15	3.170	4	94.6	4	0	1	39.33	2.291	4	0.3	3	3	1	46.18	1.966	8	2.2
1	2	1	29.50	3.028	8	100.0	2	0	2	40.13	2.247	4	5.0	3	1	2	46.29	1.961	8	9.3
2	2	1	33.19	2.699	8	2.7	4	1	1	40.90	2.206	8	3.7	2	4	0	47.77	1.904	4	0.7
3	1	1	33.48	2.676	8	0.5	4	2	0	41.38	2.182	4	2.5	4	3	0	48.56	1.875	4	1.2
1	3	0	33.95	2.640	4	4.1	2	3	1	41.56	2.173	8	7.9	1	4	1	48.86	1.864	8	0.9
3	2	0	34.04	2.633	4	1.1	2	1	2	41.68	2.167	8	1.3	5	2	0	49.47	1.842	4	1.3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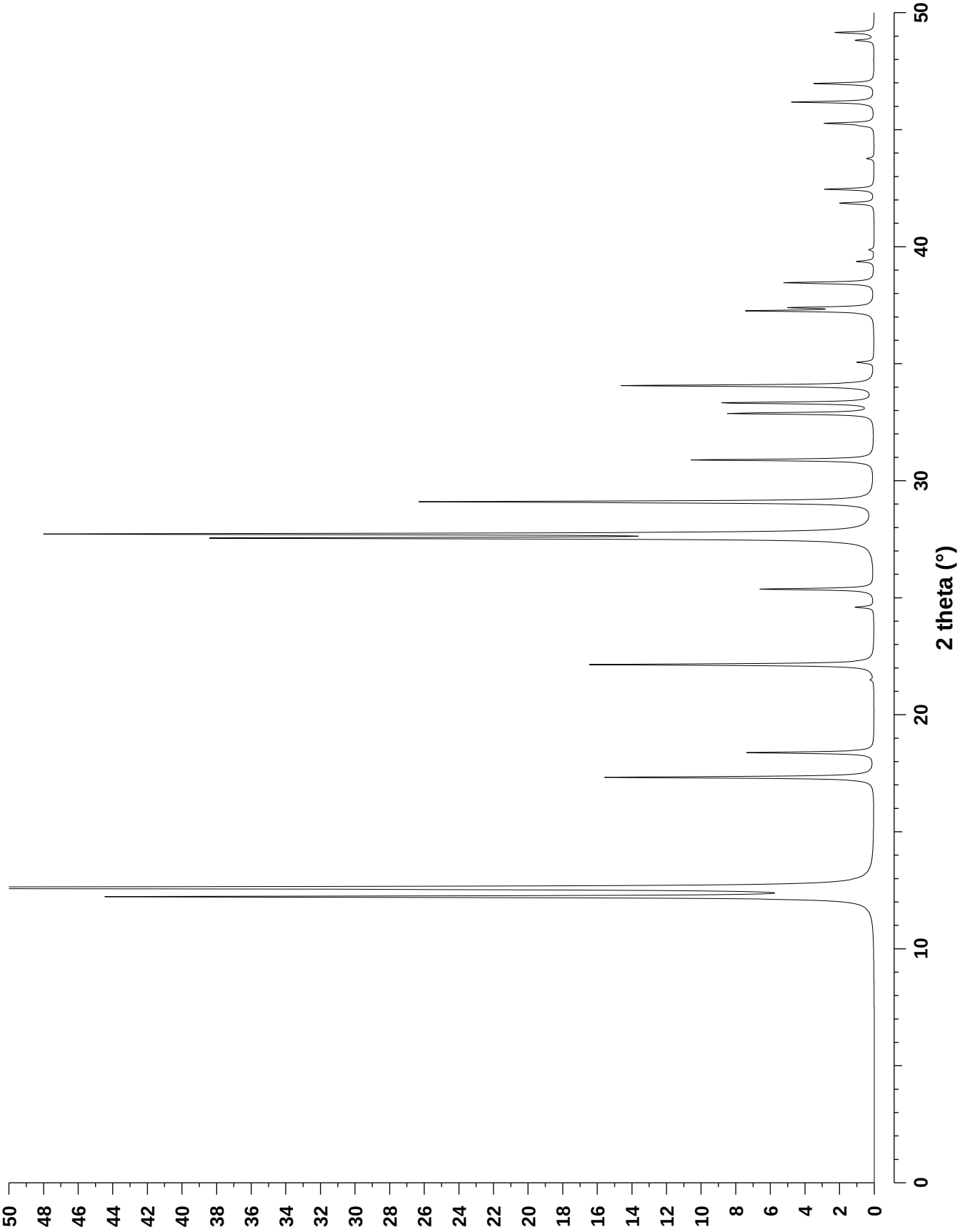
CHEMICAL COMPOSITION: $|(NH_2(CH_2)_2NH_2)_4(H_2O)_2|$ $[Al_{0.88}Co_{7.12}P_8O_{32}]$
$NH_2(CH_2)_2NH_2$ = ethylenediamine

REFINED COMPOSITION: $|C_8N_8O_2|$ $[Co_8P_8O_{32}]$

CRYSTAL DATA: $I\bar{4}2m$ (No. 121)
$a = 10.240$ Å $b = 10.240$ Å $c = 9.652$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_p = 0.0775$

REFERENCE: P. Feng, X. Bu and G. D. Stucky,
Nature **388** 735–741 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	12.22	7.241	4	43.6	1	0	3	29.09	3.069	8	26.4	4	0	2	39.86	2.262	8	0.3
1	0	1	12.60	7.024	8	100.0	2	2	2	30.88	2.896	8	10.6	3	3	2	41.85	2.159	8	2.0
2	0	0	17.32	5.120	4	15.6	3	2	1	32.87	2.725	16	8.4	3	2	3	42.45	2.129	16	2.9
0	0	2	18.38	4.826	2	7.4	3	1	2	33.32	2.689	16	8.7	4	2	2	43.76	2.069	16	0.4
2	1	1	21.48	4.137	16	0.2	2	1	3	34.06	2.633	16	14.7	2	2	4	45.16	2.008	8	0.5
1	1	2	22.14	4.016	8	16.5	4	0	0	35.05	2.560	4	1.0	4	3	1	45.26	2.003	16	2.8
2	2	0	24.59	3.620	4	1.1	3	3	0	37.25	2.414	4	7.1	4	1	3	46.17	1.966	16	4.8
2	0	2	25.36	3.512	8	6.6	4	1	1	37.39	2.405	16	4.5	3	1	4	46.96	1.935	16	3.5
3	1	0	27.54	3.238	8	36.4	3	0	3	38.45	2.341	8	5.2	5	2	1	48.81	1.866	16	1.1
3	0	1	27.72	3.218	8	46.5	1	1	4	39.36	2.289	8	1.0	5	1	2	49.14	1.854	16	2.3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AEI — AlPO–18, Calcined

CHEMICAL COMPOSITION: $[Al_{24}P_{24}O_{96}]$

REFINED COMPOSITION: $[Al_{24}P_{24}O_{96}]$

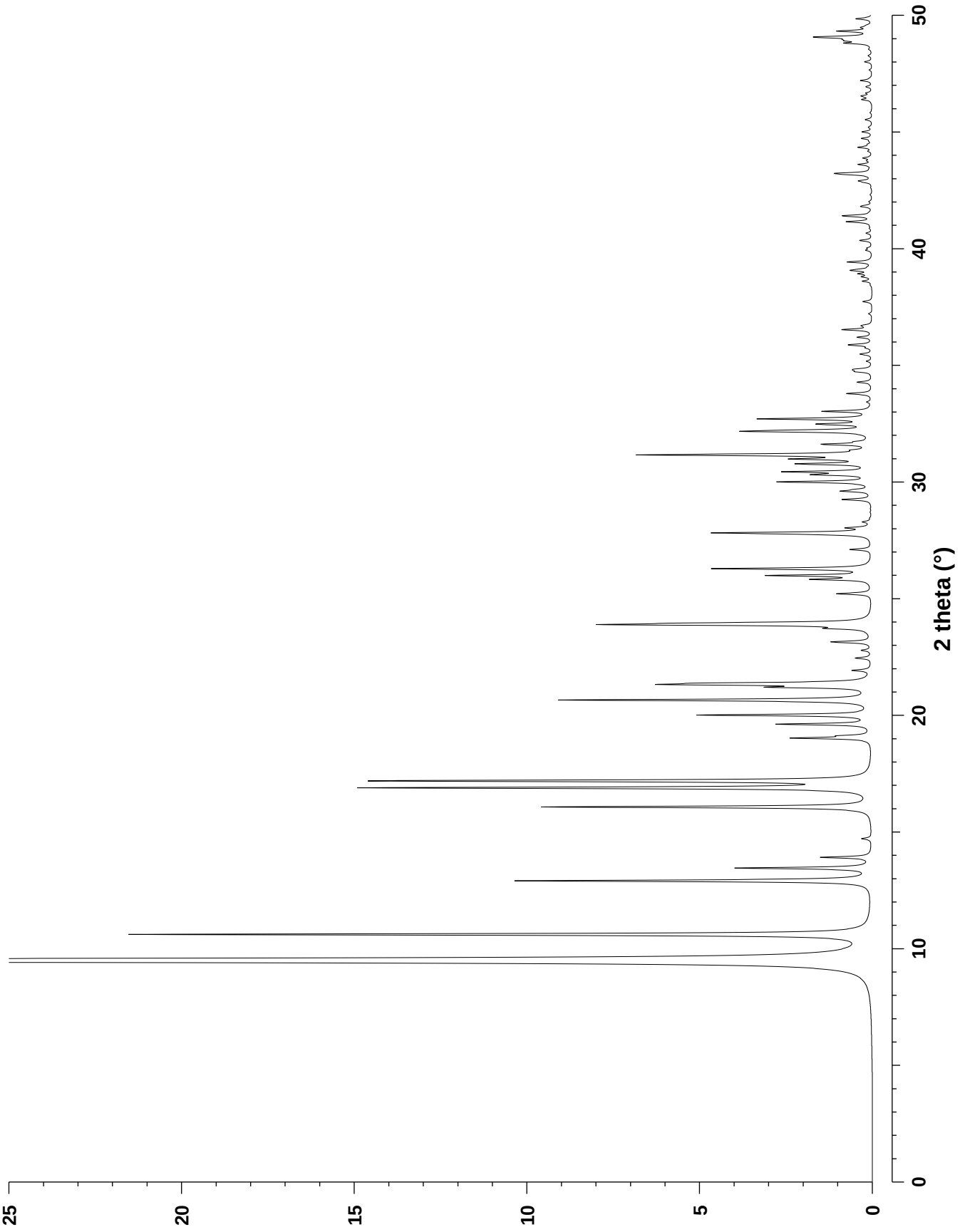
CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 13.7114$ Å $b = 12.7315$ Å $c = 18.5706$ Å
$\alpha = 90°$ $\beta = 90.01°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.047$, $R_{wp} = 0.108$, $R_F = 0.032$

REFERENCE: A. Simmen, L. B. McCusker, Ch. Baerlocher and W. M. Meier, *Zeolites* **11** 654–661 (1991). Ch. Baerlocher, Private communication.

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.48	9.330	4	100.0	0	2	5	27.81	3.208	4	5.9	-3	3	5	37.72	2.385	4	0.2
0	0	2	9.52	9.285	2	57.9	0	4	0	28.03	3.183	2	0.8	4	4	0	38.60	2.332	4	0.3
-1	1	1	10.61	8.337	4	13.5	-1	3	4	29.24	3.054	4	0.6	0	0	8	38.79	2.321	2	0.3
1	1	1	10.61	8.336	4	14.6	1	3	4	29.25	3.054	4	0.5	-4	4	1	38.91	2.314	4	0.3
2	0	0	12.91	6.856	2	13.5	4	2	0	29.60	3.018	4	1.0	4	4	1	38.92	2.314	4	0.2
-1	1	2	13.45	6.582	4	2.4	0	4	2	29.67	3.011	4	0.4	-2	2	7	39.06	2.306	4	0.5
1	1	2	13.45	6.581	4	2.8	-4	2	1	29.99	2.979	4	1.4	5	3	0	39.11	2.303	4	0.3
0	2	0	13.91	6.366	2	1.9	4	2	1	30.00	2.979	4	2.2	-5	3	1	39.42	2.286	4	0.5
0	2	1	14.71	6.022	4	0.4	-3	3	2	30.31	2.949	4	1.4	5	3	1	39.42	2.286	4	0.3
-2	0	2	16.07	5.516	2	6.5	3	3	2	30.31	2.949	4	0.6	-5	3	2	40.34	2.236	4	0.2
2	0	2	16.07	5.515	2	6.0	-1	1	6	30.43	2.938	4	1.3	5	3	2	40.35	2.235	4	0.2
0	2	2	16.89	5.250	4	19.2	1	1	6	30.43	2.938	4	1.9	-3	3	6	41.14	2.194	4	0.4
-1	1	3	17.19	5.158	4	9.3	-2	2	5	30.77	2.906	4	1.5	3	3	6	41.15	2.194	4	0.6
1	1	3	17.19	5.158	4	9.5	2	2	5	30.77	2.905	4	1.2	0	2	8	41.40	2.181	4	1.0
2	2	0	19.02	4.665	4	3.0	2	4	0	30.98	2.887	4	2.6	-4	2	6	41.80	2.161	4	0.2
0	0	4	19.12	4.643	2	0.9	-4	2	2	31.16	2.870	4	5.1	2	4	6	42.84	2.111	4	0.2
-2	2	1	19.62	4.524	4	1.6	4	2	2	31.16	2.870	4	3.7	0	6	1	42.90	2.108	4	0.4
2	2	1	19.62	4.524	4	2.0	2	4	1	31.36	2.853	4	0.2	-6	2	2	43.17	2.095	4	0.5
0	2	3	20.01	4.438	4	6.6	0	4	3	31.61	2.831	4	1.8	-3	5	3	43.22	2.093	4	0.7
3	1	0	20.65	4.302	4	11.8	2	0	6	31.72	2.821	2	0.4	3	5	3	43.22	2.093	4	0.5
3	1	1	21.20	4.191	4	3.0	0	2	6	32.16	2.784	4	4.2	1	5	5	43.60	2.076	4	0.3
-2	2	2	21.31	4.169	4	0.9	-3	3	3	32.21	2.779	4	1.0	5	3	4	43.88	2.063	4	0.2
2	2	2	21.32	4.168	4	5.6	3	3	3	32.21	2.779	4	0.9	-3	1	8	44.34	2.043	4	0.3
-1	1	4	21.38	4.157	4	4.2	-4	0	4	32.46	2.758	2	0.5	3	1	8	44.34	2.043	4	0.2
1	1	4	21.38	4.156	4	0.5	4	0	4	32.47	2.757	2	0.4	5	1	6	44.72	2.026	4	0.2
1	3	0	21.92	4.054	4	0.7	-2	4	2	32.48	2.757	4	0.5	1	3	8	45.00	2.014	4	0.2
1	3	1	22.45	3.961	4	0.4	2	4	2	32.48	2.757	4	0.5	-5	3	5	46.38	1.958	4	0.2
-3	1	2	22.78	3.903	4	0.3	-1	3	5	32.70	2.739	4	1.7	5	3	5	46.39	1.957	4	0.2
-2	0	4	23.14	3.844	2	1.5	1	3	5	32.70	2.739	4	2.5	-6	2	4	46.53	1.952	4	0.2
0	2	4	23.72	3.751	4	1.2	-4	2	3	33.02	2.713	4	0.9	7	1	0	46.93	1.936	4	0.2
-2	2	3	23.88	3.726	4	4.4	4	2	3	33.02	2.713	4	0.9	7	1	1	47.20	1.926	4	0.3
2	2	3	23.89	3.725	4	4.6	-5	1	1	33.78	2.653	4	0.5	7	1	2	48.00	1.895	4	0.2
-1	3	2	23.95	3.715	4	1.6	5	1	1	33.78	2.653	4	0.5	5	5	0	48.80	1.866	4	0.9
1	3	2	23.95	3.715	4	3.6	-2	4	3	34.27	2.616	4	0.4	4	4	6	48.90	1.863	4	0.5
-3	1	3	25.21	3.533	4	0.4	2	4	3	34.27	2.616	4	0.2	-3	3	8	48.96	1.860	4	0.2
3	1	3	25.21	3.532	4	0.9	3	3	4	34.72	2.584	4	0.4	0	0	10	49.05	1.857	2	1.1
-1	1	5	25.82	3.451	4	1.2	-2	2	6	34.78	2.579	4	0.3	-5	5	1	49.07	1.857	4	0.4
1	1	5	25.82	3.451	4	0.9	5	1	2	34.83	2.575	4	0.4	5	5	1	49.07	1.857	4	0.5
4	0	0	25.99	3.428	2	3.8	-4	2	4	35.47	2.531	4	0.4	-5	3	6	49.31	1.848	4	0.4
-1	3	3	26.28	3.392	4	3.3	1	5	0	35.87	2.503	4	0.9	-7	1	3	49.32	1.848	4	0.3
1	3	3	26.28	3.391	4	2.8	-1	5	1	36.20	2.481	4	0.2	7	1	3	49.32	1.848	4	0.3
-2	2	4	27.10	3.291	4	0.4	1	5	1	36.20	2.481	4	0.3	5	3	6	49.32	1.848	4	0.2
2	2	4	27.10	3.290	4	0.4	-5	1	3	36.52	2.460	4	0.5	0	6	5	49.47	1.842	4	0.3
-4	0	2	27.74	3.216	2	0.2	5	1	3	36.53	2.460	4	0.5	-5	5	2	49.84	1.829	4	0.2
4	0	2	27.74	3.216	2	0.4	0	2	7	36.70	2.449	4	0.3	5	5	2	49.85	1.829	4	0.4

AlPO–18, Calcined

AEI



AEL AlPO–11, Calcined

CHEMICAL COMPOSITION: $[Al_{20}P_{20}O_{80}]$

REFINED COMPOSITION: $[Al_{20}P_{20}O_{80}]$

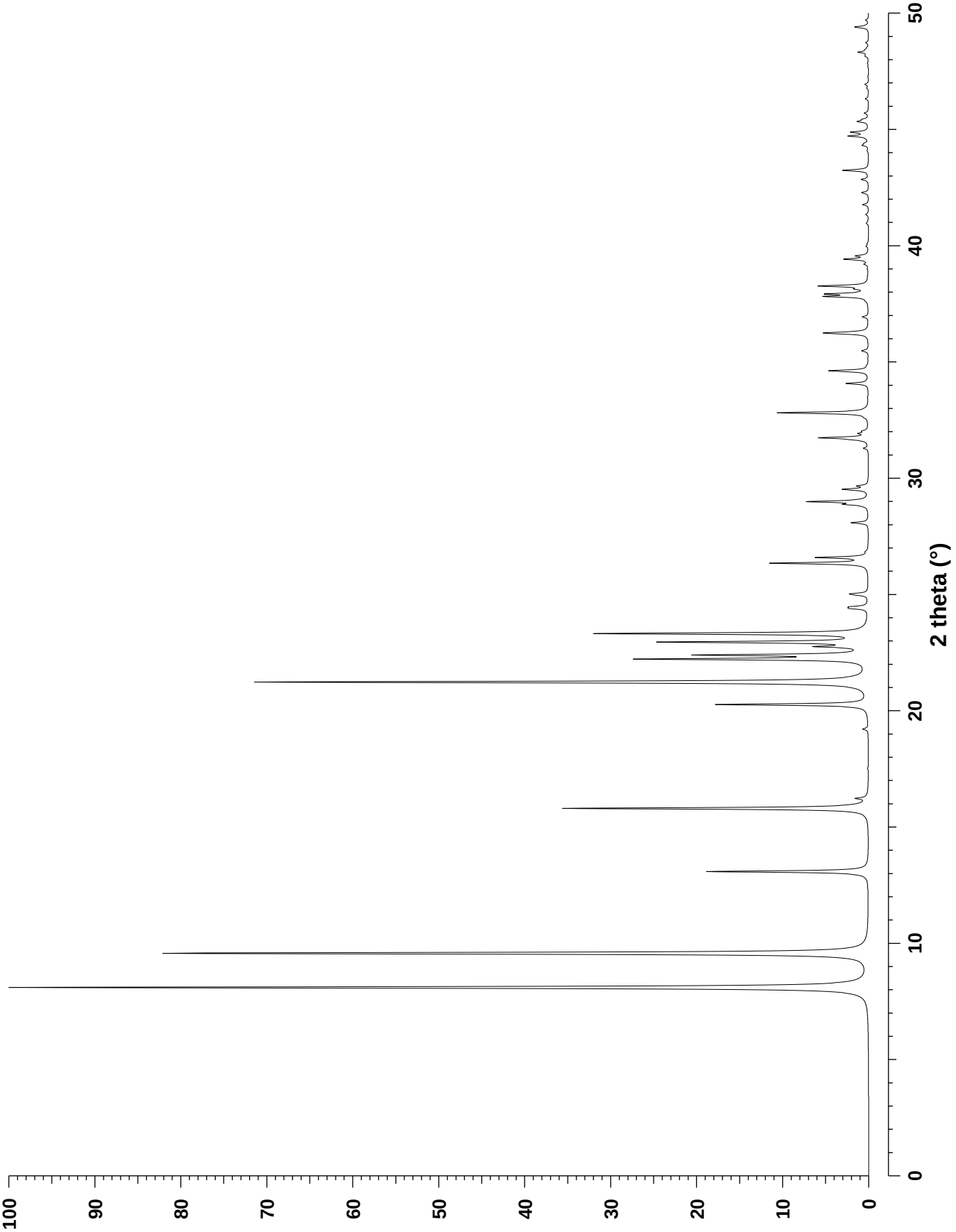
CRYSTAL DATA: *Ibm*2 (No. 46) **ba$\bar{\mathbf{c}}$** setting
$a = 13.5336$ Å $b = 18.4821$ Å $c = 8.3703$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.027$, $R_{F^2} = 0.058$

REFERENCE: J. W. Richardson, Jr., J. J. Pluth and J. V. Smith, *Acta Cryst.* **B44** 367–373 (1988).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.10	10.919	4	100.0	3	5	0	31.28	2.859	4	0.5	6	1	1	41.76	2.163	8	0.7
0	2	0	9.57	9.241	2	82.1	1	6	1	31.65	2.827	8	1.2	4	1	3	42.27	2.138	8	0.8
2	0	0	13.08	6.767	2	18.9	2	4	2	31.73	2.820	8	5.6	3	4	3	42.84	2.111	8	0.8
1	3	0	15.80	5.607	4	35.6	2	6	0	31.92	2.804	4	0.9	0	0	4	43.23	2.093	2	3.0
2	2	0	16.23	5.460	4	1.3	4	3	1	32.02	2.795	8	0.6	1	1	4	44.06	2.055	8	0.1
0	4	0	19.21	4.621	2	0.6	3	3	2	32.60	2.746	8	0.2	1	6	3	44.31	2.044	8	0.7
3	1	0	20.26	4.383	4	17.7	4	4	0	32.81	2.730	4	10.6	0	2	4	44.39	2.041	4	0.4
0	0	2	21.23	4.185	2	71.4	4	0	2	34.07	2.631	4	2.6	6	4	0	44.71	2.027	4	2.3
2	3	1	22.22	4.001	8	26.2	1	7	0	34.61	2.591	4	4.6	4	7	1	44.87	2.020	8	2.0
3	0	1	22.39	3.971	4	18.9	5	0	1	34.83	2.575	4	0.1	3	7	2	45.31	2.001	8	0.3
1	1	2	22.75	3.908	8	5.0	4	2	2	35.47	2.531	8	0.8	4	6	2	45.33	2.001	8	1.0
1	4	1	22.95	3.876	8	23.9	0	6	2	36.21	2.481	4	1.8	2	0	4	45.36	1.999	4	0.1
2	4	0	23.31	3.816	4	26.6	5	3	0	36.25	2.478	4	4.3	3	8	1	45.42	1.997	8	0.6
0	2	2	23.33	3.812	4	6.2	3	6	1	36.93	2.434	8	0.7	6	0	2	45.69	1.986	4	0.5
3	2	1	24.40	3.649	8	1.7	4	5	1	37.61	2.392	8	0.1	1	3	4	46.31	1.960	8	0.4
3	3	0	24.46	3.640	4	1.7	2	3	3	37.81	2.379	8	4.8	5	0	3	46.76	1.943	4	0.1
1	5	0	24.97	3.566	4	0.9	3	0	3	37.92	2.373	4	4.5	5	5	2	46.93	1.936	8	0.4
2	0	2	25.02	3.559	4	1.9	3	5	2	38.12	2.361	8	0.1	5	2	3	47.84	1.901	8	0.1
4	0	0	26.34	3.383	2	11.3	2	7	1	38.13	2.360	8	0.9	5	7	0	48.14	1.890	4	0.3
1	3	2	26.58	3.354	8	5.9	1	4	3	38.26	2.352	8	5.7	3	1	4	48.19	1.888	8	0.1
2	2	2	26.84	3.322	8	0.2	3	2	3	39.20	2.298	8	0.4	7	0	1	48.31	1.884	4	1.2
4	2	0	28.08	3.177	4	2.0	4	4	2	39.41	2.286	8	2.8	3	6	3	48.42	1.880	8	0.3
0	4	2	28.78	3.102	4	0.2	3	7	0	39.55	2.279	4	0.6	6	5	1	48.51	1.876	8	0.1
4	1	1	28.87	3.093	8	2.3	4	6	0	39.56	2.278	4	0.8	3	9	0	48.72	1.869	4	0.3
0	6	0	28.99	3.080	2	7.0	6	0	0	39.97	2.256	2	0.2	7	2	1	49.37	1.846	8	0.1
3	1	2	29.51	3.027	8	2.7	5	4	1	40.08	2.250	8	0.2	2	7	3	49.39	1.845	8	1.0
2	5	1	29.53	3.025	8	0.3	1	7	2	40.96	2.203	8	0.3	7	3	0	49.41	1.845	4	0.6
3	4	1	29.66	3.012	8	1.2	5	5	0	41.34	2.184	4	0.3	2	4	4	49.69	1.835	8	0.3

AlPO–11, Calcined

AEL



AEL Di-isopropylamine MnAPO–11

CHEMICAL COMPOSITION: $|(C_6H_{16}N)_2|\ [Mn_2Al_{18}P_{20}O_{80}]$
$C_6H_{16}N$ = di-isopropylamine

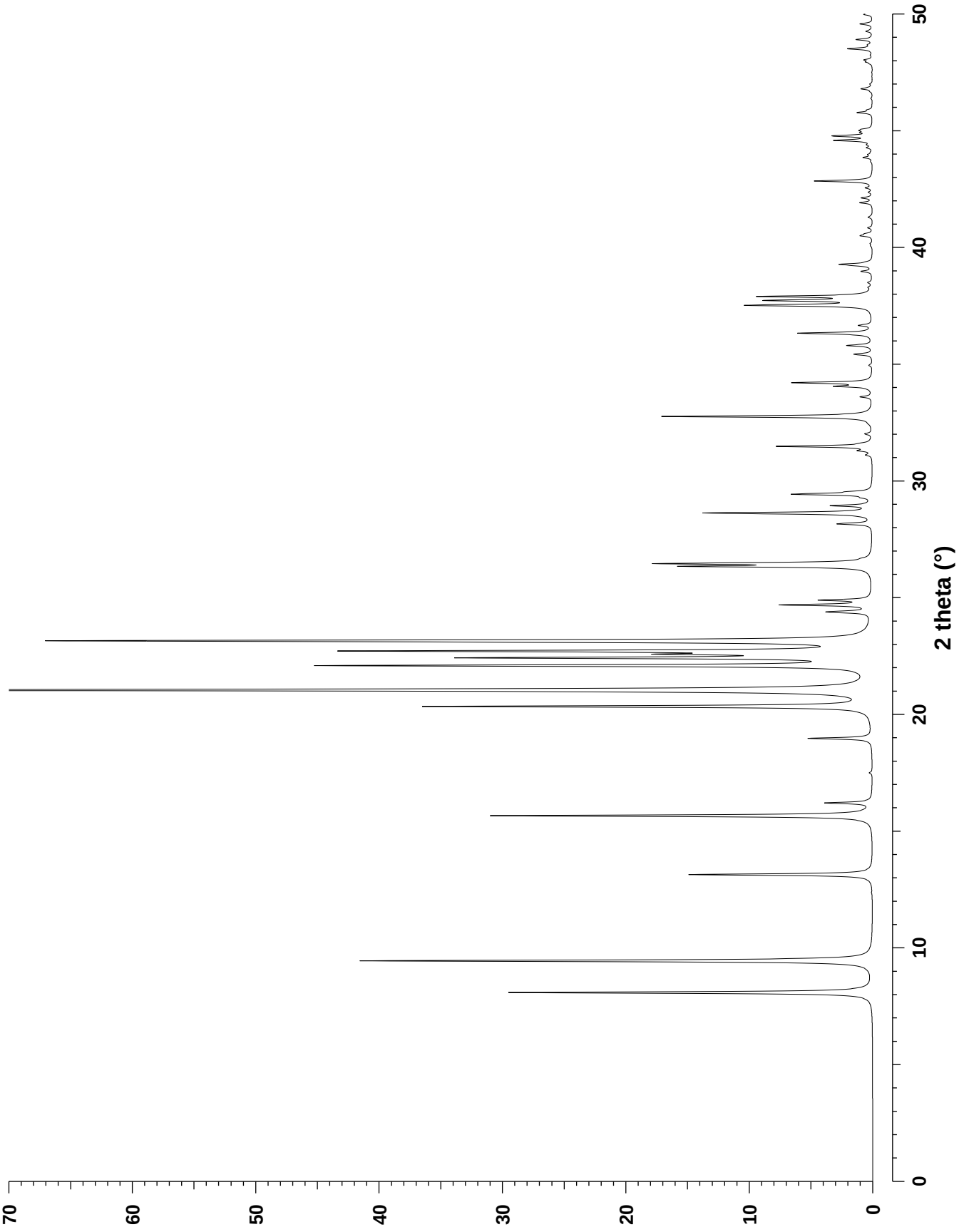
REFINED COMPOSITION: $|C_{15.5}N_{2.58}|\ [Al_{20.54}P_{18.22}O_{80}]$

CRYSTAL DATA: *Ibm*2 (No. 46) **ba$\bar{\mathbf{c}}$** setting
$a = 13.472$ Å $b = 18.712$ Å $c = 8.4431$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.042$

REFERENCE: J. J. Pluth, J. V. Smith and J. W. Richardson, Jr., *J. Phys. Chem.* **92** 2734–2738 (1988).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.09	10.933	4	29.6	4	3	1	32.01	2.796	8	0.6	0	0	4	42.84	2.111	2	4.7
0	2	0	9.45	9.356	2	41.6	3	3	2	32.45	2.759	8	0.1	1	1	4	43.67	2.073	8	0.1
2	0	0	13.14	6.736	2	14.9	4	4	0	32.76	2.733	4	17.1	1	6	3	43.85	2.065	8	0.7
1	3	0	15.66	5.660	4	31.0	5	1	0	33.60	2.667	4	1.0	0	2	4	43.97	2.059	4	0.3
2	2	0	16.21	5.467	4	3.7	4	0	2	34.05	2.633	4	2.8	0	8	2	44.27	2.046	4	0.4
2	1	1	17.50	5.069	8	0.2	1	7	0	34.20	2.622	4	6.4	4	3	3	44.39	2.041	8	0.3
0	4	0	18.97	4.678	2	5.2	5	0	1	34.95	2.567	4	0.3	4	7	1	44.58	2.032	8	3.0
3	1	0	20.34	4.367	4	36.2	4	2	2	35.42	2.534	8	1.5	6	4	0	44.77	2.024	4	3.1
0	0	2	21.04	4.222	2	100.0	0	6	2	35.80	2.508	4	2.1	3	7	2	44.92	2.018	8	0.6
2	3	1	22.09	4.024	8	44.4	5	2	1	36.29	2.475	8	0.1	3	8	1	45.00	2.015	8	0.6
3	0	1	22.42	3.965	4	31.6	5	3	0	36.32	2.473	4	6.0	2	0	4	45.01	2.014	4	0.1
1	1	2	22.58	3.938	8	11.8	3	6	1	36.66	2.451	8	1.1	4	6	2	45.06	2.012	8	0.6
1	4	1	22.71	3.915	8	41.0	4	5	1	37.47	2.400	8	0.5	6	0	2	45.77	1.982	4	1.2
0	2	2	23.11	3.848	4	12.5	2	3	3	37.52	2.397	8	9.8	1	3	4	45.88	1.978	8	0.4
2	4	0	23.15	3.842	4	60.4	3	0	3	37.72	2.385	4	6.5	2	8	2	46.38	1.958	8	0.1
3	2	1	24.38	3.651	8	3.2	2	7	1	37.74	2.384	8	2.0	5	0	3	46.67	1.946	4	0.1
3	3	0	24.42	3.644	4	0.7	1	4	3	37.90	2.374	8	8.9	5	5	2	46.79	1.942	8	0.9
1	5	0	24.69	3.606	4	7.3	2	6	2	38.29	2.351	8	0.2	6	2	2	46.85	1.939	8	0.1
2	0	2	24.89	3.577	4	4.0	0	8	0	38.49	2.339	2	0.3	2	9	1	46.99	1.934	8	0.2
1	3	2	26.34	3.384	8	14.2	3	2	3	38.97	2.311	8	0.9	3	1	4	47.86	1.900	8	0.2
4	0	0	26.46	3.368	2	16.5	3	7	0	39.22	2.297	4	0.6	5	7	0	47.94	1.898	4	0.5
2	2	2	26.68	3.341	8	0.3	4	4	2	39.27	2.294	8	2.4	3	6	3	48.03	1.894	8	0.6
4	2	0	28.16	3.169	4	2.8	4	6	0	39.37	2.288	4	0.3	3	9	0	48.23	1.887	4	0.1
0	4	2	28.48	3.134	4	0.2	5	4	1	40.07	2.250	8	0.1	6	5	1	48.49	1.877	8	0.3
0	6	0	28.62	3.119	2	13.7	6	0	0	40.16	2.245	2	0.2	7	0	1	48.51	1.876	4	1.8
4	1	1	28.94	3.085	8	3.2	1	7	2	40.50	2.227	8	0.9	0	10	0	48.66	1.871	2	0.1
2	5	1	29.28	3.050	8	0.5	1	8	1	40.58	2.223	8	0.5	4	5	3	48.68	1.871	8	0.2
3	1	2	29.43	3.035	8	6.4	2	8	0	40.84	2.210	4	0.4	2	7	3	48.90	1.863	8	1.3
3	4	1	29.53	3.025	8	1.3	5	5	0	41.29	2.187	4	0.3	2	4	4	49.25	1.850	8	0.5
3	5	0	31.11	2.875	4	0.4	6	1	1	41.91	2.155	8	1.0	7	2	1	49.54	1.840	8	0.2
1	6	1	31.29	2.859	8	0.9	4	1	3	42.12	2.145	8	0.9	7	3	0	49.57	1.839	4	0.9
2	4	2	31.48	2.842	8	7.8	2	5	3	42.36	2.134	8	0.2	6	4	2	49.97	1.825	8	0.7
2	6	0	31.61	2.830	4	0.4	3	4	3	42.55	2.125	8	0.5							

Di-isopropylamine MnAPO–11 AEL



AEN AlPO-EN3

CHEMICAL COMPOSITION: $|(C_2H_8N_2)_4(H_2O)_{16}|\ [Al_{24}P_{24}O_{96}]$
$C_2H_8N_2$ = ethylene diamine

REFINED COMPOSITION: $|(C_8N_8O_8)(H_2O)_8|\ [P_{24}Al_{24}O_{96}]$

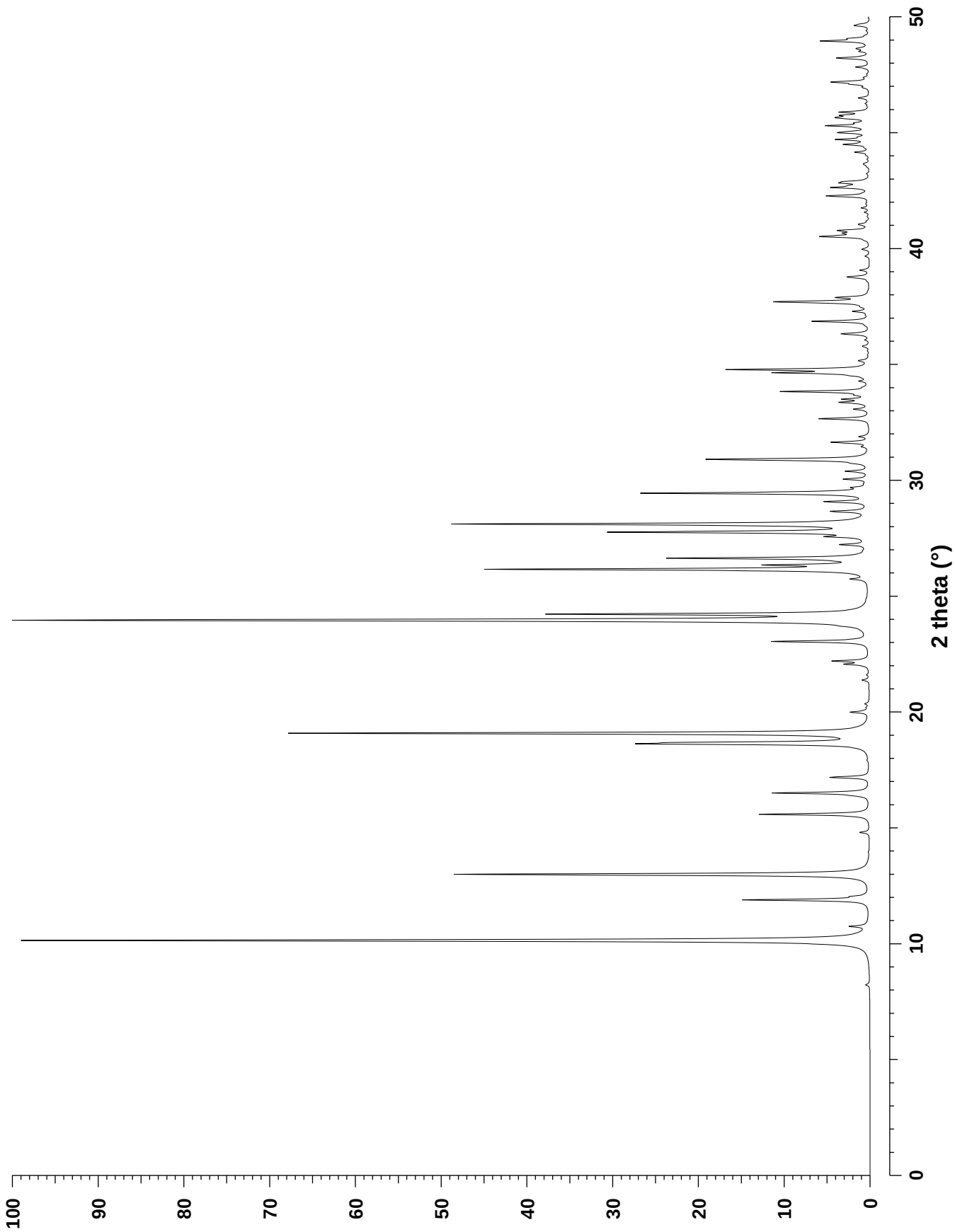
CRYSTAL DATA: $P2_12_12_1$ (No. 19)
$a = 10.321$ Å $b = 13.631$ Å $c = 17.454$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement. $R_p = 0.140$, $R_{wp} = 0.182$, $R_{F^2} = 0.103$

REFERENCE: R. M. Kirchner, R. W. Grosse-Kunstleve, J. J. Pluth, S. T. Wilson, R. W. Broach and J. V. Smith,
Microporous and Mesoporous Materials **39** 319–332 (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	1	8.23	10.743	4	0.5	3	1	3	30.90	2.894	8	16.5	4	3	2	41.56	2.173	8	0.6
0	0	2	10.14	8.727	2	100.0	0	1	6	31.44	2.845	4	0.6	1	4	6	41.75	2.163	8	0.9
1	1	0	10.75	8.228	4	2.0	2	1	5	31.63	2.828	8	4.2	1	3	7	42.26	2.138	8	5.0
1	1	1	11.89	7.443	8	14.8	2	4	1	31.88	2.807	8	1.1	3	5	1	42.63	2.121	8	4.2
0	1	2	12.04	7.350	4	1.3	1	1	6	32.65	2.743	8	5.9	3	4	4	42.71	2.117	8	1.2
0	2	0	12.99	6.815	2	49.0	3	3	1	33.06	2.710	8	1.7	4	2	4	42.82	2.112	8	2.5
1	1	2	14.80	5.987	8	1.2	2	3	4	33.35	2.687	8	2.3	1	1	8	42.88	2.109	8	2.3
1	2	0	15.58	5.687	4	13.0	0	4	4	33.36	2.686	4	1.0	3	5	2	43.61	2.075	8	0.4
1	2	1	16.39	5.408	8	1.1	0	2	6	33.49	2.675	4	2.8	1	6	3	43.66	2.073	8	0.5
0	2	2	16.50	5.372	4	11.3	2	2	5	33.67	2.662	8	0.9	4	1	5	44.15	2.051	8	1.7
2	0	0	17.18	5.161	2	4.6	3	1	4	33.82	2.650	8	10.4	1	2	8	44.48	2.037	8	2.9
1	2	2	18.62	4.765	8	22.1	1	5	0	34.01	2.636	4	0.3	2	4	6	44.56	2.033	8	0.4
1	1	3	18.68	4.750	8	16.3	3	3	2	34.27	2.617	8	1.0	5	1	1	44.70	2.027	8	3.8
2	1	1	19.08	4.652	8	68.2	1	4	4	34.51	2.599	8	1.0	2	6	2	44.81	2.023	8	0.7
2	0	2	19.99	4.442	4	2.1	1	2	6	34.63	2.590	8	10.2	0	6	4	44.99	2.015	4	3.1
0	0	4	20.35	4.364	2	0.5	4	0	0	34.77	2.580	2	16.1	2	3	7	45.04	2.013	8	1.1
0	1	4	21.38	4.156	4	0.7	2	4	3	35.12	2.555	8	0.3	3	5	3	45.21	2.006	8	0.4
0	3	2	22.06	4.030	4	2.7	4	0	1	35.16	2.553	4	0.9	4	4	2	45.29	2.002	8	4.9
2	2	1	22.20	4.004	8	4.2	3	2	4	35.75	2.512	8	0.3	3	1	7	45.41	1.997	8	1.1
2	0	3	23.04	3.861	4	10.6	4	1	1	35.79	2.509	8	0.6	3	4	5	45.60	1.989	8	1.0
1	1	4	23.07	3.855	8	1.2	2	1	6	36.05	2.491	8	0.5	0	5	6	45.60	1.989	4	0.3
1	3	2	23.70	3.754	8	0.9	4	0	2	36.31	2.474	4	3.3	2	1	8	45.63	1.988	8	0.6
2	2	2	23.91	3.721	8	3.3	2	3	5	36.85	2.439	8	6.7	5	1	2	45.65	1.987	8	2.3
2	1	3	23.96	3.715	8	98.8	3	1	5	37.28	2.412	8	1.8	4	2	5	45.71	1.985	8	0.4
0	2	4	24.22	3.675	4	35.8	1	5	3	37.46	2.401	8	0.4	2	5	5	45.74	1.984	8	2.5
1	2	4	25.73	3.462	8	1.8	4	2	1	37.63	2.390	8	1.2	1	6	4	45.88	1.978	8	3.3
0	4	0	26.15	3.408	2	44.7	2	5	1	37.67	2.388	8	3.5	5	2	1	46.25	1.963	8	0.4
1	3	3	26.34	3.383	8	10.2	1	1	7	37.70	2.386	8	8.4	1	5	6	46.49	1.953	8	1.3
2	2	3	26.53	3.359	8	0.9	2	2	6	37.88	2.375	8	3.0	3	2	7	46.94	1.936	8	0.5
2	3	1	26.63	3.347	8	23.2	1	4	5	37.91	2.373	8	0.7	4	0	6	47.08	1.930	4	1.6
3	1	1	27.22	3.276	8	3.1	2	5	2	38.75	2.324	8	0.9	2	2	8	47.15	1.927	8	0.8
2	1	4	27.56	3.237	8	0.4	3	3	4	38.78	2.322	8	1.8	5	2	2	47.17	1.927	8	1.7
1	4	0	27.56	3.236	4	3.5	3	2	5	39.06	2.306	8	1.1	5	1	3	47.19	1.926	8	2.4
1	1	5	27.76	3.214	8	30.0	0	6	0	39.67	2.272	2	0.5	3	5	4	47.37	1.919	8	0.5
1	4	1	28.04	3.182	8	4.4	1	5	4	39.96	2.256	8	0.8	1	7	1	47.82	1.902	8	1.6
0	4	2	28.11	3.174	4	47.5	4	2	3	40.47	2.229	8	0.3	1	1	9	48.21	1.888	8	3.0
3	1	2	28.65	3.116	8	4.2	2	5	3	40.51	2.227	8	4.4	4	3	5	48.21	1.887	8	0.8
3	2	0	29.07	3.071	4	4.9	4	3	1	40.54	2.225	8	1.6	2	6	4	48.50	1.877	8	1.0
1	4	2	29.44	3.034	8	26.7	4	0	4	40.62	2.221	4	0.7	1	6	5	48.62	1.873	8	1.2
3	2	1	29.53	3.025	8	0.5	1	6	0	40.66	2.219	4	1.9	3	4	6	48.95	1.861	8	2.3
1	3	4	29.68	3.010	8	1.4	2	1	7	40.73	2.215	8	0.9	4	4	4	48.95	1.861	8	3.2
1	2	5	30.04	2.975	8	2.9	2	3	6	40.77	2.213	8	1.3	4	2	6	49.05	1.857	8	1.9
2	3	3	30.38	2.942	8	2.6	0	4	6	40.78	2.212	4	1.8	3	6	2	49.18	1.853	8	0.3
0	0	6	30.73	2.909	2	0.8	1	6	1	41.01	2.201	8	0.6	0	4	8	49.61	1.837	4	1.2
3	2	2	30.86	2.897	8	5.3	0	6	2	41.05	2.199	4	0.8	1	2	9	49.67	1.836	8	0.8

AlPO-EN3

AEN



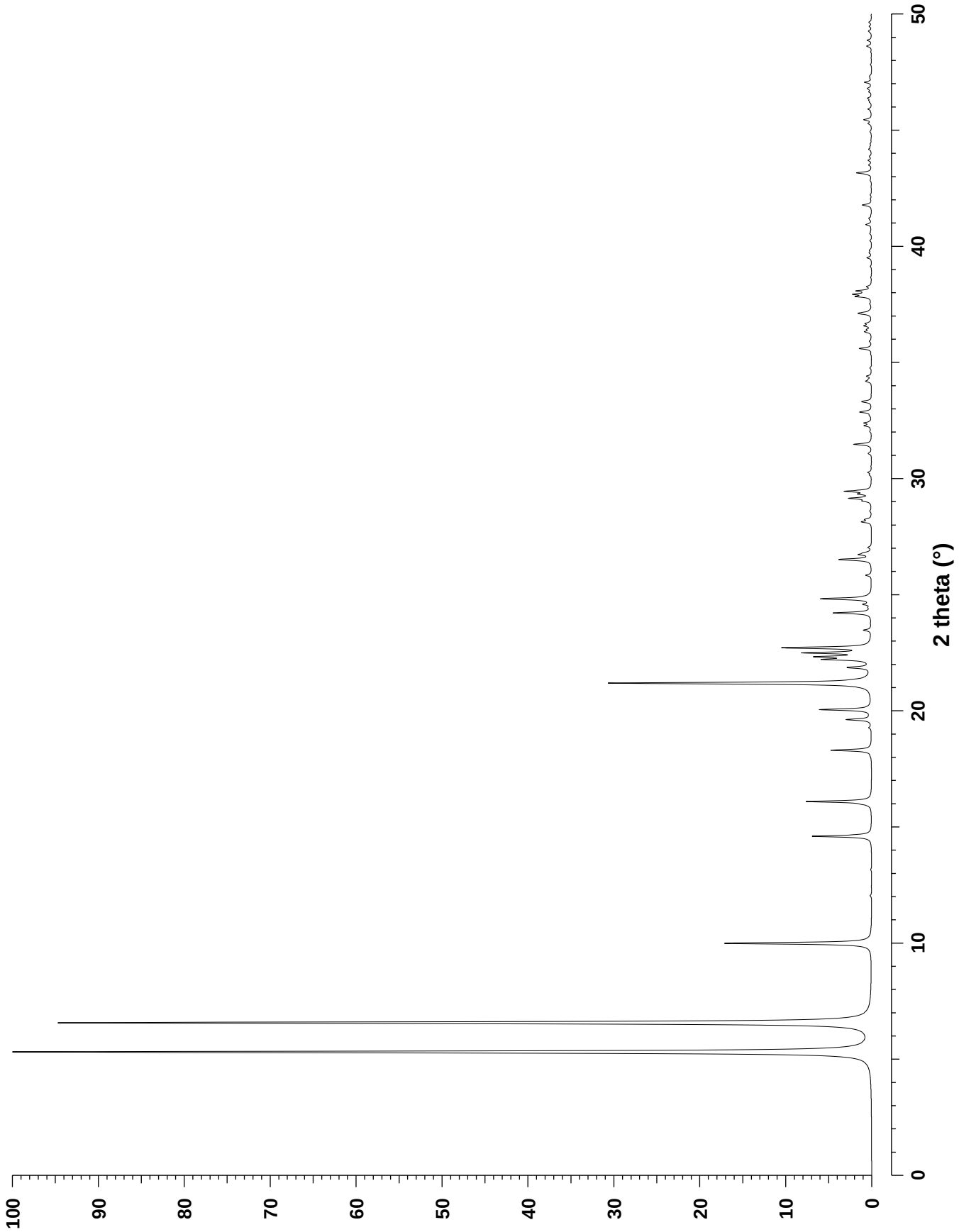
CHEMICAL COMPOSITION: $[Al_{36}P_{36}O_{144}]$

REFINED COMPOSITION: $[Si_{72}O_{144}]$

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 33.2900$ Å $b = 14.7036$ Å $c = 8.3863$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.043$, $R_{F^2} = 0.077$

REFERENCE: J. W. Richardson, Jr. and E. T. C. Vogt,
Zeolites **12** 13–19 (1992).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	5.31	16.645	2	100.0	6	4	0	29.14	3.064	4	2.5	15	1	0	41.13	2.194	4	0.1
1	1	0	6.57	13.450	4	94.7	6	2	2	29.33	3.045	8	1.3	13	3	1	41.20	2.191	8	0.3
3	1	0	9.99	8.857	4	17.1	10	2	0	29.45	3.033	4	3.0	7	3	3	41.77	2.163	8	1.0
0	2	0	12.04	7.352	2	0.2	11	1	0	30.15	2.964	4	0.2	13	1	2	41.79	2.162	8	0.1
2	2	0	13.16	6.725	4	0.1	8	0	2	30.26	2.954	4	0.4	4	4	3	42.03	2.150	8	0.1
3	1	1	14.55	6.090	8	0.1	6	4	1	31.07	2.878	8	0.3	12	4	1	42.21	2.141	8	0.2
5	1	0	14.60	6.065	4	6.9	3	5	0	31.47	2.843	4	2.1	8	6	0	42.82	2.112	4	0.1
6	0	0	15.97	5.548	2	0.5	11	1	1	32.02	2.795	8	0.2	2	6	2	43.10	2.099	8	0.2
4	2	0	16.09	5.510	4	7.6	12	0	0	32.27	2.774	2	0.8	0	0	4	43.15	2.097	2	1.7
1	3	0	18.30	4.849	4	4.7	0	4	2	32.39	2.764	4	0.8	16	0	0	43.49	2.081	2	0.3
4	2	1	19.27	4.605	8	0.3	1	1	3	32.72	2.737	8	0.1	1	1	4	43.69	2.072	8	0.4
7	1	0	19.62	4.525	4	2.9	9	1	2	32.86	2.726	8	1.4	3	7	0	43.87	2.064	4	0.2
6	2	0	20.05	4.429	4	6.0	3	5	1	33.28	2.692	8	0.2	4	6	2	44.17	2.051	8	0.3
1	3	1	21.16	4.198	8	4.3	5	5	0	33.31	2.690	4	1.0	11	5	1	44.28	2.045	8	0.1
0	0	2	21.19	4.193	2	27.9	4	4	2	34.18	2.623	8	0.6	3	1	4	44.40	2.040	8	0.1
8	0	0	21.35	4.161	2	0.5	8	4	1	34.26	2.617	8	0.3	9	5	2	44.92	2.018	8	0.2
2	0	2	21.86	4.066	4	2.6	10	0	2	34.40	2.607	4	0.6	5	7	0	45.27	2.003	4	0.3
1	1	2	22.21	4.003	8	5.0	2	2	3	34.75	2.581	8	0.2	13	3	2	45.44	1.996	8	0.8
7	1	1	22.32	3.982	8	5.7	13	1	0	35.59	2.523	4	1.5	6	6	2	45.90	1.977	8	0.4
3	3	1	22.49	3.954	8	7.3	7	5	0	35.90	2.501	4	0.2	15	3	1	46.19	1.965	8	0.2
5	3	0	22.53	3.947	4	0.2	6	4	2	36.31	2.474	8	0.7	8	4	3	46.27	1.962	8	0.2
6	2	1	22.71	3.916	8	10.1	10	4	0	36.41	2.468	4	0.4	12	4	2	46.37	1.958	8	0.4
3	1	2	23.47	3.790	8	0.9	10	2	2	36.57	2.457	8	0.8	16	2	1	46.64	1.947	8	0.3
0	4	0	24.21	3.676	2	4.4	0	6	0	36.67	2.451	2	0.6	14	4	1	46.77	1.942	8	0.2
0	2	2	24.44	3.642	4	0.2	2	6	0	37.08	2.424	4	0.7	17	1	0	46.80	1.941	4	0.3
8	2	0	24.58	3.621	4	0.8	1	3	3	37.12	2.422	8	1.2	13	5	0	47.05	1.931	4	0.8
9	1	0	24.82	3.587	4	5.9	7	5	1	37.52	2.397	8	0.2	1	3	4	47.23	1.924	8	0.1
5	3	1	24.93	3.571	8	0.2	7	1	3	37.83	2.378	8	1.6	7	7	0	47.31	1.921	4	0.1
2	2	2	25.03	3.558	8	0.1	3	3	3	37.93	2.372	8	1.9	10	6	1	47.32	1.921	8	0.1
5	1	2	25.83	3.449	8	0.7	10	4	1	38.01	2.367	8	0.2	7	1	4	47.81	1.902	8	0.1
0	4	1	26.47	3.367	4	0.2	6	2	3	38.07	2.364	8	1.6	7	7	1	48.61	1.873	8	0.4
4	4	0	26.51	3.363	4	3.7	3	5	2	38.25	2.353	8	0.3	13	1	3	48.61	1.873	8	0.1
4	2	2	26.72	3.337	8	1.2	0	6	1	38.26	2.352	4	0.2	7	5	3	48.86	1.864	8	0.2
10	0	0	26.78	3.329	2	0.4	9	5	0	39.13	2.302	4	0.1	16	0	2	48.86	1.864	4	0.3
8	2	1	26.81	3.325	8	0.4	5	3	3	39.50	2.281	8	0.6	3	7	2	49.20	1.852	8	0.1
9	1	1	27.03	3.298	8	0.3	13	3	0	39.71	2.270	4	0.3	10	4	3	49.26	1.850	8	0.3
1	3	2	28.13	3.172	8	1.1	5	5	2	39.81	2.264	8	0.2	0	6	3	49.46	1.843	4	0.3
7	3	1	28.23	3.161	8	0.7	6	6	0	40.23	2.242	4	0.2	12	6	0	49.64	1.837	4	0.3
4	4	1	28.60	3.121	8	0.2	0	4	3	40.54	2.225	4	0.2							
7	1	2	29.03	3.076	8	0.8	9	1	3	40.93	2.205	8	0.7							


100
90
80
70
60
50
40
30
20
10
0
0
10
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30
40
50
2 theta (°)

AFG Afghanite

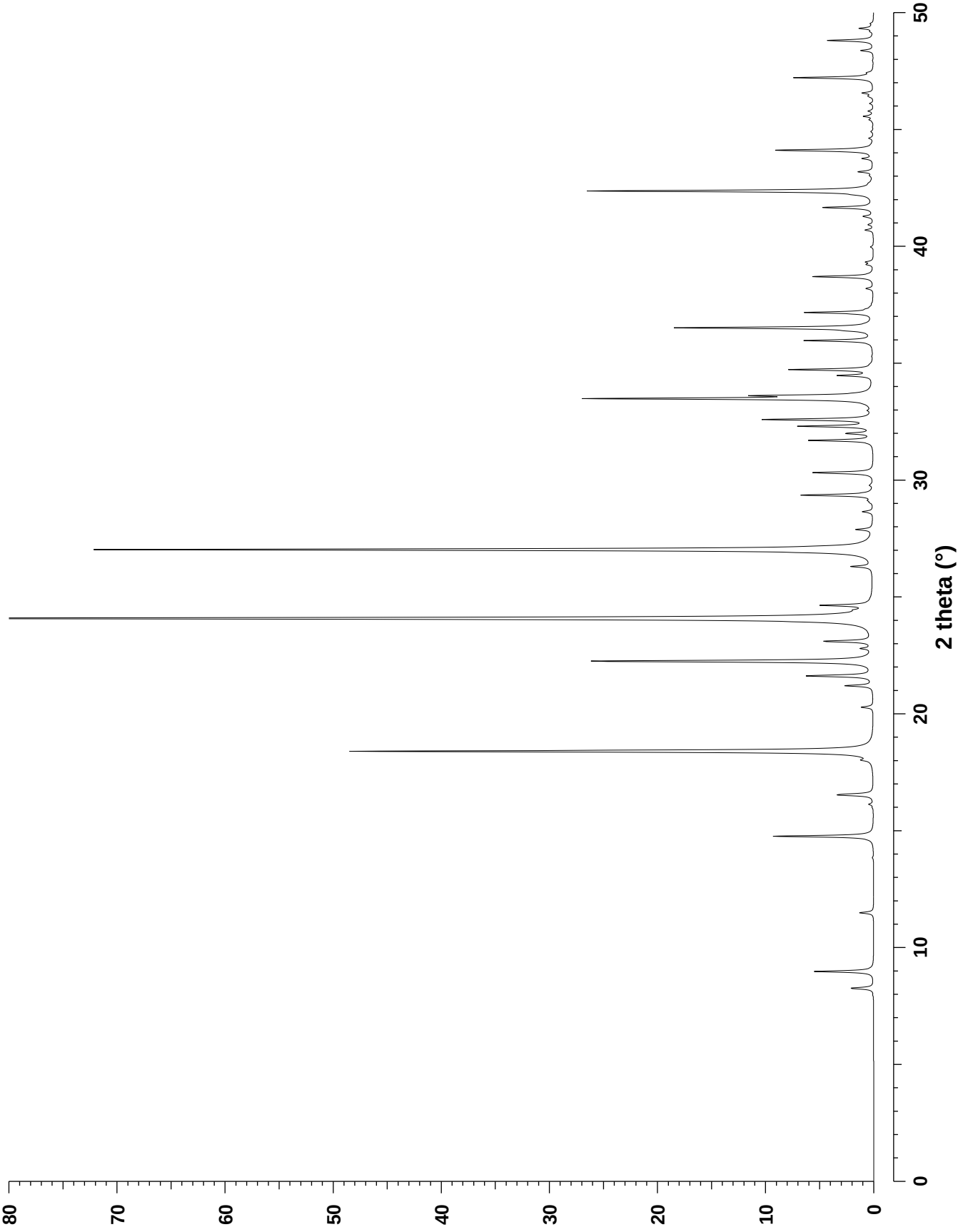
CHEMICAL COMPOSITION: $|(Na_{17.28}K_{4.72}Ca_{10})(SO_4)_6Cl_{5.8}F_{0.2}|\ [Si_{24}Al_{24}O_{96}]$
Pitigliano, Tuscany, Italy

REFINED COMPOSITION: $|(Na_{10.134}K_{5.304}Ca_{9.332})((SO_4)_6Cl_{5.8}F_{0.18})|\ [Si_{24}Al_{24}O_{96}]$

CRYSTAL DATA: $P31c$ (No. 159)
$a = 12.801$ Å $b = 12.801$ Å $c = 21.412$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_p = 0.045$, $R_{wp} = 0.102$

REFERENCE: P. Ballirano, E. Bonaccorsi, A. Maras and S. Merlino, *Eur. J. Mineral.* **9** 21–30 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	8.26	10.706	2	2.1	1	0	7	30.31	2.949	12	5.6	2	0	9	41.29	2.186	12	0.2
1	0	1	8.98	9.845	12	5.5	4	-1	3	31.69	2.824	12	3.1	3	1	7	41.65	2.169	12	1.5
1	0	2	11.49	7.701	12	1.3	3	1	3	31.69	2.824	12	2.9	4	-1	7	41.65	2.169	12	1.6
1	1	0	13.84	6.400	6	0.1	3	0	5	31.99	2.798	12	2.3	3	0	8	41.67	2.168	12	1.8
1	0	3	14.76	6.001	12	9.3	4	0	0	32.30	2.771	6	6.7	0	0	10	42.20	2.141	2	0.4
2	-1	2	16.13	5.494	6	0.2	4	0	1	32.58	2.749	12	8.1	3	3	0	42.36	2.133	6	26.5
1	1	2	16.13	5.494	6	0.2	4	-2	4	32.60	2.747	6	1.4	5	0	3	42.70	2.117	12	0.1
2	0	1	16.52	5.366	12	2.4	2	2	4	32.60	2.747	6	1.1	1	0	10	43.02	2.102	12	0.2
0	0	4	16.56	5.353	2	1.7	3	-1	6	32.97	2.717	12	0.1	4	2	0	43.18	2.095	12	1.4
2	0	2	18.02	4.922	12	0.7	2	1	6	32.97	2.717	12	0.1	3	-1	9	43.75	2.069	12	0.5
1	0	4	18.40	4.820	12	48.5	2	0	7	33.46	2.678	12	0.2	2	1	9	43.75	2.069	12	0.5
2	0	3	20.28	4.378	12	1.1	0	0	8	33.48	2.677	2	26.0	6	-2	2	44.04	2.056	12	0.2
2	1	0	21.20	4.190	12	2.6	3	1	4	33.61	2.666	12	4.7	4	2	2	44.04	2.056	12	0.1
3	-1	1	21.61	4.112	12	2.1	4	-1	4	33.61	2.666	12	4.6	4	0	7	44.09	2.054	12	2.9
2	1	1	21.61	4.112	12	2.2	1	0	8	34.47	2.602	12	3.1	4	-2	8	44.11	2.053	6	3.4
2	-1	4	21.64	4.106	6	1.2	4	0	3	34.72	2.584	12	7.7	2	2	8	44.11	2.053	6	3.2
1	1	4	21.64	4.106	6	1.4	3	0	6	34.95	2.567	12	0.1	5	0	4	44.21	2.048	12	0.2
1	0	5	22.25	3.995	12	26.1	4	-1	5	35.96	2.498	12	3.2	1	1	10	44.62	2.031	6	0.2
2	1	2	22.79	3.902	12	0.5	3	1	5	35.96	2.498	12	3.1	2	-1	10	44.62	2.031	6	0.2
3	-1	2	22.79	3.902	12	0.5	1	1	8	36.38	2.469	6	0.6	3	1	8	44.90	2.019	12	0.1
2	0	4	23.10	3.851	12	4.4	2	-1	8	36.38	2.469	6	0.5	2	0	10	45.41	1.997	12	0.3
3	0	0	24.08	3.695	6	100.0	4	0	4	36.51	2.461	12	18.3	5	1	0	45.56	1.991	12	0.9
3	0	1	24.44	3.641	12	0.6	4	1	0	37.16	2.419	12	6.3	3	3	4	45.78	1.982	6	0.2
3	-1	3	24.64	3.613	12	2.2	2	0	8	37.31	2.410	12	0.3	6	-3	4	45.78	1.982	6	0.2
2	1	3	24.64	3.613	12	2.2	3	0	7	38.19	2.356	12	0.7	5	0	5	46.10	1.969	12	0.3
2	0	5	26.30	3.389	12	1.9	4	-1	6	38.65	2.329	12	0.1	3	2	7	46.43	1.956	12	0.2
3	-1	4	27.02	3.299	12	36.4	4	0	5	38.70	2.327	12	4.6	5	-2	7	46.43	1.956	12	0.1
2	1	4	27.02	3.299	12	35.7	1	0	9	38.71	2.326	12	1.1	4	2	4	46.55	1.951	12	0.5
3	0	3	27.17	3.282	12	1.0	5	-2	4	39.22	2.297	12	0.3	6	-2	4	46.55	1.951	12	0.5
2	2	0	27.88	3.200	6	1.5	3	2	4	39.22	2.297	12	0.2	4	0	8	47.21	1.925	12	7.4
2	-1	6	28.64	3.117	6	0.5	5	-1	3	39.32	2.291	12	0.3	1	0	11	47.42	1.917	12	0.4
1	1	6	28.64	3.117	6	0.5	4	1	3	39.32	2.291	12	0.4	4	2	5	48.36	1.882	12	0.1
3	1	0	29.04	3.075	12	0.2	2	1	8	39.97	2.256	12	0.1	3	1	9	48.37	1.882	12	0.5
4	-2	2	29.12	3.066	6	0.2	3	-1	8	39.97	2.256	12	0.1	4	-1	9	48.37	1.882	12	0.5
2	2	2	29.12	3.066	6	0.1	5	0	0	40.69	2.217	6	0.8	5	1	4	48.80	1.866	12	2.0
3	1	1	29.35	3.043	12	2.6	5	0	1	40.92	2.205	12	0.4	6	-1	4	48.80	1.866	12	2.3
4	-1	1	29.35	3.043	12	2.7	4	0	6	41.24	2.189	12	0.2	3	0	10	49.18	1.853	12	0.2
3	0	4	29.37	3.041	12	1.7	5	-2	5	41.28	2.187	12	0.3	6	0	0	49.32	1.848	6	1.3
2	0	6	29.77	3.001	12	0.3	3	2	5	41.28	2.187	12	0.3	6	0	1	49.52	1.841	12	0.3


0
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40
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0
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30
40
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60
70
80

AFI Tetrapropylammonium Fluoride AlPO-5

CHEMICAL COMPOSITION: $|(C_3H_7)_4NF|\ [Al_{12}P_{12}O_{48}]$
$(C_3H_7)_4NF$ = tetrapropylammonium fluoride

REFINED COMPOSITION: $|C_{12}NF|\ [Al_{12}P_{12}O_{48}]$

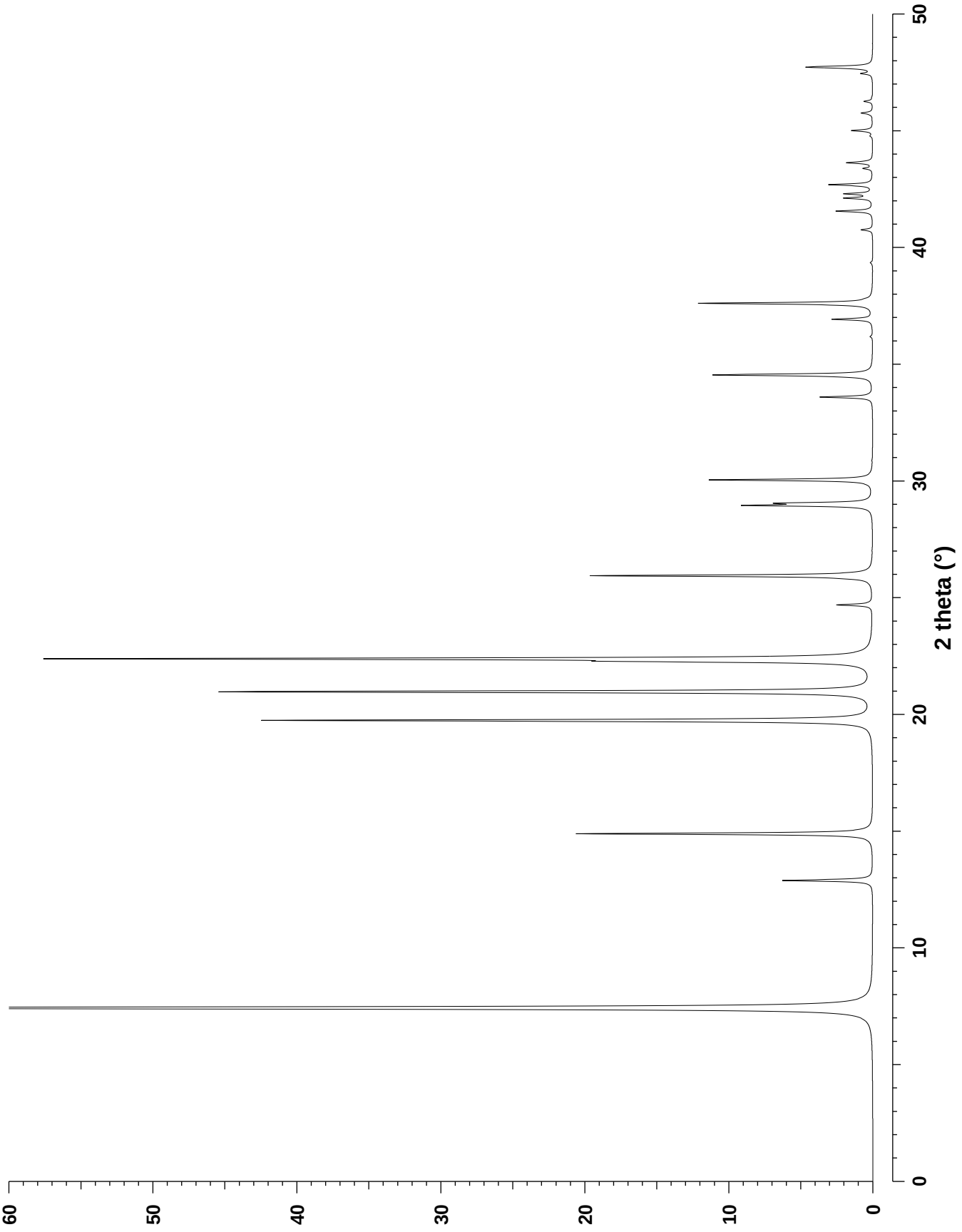
CRYSTAL DATA: *P*6*cc* (No. 184)
$a = 13.740$ Å $b = 13.740$ Å $c = 8.474$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.042$

REFERENCE: S. Qiu, W. Pang, H. Kessler and J. L. Guth, *Zeolites* **9** 440–444 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.43	11.899	6	100.0	4	0	0	30.04	2.975	6	11.4	5	1	0	42.29	2.137	12	1.9
1	1	0	12.89	6.870	6	6.3	2	2	2	33.59	2.668	12	3.7	0	0	4	42.68	2.118	2	3.0
2	0	0	14.89	5.950	6	20.6	3	1	2	34.45	2.604	24	0.4	1	0	4	43.38	2.086	12	0.6
2	1	0	19.74	4.497	12	42.4	3	2	1	34.52	2.598	24	1.0	5	0	2	43.62	2.075	12	1.8
0	0	2	20.97	4.237	2	45.3	4	1	0	34.54	2.597	12	10.3	5	1	1	43.68	2.072	24	0.2
1	0	2	22.27	3.992	12	12.5	4	1	1	36.18	2.483	24	0.2	1	1	4	44.77	2.024	12	0.2
2	1	1	22.38	3.973	24	55.3	4	0	2	36.92	2.435	12	2.8	3	3	2	45.00	2.015	12	1.5
3	0	0	22.41	3.966	6	1.3	2	1	3	37.60	2.392	24	12.1	6	0	0	45.75	1.983	6	0.8
1	1	2	24.69	3.606	12	2.5	5	0	0	37.80	2.380	6	0.2	3	2	3	46.25	1.963	24	0.6
2	0	2	25.81	3.451	12	0.5	3	3	0	39.34	2.290	6	0.2	2	1	4	47.44	1.917	24	0.8
2	2	0	25.94	3.435	6	19.6	4	1	2	40.75	2.214	24	0.8	5	1	2	47.66	1.908	24	0.4
2	1	2	28.95	3.084	24	8.2	4	2	1	41.55	2.174	24	2.6	4	3	1	47.71	1.906	24	2.4
3	1	1	29.04	3.075	24	5.6	3	1	3	42.11	2.146	24	1.9	5	2	0	47.73	1.905	12	2.4

Tetrapropylammonium Fluoride AlPO-5

AFI



AFN AlPO–14, Calcined

CHEMICAL COMPOSITION: $[Al_8P_8O_{32}]$

REFINED COMPOSITION: $[Al_8P_8O_{32}]$

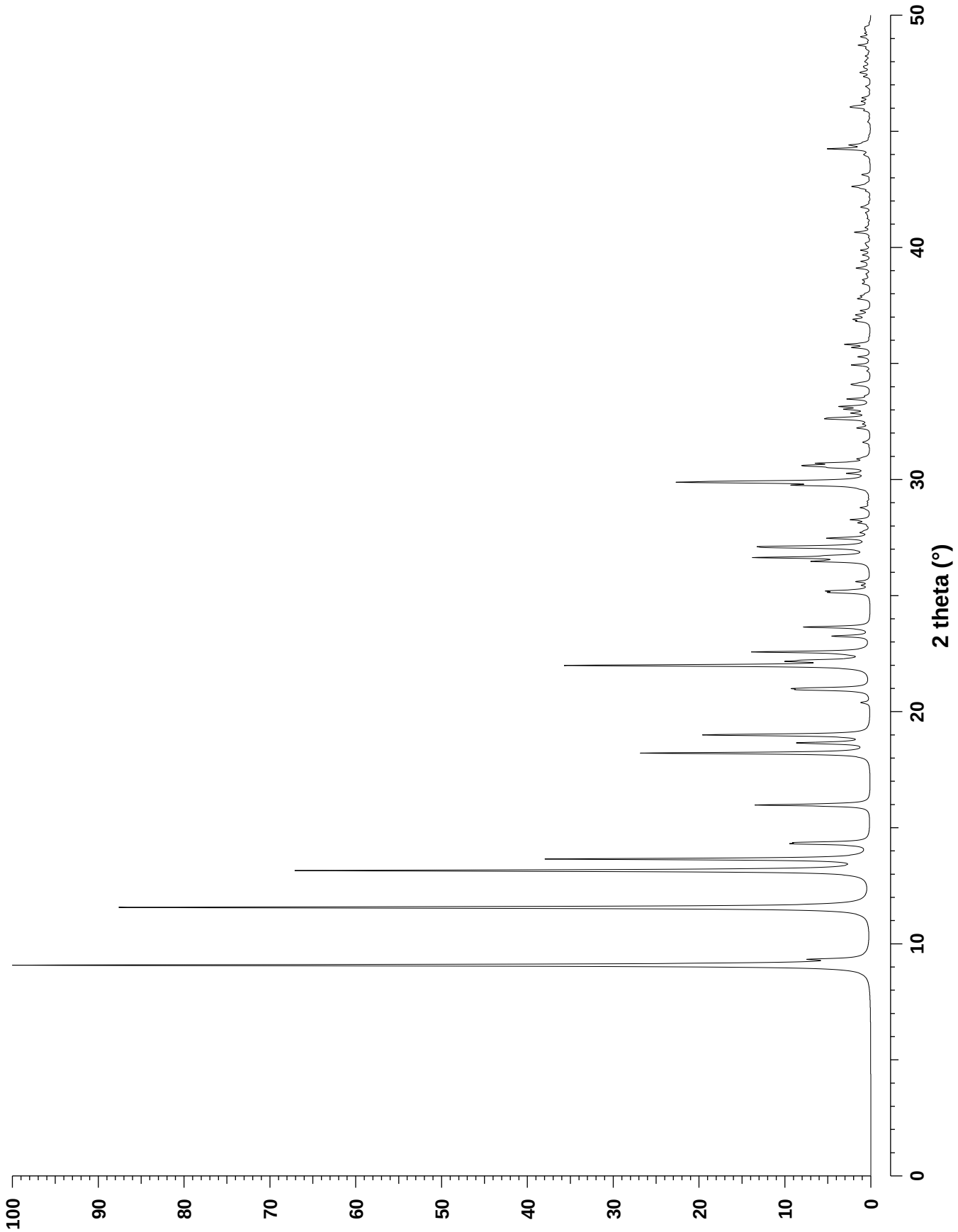
CRYSTAL DATA: $P\overline{1}$ (No. 2)
$a = 9.7041$ Å $b = 9.7361$ Å $c = 10.202$ Å
$\alpha = 77.811°$ $\beta = 77.504°$ $\gamma = 87.691°$
X-ray Rietveld refinement, $R_F = 0.059$, $R_P = 0.114$, $R_{wP} = 0.135$

REFERENCE: R. W. Broach, S. T. Wilson and R. M. Kirchner,
in *Proceedings of the 12th International Zeolite Conference*,
Ed. by M. M. J. Treacy, B. K. Marcus, J. B. Higgins and M. E. Bisher
(Materials Research Society: Warrendale) vol. **III** 1715–1722 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	9.08	9.744	2	100.0	0	3	1	27.71	3.219	2	0.9	-3	1	2	37.27	2.413	2	0.9
1	0	0	9.33	9.474	2	4.9	3	0	1	27.78	3.211	2	0.4	1	4	1	37.78	2.381	2	1.2
1	0	1	11.56	7.655	2	36.1	0	3	0	28.13	3.172	2	1.2	4	1	1	37.90	2.374	2	0.6
0	1	1	11.57	7.647	2	53.6	3	0	0	28.26	3.158	2	2.2	2	-2	3	38.43	2.343	2	0.8
1	-1	0	13.15	6.733	2	66.3	3	1	1	28.78	3.102	2	1.1	0	4	2	38.51	2.338	2	0.4
1	1	0	13.22	6.695	2	2.5	1	2	3	29.58	3.020	2	0.4	-2	2	3	38.60	2.332	2	0.7
1	1	1	13.65	6.488	2	37.5	1	-3	0	29.65	3.013	2	0.4	4	1	2	38.85	2.318	2	0.4
0	-1	1	14.30	6.196	2	7.1	1	3	0	29.75	3.003	2	6.8	3	3	2	39.10	2.304	2	1.6
-1	0	1	14.36	6.168	2	6.5	3	1	0	29.86	2.992	2	2.7	-1	1	4	39.39	2.287	2	0.9
1	-1	1	15.97	5.551	2	13.0	2	0	3	29.86	2.992	2	1.0	2	-3	2	39.67	2.272	2	0.9
-1	1	1	16.03	5.528	2	1.7	-1	3	1	29.88	2.990	2	15.3	-3	2	2	39.87	2.261	2	1.1
0	0	2	18.21	4.872	2	26.7	3	-1	1	29.92	2.987	2	6.7	-1	4	2	40.63	2.220	2	0.7
1	0	2	18.62	4.764	2	3.0	0	2	3	29.92	2.987	2	0.8	4	-1	2	40.65	2.220	2	1.2
0	2	0	18.65	4.758	2	1.8	0	3	2	30.26	2.953	2	1.8	2	-1	4	40.85	2.209	2	0.5
0	1	2	18.66	4.755	2	4.5	3	0	2	30.27	2.952	2	0.5	1	-4	1	41.49	2.176	2	0.4
2	0	0	18.73	4.737	2	0.4	1	-1	3	30.50	2.930	2	3.0	3	0	4	41.73	2.164	2	0.8
0	2	1	18.98	4.675	2	12.8	1	3	2	30.57	2.924	2	4.0	2	-4	0	42.42	2.131	2	0.4
2	0	1	19.01	4.669	2	9.2	3	1	2	30.61	2.921	2	1.5	4	-2	0	42.54	2.125	2	0.5
2	1	1	20.39	4.356	2	0.9	-1	1	3	30.61	2.920	2	3.0	-2	4	1	42.61	2.122	2	1.2
1	2	0	20.94	4.242	2	6.3	-2	-2	1	30.70	2.912	2	5.2	2	4	0	42.62	2.121	2	0.4
2	1	0	21.00	4.231	2	7.1	0	-1	3	30.88	2.896	2	1.1	4	-2	1	42.64	2.120	2	0.4
2	-1	1	21.98	4.044	2	28.1	-1	0	3	30.95	2.889	2	0.4	-1	-1	4	43.12	2.098	2	1.0
-1	2	1	22.00	4.041	2	8.9	-3	0	1	31.59	2.833	2	0.4	4	2	3	43.99	2.058	2	0.4
0	-1	2	22.16	4.012	2	6.6	-1	-2	2	31.61	2.830	2	0.4	-2	-2	3	44.24	2.047	2	3.4
-1	0	2	22.22	4.000	2	4.8	2	2	3	32.21	2.779	2	1.3	-3	-3	1	44.24	2.047	2	1.5
0	-2	1	22.43	3.964	2	0.6	2	3	1	32.60	2.746	2	3.9	1	1	5	44.40	2.040	2	2.0
1	-1	2	22.48	3.955	2	1.0	3	2	1	32.65	2.743	2	3.2	-3	3	2	44.52	2.035	2	0.4
-1	1	2	22.57	3.939	2	13.2	-1	3	2	32.86	2.725	2	1.8	2	-2	4	45.88	1.978	2	0.6
2	0	2	23.24	3.828	2	2.9	2	-1	3	33.02	2.712	2	2.6	3	4	2	46.02	1.972	2	0.8
0	2	2	23.26	3.824	2	1.7	-1	2	3	33.14	2.703	2	3.4	3	4	1	46.03	1.972	2	0.6
1	2	2	23.63	3.764	2	4.4	-1	-3	1	33.46	2.678	2	2.7	4	3	2	46.06	1.971	2	1.0
2	1	2	23.64	3.764	2	1.6	-3	-1	1	33.60	2.668	2	0.4	-1	-3	3	46.28	1.962	2	0.8
-2	1	1	23.65	3.763	2	2.0	-1	-1	3	34.06	2.632	2	1.0	-3	-1	3	46.43	1.956	2	0.5
-1	-2	1	25.13	3.543	2	3.9	2	3	0	34.10	2.629	2	1.5	2	2	5	46.45	1.955	2	0.5
-2	-1	1	25.20	3.534	2	4.3	3	2	0	34.16	2.624	2	0.8	1	5	1	47.35	1.920	2	0.8
2	2	1	25.44	3.501	2	0.8	3	1	3	34.93	2.569	2	0.8	4	0	4	47.51	1.914	2	0.5
-1	-1	2	25.60	3.479	2	1.6	1	3	3	34.93	2.568	2	1.4	5	1	1	47.52	1.913	2	0.5
2	-2	0	26.47	3.367	2	5.6	1	1	4	35.28	2.544	2	1.4	0	4	4	47.56	1.912	2	0.4
-1	2	2	26.52	3.361	2	1.2	2	-3	1	35.68	2.516	2	2.0	3	-4	0	47.73	1.905	2	0.5
2	2	0	26.63	3.348	2	12.7	-3	2	1	35.82	2.507	2	2.9	4	-3	0	47.79	1.903	2	0.5
1	1	3	26.72	3.336	2	2.9	-2	-2	2	36.81	2.442	2	1.3	5	-1	1	48.23	1.887	2	0.5
1	0	3	27.06	3.295	2	8.4	0	-3	2	36.88	2.437	2	0.5	-1	1	5	48.70	1.870	2	1.4
0	1	3	27.11	3.289	2	9.4	0	0	4	36.90	2.436	2	1.3	3	-4	1	49.06	1.857	2	1.0
0	0	3	27.46	3.248	2	4.2	1	2	4	37.05	2.426	2	0.4	-4	3	1	49.21	1.852	2	0.5
2	2	2	27.49	3.244	2	1.0	4	0	1	37.10	2.423	2	1.2	5	-1	2	49.41	1.845	2	0.5

AlPO–14, Calcined

AFN



AFO AlPO–41, Calcined

CHEMICAL COMPOSITION: $[Al_{10}P_{10}O_{40}]$

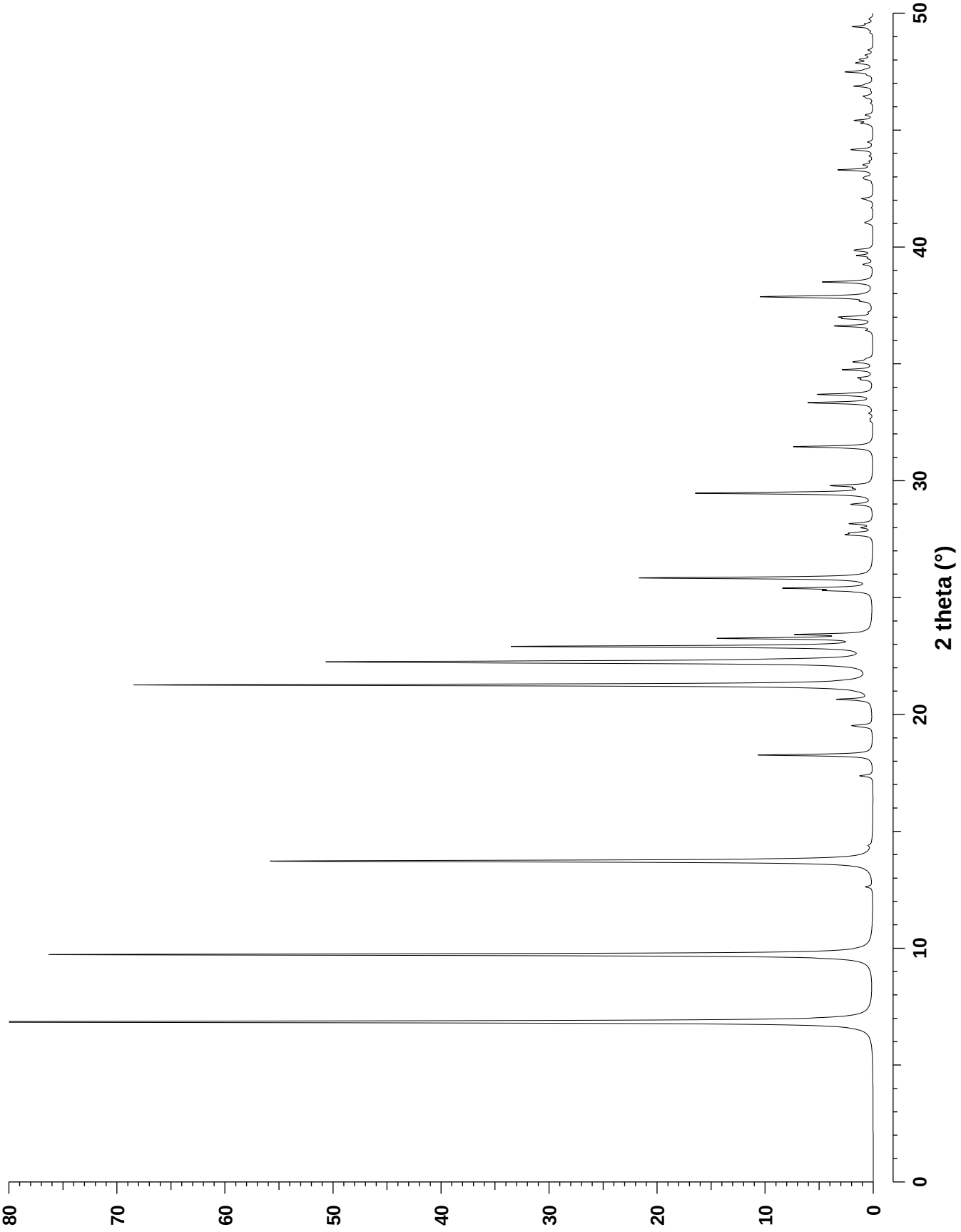
REFINED COMPOSITION: $[Al_{10}P_{10}O_{40}]$

CRYSTAL DATA: $P112_1$ (No. 4) unique axis **c**
$a = 9.7179$ Å $b = 13.7915$ Å $c = 8.3591$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 110.6°$
X-ray Rietveld refinement, $R_{exp} = 0.023$, $R_{wp} = 0.164$, $R_F = 0.074$

REFERENCE: R. M. Kirchner and J. M. Bennett,
Zeolites **14** 523–528 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	6.85	12.910	2	100.0	3	0	0	29.46	3.032	2	11.6	2	-5	2	39.88	2.261	4	0.7
1	0	0	9.72	9.097	2	42.8	3	-3	0	29.47	3.031	2	5.1	1	5	1	41.00	2.201	4	0.2
1	-1	0	9.73	9.094	2	35.6	0	4	1	29.67	3.011	4	0.9	2	-6	1	41.04	2.199	4	0.4
0	1	1	12.62	7.017	4	0.6	3	-1	1	29.78	3.000	4	1.4	0	6	0	41.99	2.152	2	0.3
0	2	0	13.72	6.455	2	41.9	3	-2	1	29.78	3.000	4	1.0	3	3	0	42.06	2.148	2	0.9
1	1	0	13.74	6.445	2	10.1	0	3	2	29.80	2.998	4	1.4	0	4	3	42.88	2.109	4	0.3
1	-2	0	13.75	6.441	2	8.6	3	0	1	31.38	2.850	4	0.4	2	-4	3	42.92	2.107	4	0.3
1	-1	1	14.39	6.154	4	0.2	2	1	2	31.45	2.845	4	2.8	3	-1	3	42.96	2.105	4	0.4
0	2	1	17.36	5.109	4	0.6	2	-3	2	31.45	2.844	4	4.4	3	-5	2	43.01	2.103	4	0.3
1	1	1	17.37	5.104	4	0.3	0	1	3	32.88	2.724	4	0.3	0	0	4	43.29	2.090	2	3.2
1	-2	1	17.38	5.102	4	0.4	2	3	0	33.32	2.689	2	1.4	3	3	1	43.50	2.081	4	0.4
2	-1	0	18.26	4.859	2	10.6	2	-5	0	33.33	2.688	2	4.6	3	-6	1	43.52	2.080	4	0.4
1	-3	0	19.47	4.559	2	0.5	1	-1	3	33.64	2.664	4	0.8	0	1	4	43.89	2.063	4	0.3
2	0	0	19.52	4.548	2	0.8	1	3	2	33.69	2.660	4	4.2	3	0	3	44.14	2.052	4	0.3
2	-2	0	19.52	4.547	2	0.9	1	-4	2	33.70	2.660	4	0.6	4	1	1	44.15	2.051	4	0.9
0	3	0	20.64	4.303	2	3.1	1	4	1	34.31	2.614	4	0.5	4	-5	1	44.17	2.051	4	0.8
2	-1	1	21.15	4.201	4	0.3	1	-5	1	34.32	2.613	4	0.4	1	-1	4	44.48	2.037	4	0.5
0	0	2	21.26	4.180	2	68.3	3	1	1	34.39	2.608	4	0.2	1	5	2	45.28	2.003	4	0.7
1	2	1	22.20	4.004	4	10.5	3	-4	1	34.40	2.607	4	1.0	2	4	2	45.30	2.002	4	0.2
1	-3	1	22.21	4.002	4	9.7	0	5	0	34.74	2.582	2	2.8	4	0	2	45.40	1.998	4	0.8
2	0	1	22.25	3.995	4	19.5	2	3	1	35.05	2.560	4	0.5	4	-4	2	45.41	1.997	4	0.9
2	-2	1	22.26	3.994	4	23.0	2	-5	1	35.07	2.559	4	0.5	1	1	4	45.64	1.988	4	0.2
0	1	2	22.36	3.976	4	3.3	0	2	3	35.08	2.558	4	0.3	1	-2	4	45.64	1.988	4	0.4
2	1	0	22.90	3.883	2	18.0	1	1	3	35.09	2.558	4	0.3	1	4	3	46.37	1.958	4	0.2
2	-3	0	22.91	3.881	2	15.9	1	-2	3	35.09	2.557	4	0.3	1	-5	3	46.38	1.958	4	0.3
0	3	1	23.25	3.826	4	13.5	2	2	2	35.17	2.552	4	0.3	3	-4	3	46.45	1.955	4	0.6
1	0	2	23.42	3.798	4	1.6	3	-2	2	35.23	2.548	4	0.3	5	-2	0	46.87	1.938	2	1.0
1	-1	2	23.42	3.798	4	4.7	0	5	1	36.42	2.467	4	0.5	5	-3	0	46.88	1.938	2	0.7
2	1	1	25.29	3.522	4	1.7	3	0	2	36.61	2.454	4	1.4	2	-5	3	46.97	1.934	4	0.3
2	-3	1	25.30	3.520	4	1.8	3	-3	2	36.62	2.454	4	2.2	2	-1	4	47.35	1.920	4	0.3
0	2	2	25.39	3.508	4	2.8	3	2	0	36.92	2.435	2	1.2	2	5	1	47.47	1.915	4	0.9
1	1	2	25.40	3.507	4	3.0	3	-5	0	36.94	2.433	2	1.1	2	-7	1	47.48	1.915	4	1.6
1	-2	2	25.40	3.506	4	2.1	4	-2	0	37.00	2.429	2	2.6	0	6	2	47.53	1.913	4	0.3
1	3	0	25.83	3.449	2	10.7	2	-1	3	37.20	2.417	4	0.3	3	3	2	47.59	1.911	4	0.4
1	-4	0	25.84	3.448	2	11.5	4	-1	0	37.67	2.388	2	0.8	3	4	0	47.84	1.901	2	0.9
2	2	0	27.68	3.222	2	1.6	1	-3	3	37.84	2.377	4	2.9	3	-7	0	47.87	1.900	2	0.4
2	-4	0	27.70	3.221	2	0.7	2	0	3	37.87	2.376	4	6.2	1	-3	4	47.88	1.900	4	0.3
3	-2	0	27.76	3.214	2	1.7	2	-2	3	37.87	2.376	4	2.2	1	6	1	48.00	1.895	4	0.3
1	3	1	27.98	3.188	4	0.6	0	3	3	38.49	2.339	4	4.5	1	-7	1	48.01	1.895	4	0.4
1	-4	1	27.99	3.187	4	0.3	4	-3	1	39.25	2.296	4	0.6	0	5	3	48.04	1.894	4	0.5
2	-1	2	28.16	3.169	4	2.1	1	-6	0	39.50	2.281	2	0.2	5	-2	1	48.20	1.888	4	0.4
1	2	2	28.98	3.081	4	0.9	4	0	0	39.63	2.274	2	1.4	0	3	4	48.42	1.880	4	0.4
1	-3	2	28.98	3.081	4	0.7	2	1	3	39.82	2.264	4	0.2	5	-4	1	49.29	1.849	4	0.2
2	0	2	29.01	3.077	4	0.3	2	-3	3	39.83	2.263	4	0.8	0	7	0	49.42	1.844	2	1.9
2	-2	2	29.02	3.077	4	0.3	2	3	2	39.86	2.261	4	0.4	2	-3	4	49.54	1.840	4	0.5

AlPO–41, Calcined AFO



AFR Tetrapropylammonium SAPO–40

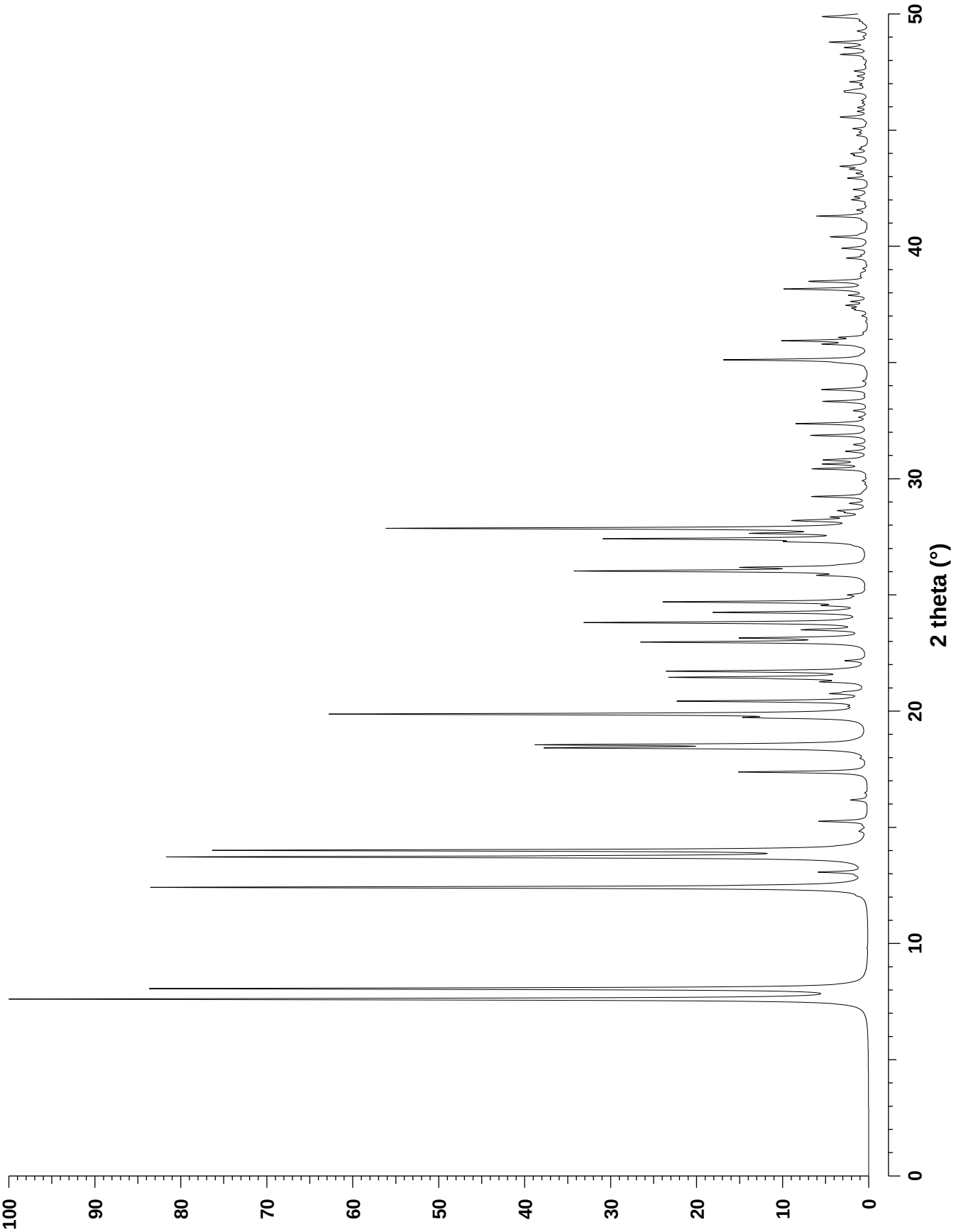
CHEMICAL COMPOSITION: $|((C_3H_7)_4NOH)_4|\ [Si_7Al_{29}P_{28}O_{128}]$
$(C_3H_7)_4NOH$ = tetrapropylammonium hydroxide

REFINED COMPOSITION: $|((C_3H_7)_4N)_4|\ [Al_{32}P_{32}O_{128}]$

CRYSTAL DATA: *Pccn* (No. 56)
$a = 21.9443$ Å $b = 13.6911$ Å $c = 14.2486$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.149$, $R_{wp} = 0.161$, $R_F = 0.066$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
Microporous Materials **6** 51–54 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	7.61	11.616	4	100.0	6	0	2	27.41	3.254	4	29.6	0	6	0	39.49	2.282	2	2.5
2	0	0	8.06	10.972	2	83.4	6	2	0	27.65	3.226	4	11.1	9	1	2	39.62	2.275	8	0.6
0	0	2	12.42	7.124	2	83.9	3	0	4	27.86	3.203	4	55.7	3	0	6	39.91	2.259	4	2.8
1	0	2	13.07	6.776	4	5.2	6	1	2	28.19	3.166	8	7.1	5	2	5	39.95	2.257	8	0.5
3	1	0	13.73	6.452	4	80.7	0	2	4	28.24	3.160	4	1.7	8	3	2	40.40	2.233	8	1.8
0	1	2	14.01	6.320	4	75.2	4	3	2	28.35	3.147	8	3.2	1	2	6	40.41	2.232	8	2.7
2	0	2	14.83	5.975	4	0.7	1	2	4	28.54	3.128	8	1.7	7	2	4	40.53	2.226	8	0.5
2	2	0	15.26	5.808	4	5.7	3	1	4	28.62	3.118	8	2.9	10	0	0	41.13	2.194	2	0.5
2	1	2	16.18	5.476	8	1.8	0	4	2	28.94	3.085	4	1.8	9	2	2	41.30	2.186	8	6.0
3	0	2	17.38	5.104	4	15.1	1	4	2	29.23	3.055	8	6.5	0	6	2	41.56	2.173	4	0.7
0	2	2	17.97	4.936	4	0.5	4	0	4	29.91	2.988	4	0.5	5	4	4	42.00	2.151	8	1.4
1	2	2	18.42	4.816	8	34.7	6	2	2	30.42	2.939	8	6.4	3	2	6	42.13	2.145	8	1.3
4	1	1	18.50	4.795	8	0.8	4	1	4	30.63	2.919	8	4.8	2	5	4	42.44	2.130	8	1.7
3	1	2	18.55	4.782	8	35.6	4	4	0	30.79	2.904	4	3.3	4	6	0	42.93	2.107	4	2.1
2	2	2	19.72	4.502	8	10.4	3	2	4	30.82	2.901	8	2.3	10	0	2	43.13	2.097	4	1.2
1	3	0	19.87	4.468	4	62.3	7	0	2	31.17	2.869	4	2.5	5	0	6	43.32	2.089	4	1.5
1	1	3	20.20	4.396	8	0.7	3	4	2	31.47	2.843	8	1.4	3	6	2	43.44	2.083	8	2.9
4	0	2	20.43	4.347	4	21.9	7	1	2	31.86	2.808	8	5.2	7	5	0	43.90	2.062	4	1.3
4	2	0	20.75	4.281	4	3.6	0	3	4	31.87	2.808	4	1.6	9	3	2	43.98	2.059	8	1.8
1	3	1	20.83	4.263	8	1.7	5	0	4	32.37	2.766	4	8.4	8	4	2	44.18	2.050	8	0.9
5	1	0	21.26	4.179	4	4.2	8	0	0	32.64	2.743	2	0.9	6	4	4	44.27	2.046	8	0.7
2	1	3	21.39	4.153	8	2.9	2	3	4	32.92	2.720	8	1.6	3	3	6	44.77	2.024	8	1.2
4	1	2	21.45	4.143	8	21.7	4	4	2	33.32	2.689	8	5.3	4	5	4	44.90	2.019	8	0.7
4	2	1	21.68	4.100	8	1.9	6	3	2	33.83	2.649	8	4.9	9	0	4	45.06	2.012	4	1.7
3	2	2	21.72	4.092	8	22.1	7	2	2	33.87	2.646	8	1.0	6	0	6	45.54	1.992	4	1.5
5	1	1	22.17	4.010	8	2.4	3	3	4	34.20	2.622	8	0.5	9	1	4	45.57	1.991	8	2.0
3	3	0	22.97	3.872	4	25.8	5	2	4	34.99	2.564	8	1.8	7	5	2	45.80	1.981	8	1.1
0	3	2	23.14	3.843	4	10.4	8	0	2	35.05	2.560	4	0.7	11	1	0	45.97	1.974	4	1.1
1	2	3	23.15	3.842	8	3.3	0	5	2	35.11	2.556	4	16.4	4	3	6	46.16	1.967	8	0.5
1	3	2	23.50	3.785	8	7.0	8	1	2	35.68	2.516	8	0.5	8	3	4	46.27	1.962	8	0.6
5	0	2	23.81	3.737	4	32.8	6	1	4	35.79	2.509	8	4.6	1	7	0	46.62	1.948	4	1.7
4	2	2	24.25	3.669	8	17.4	4	3	4	35.93	2.500	8	3.5	5	5	4	46.68	1.946	8	1.8
6	0	0	24.34	3.657	2	0.7	6	4	0	35.93	2.499	4	6.1	1	4	6	46.74	1.943	8	0.8
2	3	2	24.54	3.627	8	3.6	2	5	2	36.08	2.489	8	2.8	6	6	0	46.93	1.936	4	0.7
5	1	2	24.70	3.605	8	23.5	7	3	2	37.01	2.429	8	0.7	9	2	4	47.07	1.930	8	2.0
5	2	1	24.90	3.576	8	0.6	3	5	2	37.26	2.413	8	1.1	2	4	6	47.32	1.921	8	1.0
0	0	4	25.00	3.562	2	1.8	2	4	4	37.34	2.408	8	1.4	6	2	6	47.54	1.912	8	1.3
0	1	4	25.84	3.447	4	4.4	9	1	0	37.46	2.400	4	2.3	0	7	2	48.25	1.886	4	3.2
0	4	0	26.03	3.423	2	33.2	6	2	4	37.62	2.391	8	1.8	7	1	6	48.55	1.875	8	2.6
4	3	1	26.16	3.407	8	0.7	0	0	6	37.89	2.375	2	2.0	6	5	4	48.78	1.867	8	4.3
1	1	4	26.17	3.406	8	5.4	6	4	2	38.16	2.358	8	9.4	11	2	2	49.26	1.850	8	1.1
3	3	2	26.19	3.402	8	7.4	0	1	6	38.47	2.340	4	4.0	8	4	4	49.69	1.835	8	0.7
2	0	4	26.30	3.388	4	1.3	3	4	4	38.50	2.339	8	3.8	12	0	0	49.87	1.829	2	4.8
2	1	4	27.11	3.289	8	0.5	1	1	6	38.70	2.327	8	0.5	3	7	2	49.93	1.826	8	1.0
2	4	0	27.29	3.267	4	6.4	9	0	2	39.04	2.307	4	0.6	6	3	6	49.96	1.825	8	0.5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2 theta (°)
100
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Di-n-propylamine MAPSO–46

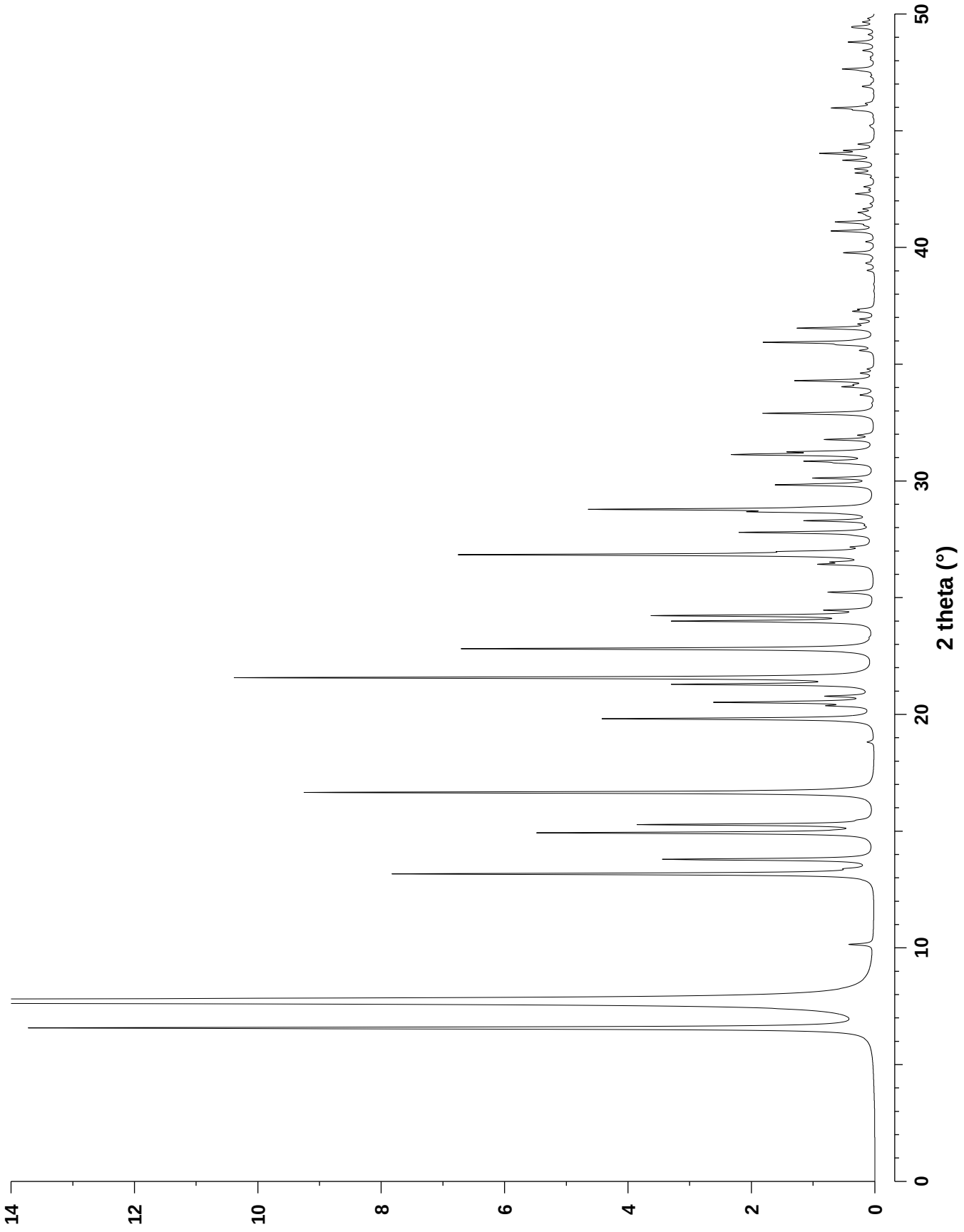
CHEMICAL COMPOSITION: $|((C_3H_7)_2NH_2)_8(H_2O)_{14}|$ $[Mg_6Al_{22}P_{26}Si_2O_{112}]$
$(C_3H_7)_2NH_2$ = di-n-propylamine

REFINED COMPOSITION: $|(C_4N)_6|$ $[Al_{28}P_{28}O_{112}]$

CRYSTAL DATA: *P*3*c*1 (No. 158)
$a = 13.2251$ Å $b = 13.2251$ Å $c = 26.8922$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.119$

REFERENCE: J. M. Bennett and B. K. Marcus,
in *Innovations in Zeolite Material Science* (*Stud. Surf. Sci. Catal. No. 37*)
Ed. by P. J. Grobet, W. J. Mortier, E. F. Vansant and G. Schulz-Ekloff
(Elsevier: Amsterdam) 269–279 (1988).
And J. M. Bennett, Private communication.

h	k	l	2θ	d	M	I_{rel}
0	0	2	6.57	13.446	2	13.6
1	0	0	7.72	11.453	6	100.0
0	1	2	10.15	8.719	6	0.1
1	0	2	10.15	8.719	6	0.2
0	0	4	13.17	6.723	2	7.8
1	1	0	13.39	6.613	6	0.2
1	1	1	13.79	6.421	12	3.4
1	1	2	14.93	5.934	12	5.4
1	0	4	15.28	5.798	6	2.2
0	1	4	15.28	5.798	6	1.6
1	1	3	16.66	5.321	12	9.2
1	1	4	18.82	4.714	12	0.1
0	0	6	19.81	4.482	2	4.4
0	2	4	20.37	4.359	6	0.5
2	1	0	20.52	4.329	12	2.5
1	2	1	20.78	4.274	12	0.1
2	1	1	20.78	4.274	12	0.6
1	0	6	21.29	4.174	6	1.0
1	1	5	21.29	4.173	12	2.0
2	1	2	21.57	4.121	12	6.7
1	2	2	21.57	4.121	12	3.6
2	1	3	22.81	3.898	12	1.4
1	2	3	22.81	3.898	12	5.3
1	1	6	23.99	3.710	12	3.2
3	0	2	24.23	3.673	6	2.1
0	3	2	24.23	3.673	6	1.4
2	1	4	24.46	3.640	12	0.6
2	0	6	25.23	3.530	6	0.2
0	2	6	25.23	3.530	6	0.5
1	2	5	26.43	3.372	12	0.5
2	1	5	26.43	3.372	12	0.3
0	0	8	26.52	3.362	2	0.5
1	1	7	26.84	3.322	12	5.7
0	3	4	26.85	3.320	6	0.7
3	0	4	26.85	3.320	6	0.3
2	2	0	26.97	3.306	6	0.9
2	2	1	27.17	3.282	12	0.2
2	2	2	27.79	3.211	12	2.2
1	3	1	28.29	3.155	12	0.6
3	1	1	28.29	3.155	12	0.5
1	2	6	28.67	3.114	12	0.6
2	1	6	28.67	3.114	12	0.9
2	2	3	28.78	3.102	12	4.4
3	1	2	28.88	3.091	12	0.1
1	3	2	28.88	3.091	12	0.3
1	1	8	29.82	2.997	12	0.6
1	3	3	29.84	2.994	12	0.3
3	1	3	29.84	2.994	12	0.8
2	2	4	30.12	2.967	12	1.0
3	0	6	30.76	2.906	6	0.2
0	3	6	30.76	2.906	6	0.3
0	2	8	30.84	2.899	6	0.5
2	0	8	30.84	2.899	6	0.5
2	1	7	31.12	2.873	12	0.7
1	2	7	31.12	2.873	12	0.7
3	1	4	31.14	2.872	12	0.3
1	3	4	31.14	2.872	12	0.6
4	0	0	31.24	2.863	6	1.1
2	2	5	31.77	2.817	12	0.8
4	0	2	31.96	2.801	6	0.1
1	1	9	32.89	2.723	12	1.8
2	2	6	33.68	2.661	12	0.2
0	4	4	34.03	2.634	6	0.2
4	0	4	34.03	2.634	6	0.3
3	2	0	34.12	2.628	12	0.2
2	3	1	34.29	2.615	12	0.6
3	2	1	34.29	2.615	12	0.7
3	1	6	34.61	2.592	12	0.1
2	2	7	35.83	2.506	12	0.4
4	1	0	35.93	2.499	12	1.7
1	1	10	36.05	2.491	12	0.1
1	2	9	36.54	2.459	12	0.5
2	1	9	36.54	2.459	12	0.7
2	0	10	36.93	2.434	6	0.1
4	0	6	37.26	2.413	6	0.2
1	4	3	37.35	2.407	12	0.1
5	0	0	39.33	2.291	6	0.1
3	2	6	39.76	2.267	12	0.1
2	3	6	39.76	2.267	12	0.1
4	1	5	39.77	2.267	12	0.2
0	0	12	40.24	2.241	2	0.1
2	2	9	40.70	2.217	12	0.7
3	3	1	41.09	2.197	12	0.5
1	3	9	41.49	2.176	12	0.1
4	2	2	42.29	2.137	12	0.1
2	4	2	42.29	2.137	12	0.2
1	1	12	42.60	2.122	12	0.2
4	1	7	43.18	2.095	12	0.1
1	4	7	43.18	2.095	12	0.1
2	0	12	43.36	2.087	6	0.1
2	2	10	43.37	2.086	12	0.1
2	3	8	43.73	2.070	12	0.2
3	2	8	43.73	2.070	12	0.3
5	1	0	44.02	2.057	12	0.8
1	5	1	44.15	2.051	12	0.2
5	1	1	44.15	2.051	12	0.2
3	3	5	44.42	2.040	12	0.2
3	3	6	45.88	1.978	12	0.2
1	1	13	45.97	1.974	12	0.6
3	1	11	46.89	1.937	12	0.1
3	3	7	47.56	1.912	12	0.1
6	0	0	47.64	1.909	6	0.5
1	2	13	48.79	1.866	12	0.2
2	1	13	48.79	1.866	12	0.3
1	1	14	49.41	1.845	12	0.2
3	3	8	49.45	1.843	12	0.2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2 theta (°)
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14

AFT AlPO–52, Calcined, Rehydrated

CHEMICAL COMPOSITION: $|(H_2O)_x|$ $[Al_{36}P_{36}O_{144}]$
Partially Rehydrated.

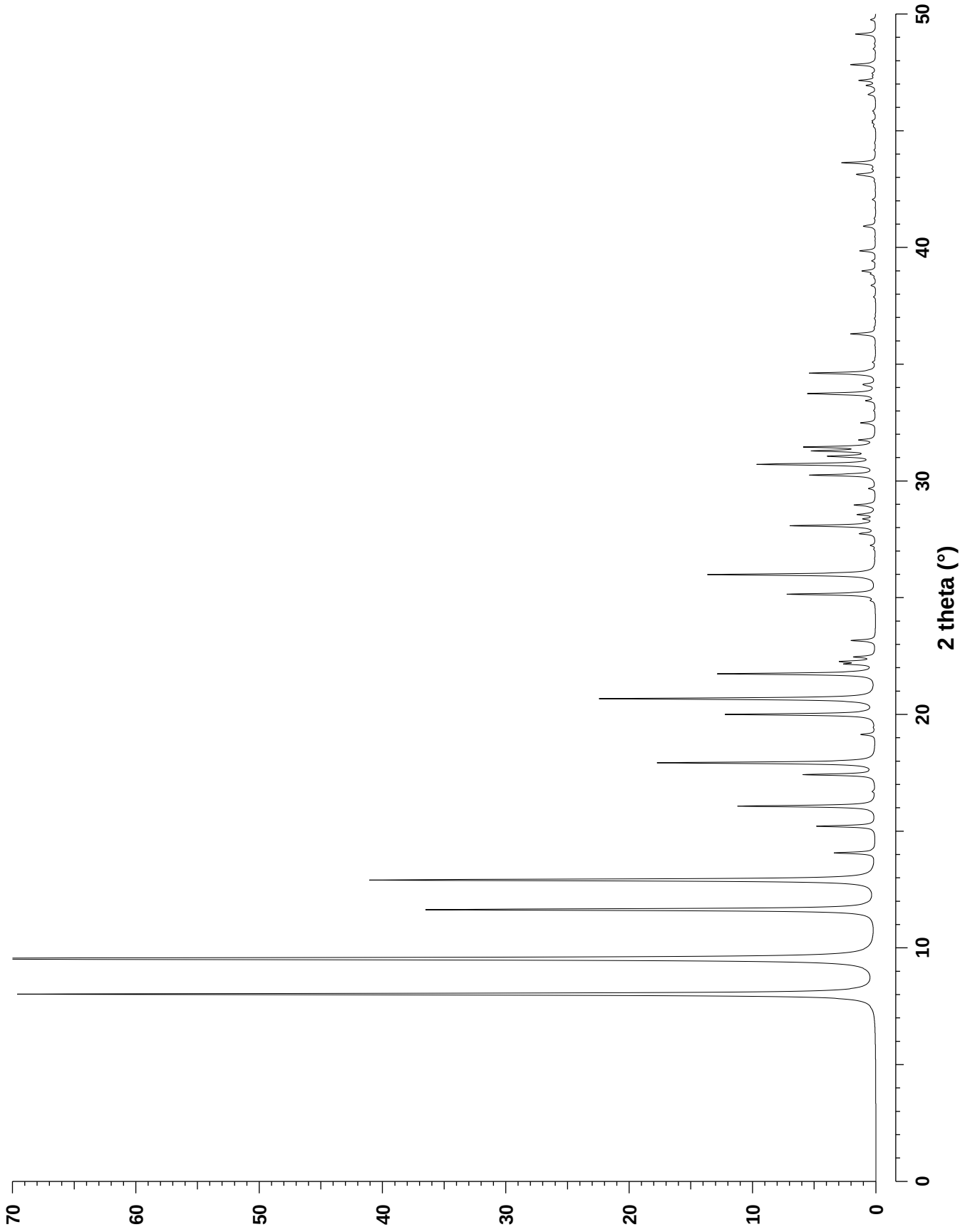
REFINED COMPOSITION: $[Al_{36}P_{36}O_{144}]$

CRYSTAL DATA: $P\overline{3}1c$ (No. 163)
$a = 13.715$ Å $b = 13.715$ Å $c = 29.676$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.130$, $R_{wp} = 0.197$, $R_p = 0.173$

REFERENCE: N. K. McGuire, C. A. Bateman, C. S. Blackwell, S. T. Wilson and R. M. Kirchner, *Zeolites* **15** 460–469 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	8.02	11.027	12	69.6	2	0	8	28.37	3.146	12	0.9	2	1	10	36.29	2.476	12	0.8
1	0	2	9.54	9.273	12	100.0	4	-1	3	28.56	3.125	12	0.9	4	0	7	36.96	2.432	12	0.1
1	0	3	11.64	7.601	12	36.5	3	1	3	28.56	3.125	12	0.5	5	-1	5	37.88	2.375	12	0.1
1	1	0	12.91	6.857	6	41.0	3	0	6	28.89	3.091	12	0.2	5	0	2	38.37	2.346	12	0.4
1	0	4	14.07	6.292	12	3.3	2	1	7	28.97	3.082	12	0.5	4	0	8	38.85	2.318	12	0.3
2	0	1	15.21	5.823	12	4.8	3	-1	7	28.97	3.082	12	1.2	3	-1	11	38.95	2.312	12	0.1
2	0	2	16.07	5.514	12	11.2	4	-1	4	29.67	3.011	12	0.5	5	0	3	38.99	2.310	12	1.0
1	0	5	16.70	5.309	12	0.2	4	0	1	30.25	2.955	12	5.3	3	3	0	39.42	2.286	6	0.3
2	0	3	17.42	5.092	12	5.8	4	0	2	30.71	2.912	12	9.5	5	0	4	39.85	2.262	12	1.3
0	0	6	17.93	4.946	2	17.7	2	0	9	31.02	2.883	12	0.7	4	0	9	40.90	2.207	12	0.6
2	0	4	19.14	4.636	12	1.2	4	-1	5	31.05	2.880	12	0.1	5	0	5	40.92	2.205	12	0.4
3	-1	1	20.00	4.439	12	4.9	1	0	10	31.06	2.879	12	3.1	4	2	4	42.05	2.148	12	0.1
2	1	1	20.00	4.439	12	7.2	3	-1	8	31.28	2.860	12	3.3	6	-2	4	42.05	2.148	12	0.1
2	1	2	20.67	4.297	12	15.5	2	1	8	31.28	2.860	12	1.4	4	2	5	43.08	2.100	12	0.1
3	-1	2	20.67	4.297	12	6.9	4	0	3	31.45	2.844	12	5.5	4	0	10	43.09	2.099	12	0.5
2	1	3	21.74	4.088	12	9.7	2	2	6	31.75	2.818	6	0.3	3	0	12	43.13	2.097	12	1.2
3	-1	3	21.74	4.088	12	3.1	4	-2	6	31.75	2.818	6	1.0	6	-3	6	43.62	2.075	6	1.8
2	-1	6	22.16	4.011	6	2.1	4	0	4	32.48	2.757	12	1.2	3	3	6	43.62	2.075	6	1.0
1	0	7	22.26	3.993	12	2.5	5	-2	2	33.43	2.680	12	0.2	5	0	8	45.33	2.000	12	0.2
3	0	0	22.46	3.959	6	1.6	3	2	2	33.43	2.680	12	0.5	4	0	11	45.42	1.997	12	0.3
2	1	4	23.16	3.841	12	1.9	3	-1	9	33.73	2.658	12	3.2	6	0	0	45.84	1.980	6	0.2
3	-1	4	23.16	3.841	12	0.1	2	1	9	33.73	2.658	12	1.9	1	0	15	46.54	1.952	12	0.6
3	-1	5	24.87	3.580	12	0.3	2	0	10	33.76	2.655	12	0.6	4	3	1	46.61	1.948	12	0.2
1	0	8	25.15	3.541	12	7.2	1	0	11	34.08	2.631	12	0.4	7	-3	2	46.93	1.936	12	0.1
2	0	7	25.82	3.450	12	0.1	5	-2	3	34.13	2.627	12	0.4	4	3	2	46.93	1.936	12	0.6
2	2	0	25.99	3.429	6	13.6	3	2	3	34.13	2.627	12	0.4	5	0	9	47.15	1.927	12	1.3
3	0	5	27.07	3.294	12	0.1	4	1	0	34.61	2.592	12	5.4	6	-2	8	47.33	1.920	12	0.1
3	1	1	27.24	3.274	12	0.4	4	1	1	34.74	2.582	12	0.1	5	2	0	47.82	1.902	12	2.0
4	-1	2	27.74	3.216	12	0.3	5	-2	4	35.08	2.558	12	0.2	2	0	15	48.50	1.877	12	0.1
3	1	2	27.74	3.216	12	0.9	5	-2	5	36.28	2.476	12	0.1	5	0	10	49.13	1.855	12	1.6
1	0	9	28.08	3.177	12	6.9	3	-1	10	36.29	2.476	12	1.1	1	0	16	49.75	1.833	12	0.4

AlPO–52, Calcined, Rehydrated AFT



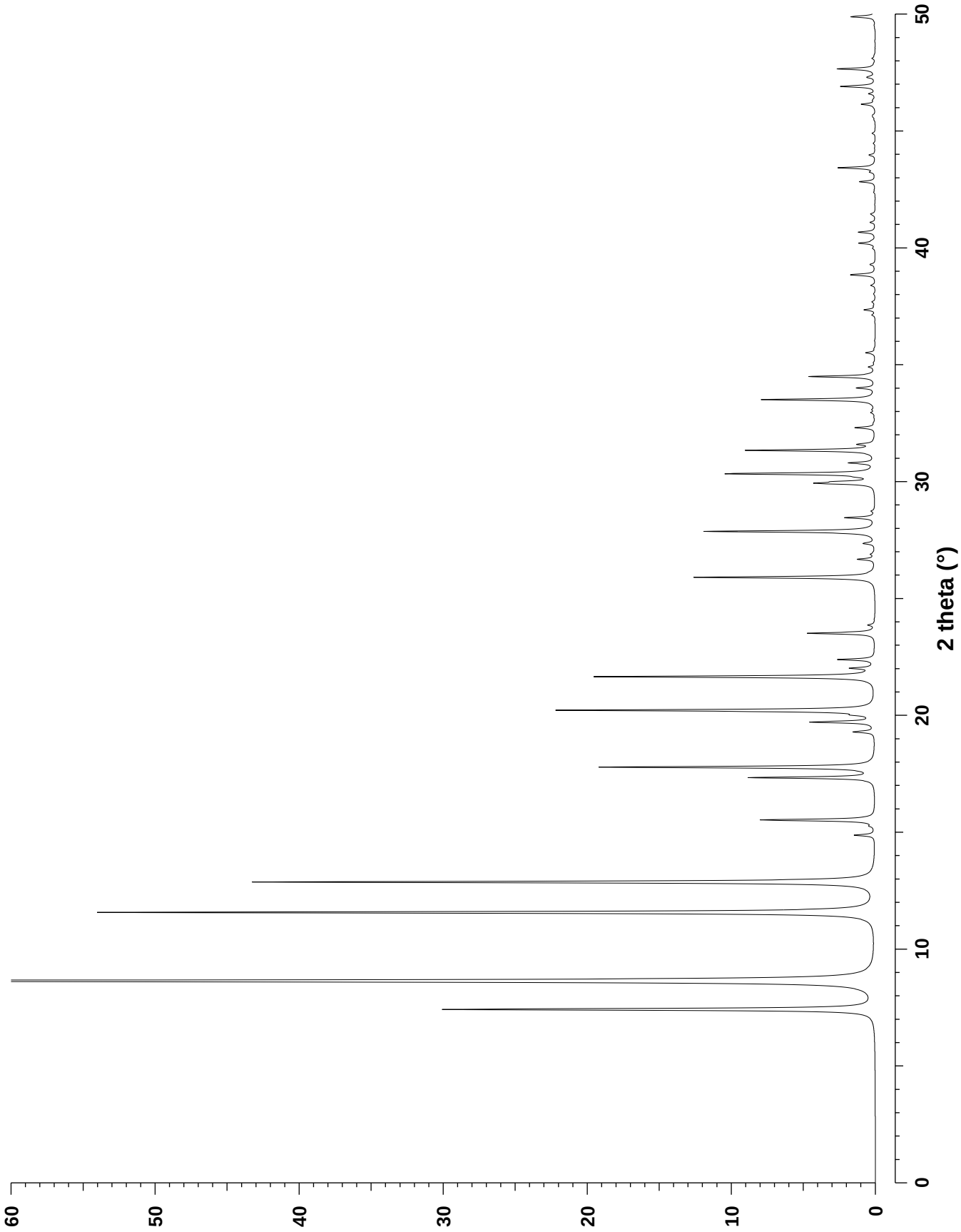
CHEMICAL COMPOSITION: $[Si_5Al_{23}P_{20}O_{96}]$

REFINED COMPOSITION: $[Al_{24}P_{24}O_{96}]$

CRYSTAL DATA: $P\bar{3}1c$ (No. 163)
$a = 13.7617$ Å $b = 13.7617$ Å $c = 19.949$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.068$, $R_{wp} = 0.219$

REFERENCE: N. K. McGuire, C. S. Blackwell, C. A. Bateman, S. T. Wilson and R. M. Kirchner, *Microporous and Mesoporous Materials* **28** 125–137 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.42	11.918	6	30.0	4	-1	2	28.45	3.138	12	0.9	5	0	1	38.02	2.367	12	0.1
1	0	1	8.64	10.231	12	100.0	3	1	2	28.45	3.138	12	1.2	2	-1	8	38.39	2.344	6	0.3
1	0	2	11.57	7.649	12	54.0	3	0	4	28.73	3.107	12	0.2	5	0	2	38.84	2.318	12	1.7
1	1	0	12.87	6.881	6	43.2	3	-1	5	29.92	2.987	12	1.1	3	3	0	39.28	2.294	6	0.4
2	0	0	14.87	5.959	6	1.4	2	1	5	29.92	2.987	12	2.6	5	0	3	40.19	2.244	12	1.1
1	0	3	15.26	5.807	12	0.2	4	0	0	29.99	2.979	6	2.0	6	-2	1	40.30	2.238	12	0.2
2	0	1	15.52	5.710	12	8.0	3	1	3	30.19	2.960	12	0.5	4	0	6	40.66	2.219	12	1.2
2	0	2	17.33	5.116	12	8.7	4	-1	3	30.19	2.960	12	0.1	6	-2	2	41.08	2.197	12	0.2
0	0	4	17.78	4.987	2	19.1	4	0	1	30.33	2.947	12	10.3	4	2	2	41.08	2.197	12	0.1
1	0	4	19.29	4.601	12	1.5	2	0	6	30.79	2.903	12	1.8	5	-1	5	41.44	2.179	12	0.2
2	1	0	19.71	4.505	12	4.4	4	0	2	31.33	2.855	12	9.0	4	1	5	41.44	2.179	12	0.1
2	0	3	20.01	4.438	12	0.8	4	-2	4	31.59	2.832	6	0.2	3	0	8	42.82	2.112	12	1.1
2	1	1	20.21	4.394	12	7.3	2	2	4	31.59	2.832	6	0.9	6	-1	2	43.23	2.093	12	0.3
3	-1	1	20.21	4.394	12	14.8	1	0	7	32.30	2.772	12	1.4	6	-3	4	43.42	2.084	6	1.0
3	-1	2	21.65	4.105	12	15.7	4	0	3	32.94	2.719	12	0.3	3	3	4	43.42	2.084	6	1.6
2	1	2	21.65	4.105	12	3.8	3	-1	6	33.50	2.675	12	3.9	4	0	7	43.96	2.059	12	0.4
1	1	4	22.01	4.038	6	1.5	2	1	6	33.50	2.675	12	4.0	4	-2	8	44.89	2.019	6	0.2
3	0	0	22.38	3.973	6	2.5	5	-2	2	34.00	2.637	12	0.2	6	0	0	45.67	1.986	6	0.1
1	0	5	23.51	3.783	12	4.7	3	2	2	34.00	2.637	12	1.0	1	0	10	46.13	1.968	12	0.9
2	1	3	23.86	3.729	12	0.1	4	1	0	34.49	2.601	12	4.6	7	-3	1	46.58	1.950	12	0.4
3	-1	3	23.86	3.729	12	0.3	2	0	7	34.90	2.571	12	0.4	5	0	6	46.90	1.937	12	2.4
2	2	0	25.90	3.440	6	12.6	5	-2	3	35.50	2.529	12	0.2	7	-3	2	47.28	1.923	12	0.1
2	1	4	26.67	3.343	12	0.8	3	2	3	35.50	2.529	12	0.5	4	3	2	47.28	1.923	12	0.3
3	-1	4	26.67	3.343	12	0.4	4	1	3	37.12	2.422	12	0.2	5	-1	7	47.32	1.921	12	0.2
2	0	5	26.89	3.315	12	0.3	2	1	7	37.34	2.408	12	0.6	5	2	0	47.65	1.908	12	2.6
4	-1	1	27.35	3.261	12	0.7	3	-1	7	37.34	2.408	12	0.2	2	0	10	48.10	1.892	12	0.2
1	0	6	27.86	3.203	12	11.9	4	0	5	37.68	2.387	12	0.2	5	0	7	49.88	1.828	12	1.7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AFY Di-n-propylamine CoAPO–50

CHEMICAL COMPOSITION: $|((C_3H_7)_2NH)_3(H_2O)_{6.7}|\ [Co_3Al_5P_8O_{32}]$
$(C_3H_7)_2NH$ = di-n-propylamine

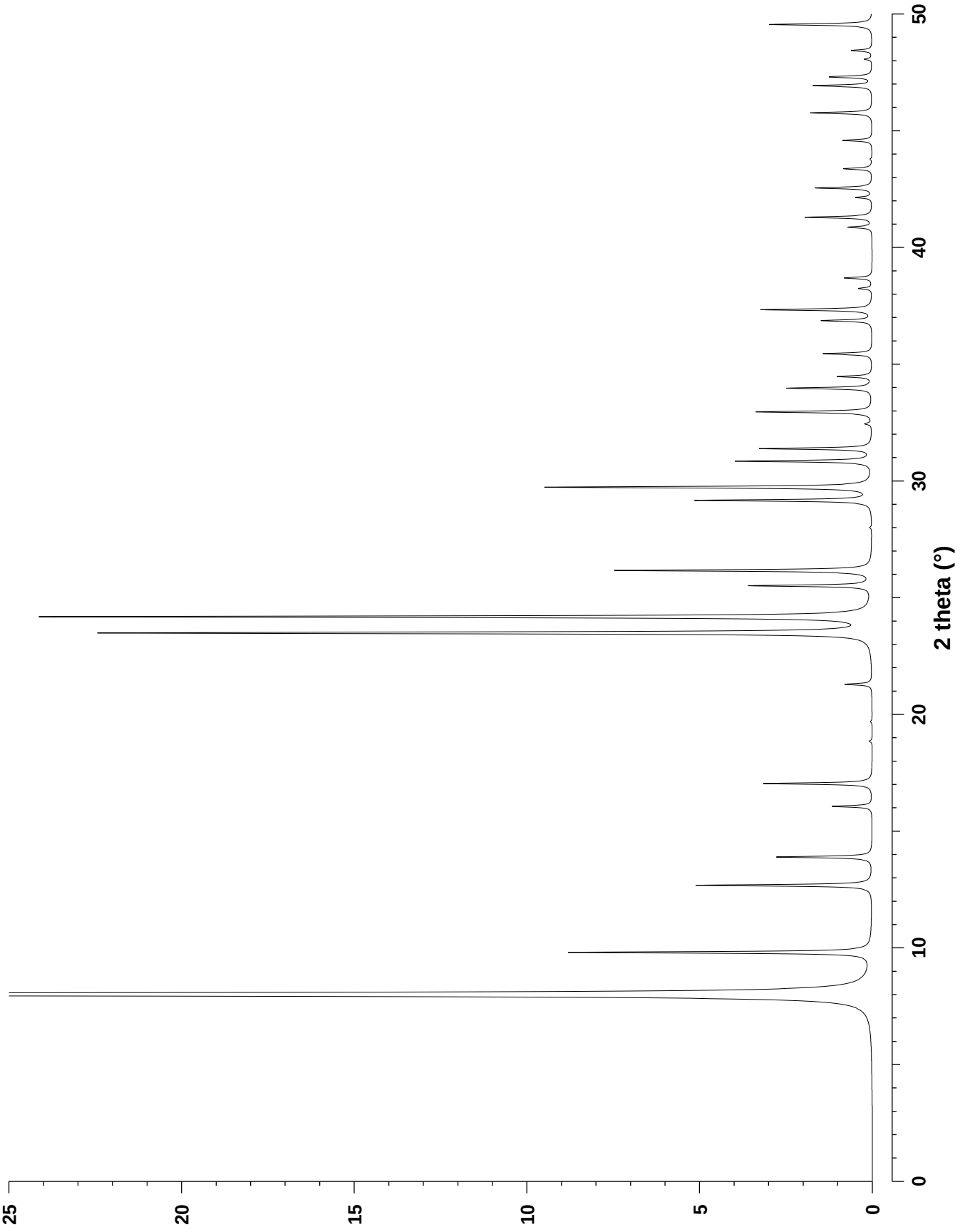
REFINED COMPOSITION: $|(C_4N)_6|\ [Al_6Co_2P_8O_{32}]$

CRYSTAL DATA: $P\overline{3}$ (No. 147)
$a = 12.7468$ Å $b = 12.7468$ Å $c = 9.0153$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.071$

REFERENCE: J. M. Bennett and B. K. Marcus,
in *Innovations in Zeolite Material Science* (*Stud. Surf. Sci. Catal. No. 37*)
Ed. by P. J. Grobet, W. J. Mortier, E. F. Vansant and G. Schulz-Ekloff
(Elsevier: Amsterdam) 269–279 (1988).
and J. M. Bennett, Private communication.

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	8.01	11.039	6	100.0	0	3	2	31.38	2.851	6	1.6	4	-2	3	41.29	2.186	6	0.2
0	0	1	9.81	9.015	2	8.8	3	0	2	31.38	2.851	6	1.7	2	2	3	41.29	2.186	6	1.7
0	1	1	12.68	6.983	6	5.1	0	4	0	32.44	2.760	6	0.2	0	5	1	42.14	2.144	6	0.3
1	1	0	13.89	6.373	6	2.8	1	1	3	32.95	2.718	6	3.2	1	1	4	42.54	2.125	6	0.5
0	2	0	16.06	5.520	6	1.2	2	-1	3	32.95	2.718	6	0.1	2	-1	4	42.54	2.125	6	0.2
2	-1	1	17.04	5.204	6	3.1	0	2	3	33.97	2.639	6	0.9	5	-4	2	42.55	2.125	6	0.3
2	1	0	21.29	4.172	6	0.5	2	0	3	33.97	2.639	6	0.3	3	3	0	42.55	2.124	6	0.5
1	2	0	21.29	4.172	6	0.2	0	4	1	33.97	2.639	6	1.1	2	0	4	43.36	2.087	6	0.3
1	2	1	23.49	3.787	6	0.3	4	0	1	33.97	2.639	6	0.1	4	2	0	43.37	2.086	6	0.5
3	-1	1	23.49	3.787	6	12.5	4	-2	2	34.47	2.602	6	0.4	4	0	3	44.58	2.033	6	0.1
3	-2	1	23.49	3.787	6	9.5	2	2	2	34.47	2.602	6	0.6	4	2	1	44.58	2.032	6	0.2
1	1	2	24.18	3.680	6	1.3	4	-3	2	35.44	2.533	6	0.3	6	-4	1	44.58	2.032	6	0.5
2	-1	2	24.18	3.680	6	19.4	4	-1	2	35.44	2.533	6	0.8	1	2	4	45.75	1.983	6	0.5
0	3	0	24.19	3.680	6	3.6	2	3	0	35.44	2.533	6	0.2	5	0	2	45.76	1.983	6	0.3
0	2	2	25.51	3.491	6	0.5	1	2	3	36.86	2.438	6	0.7	0	5	2	45.76	1.983	6	0.2
2	0	2	25.51	3.491	6	3.1	2	1	3	36.86	2.438	6	0.4	1	5	0	45.76	1.983	6	0.4
3	0	1	26.16	3.407	6	4.4	3	2	1	36.86	2.438	6	0.2	5	1	0	45.76	1.983	6	0.3
0	3	1	26.16	3.407	6	3.0	1	4	0	37.33	2.409	6	1.3	5	-3	3	46.92	1.937	6	0.8
3	-2	2	29.16	3.062	6	3.6	4	1	0	37.33	2.409	6	1.9	5	-2	3	46.92	1.937	6	0.5
3	-1	2	29.16	3.062	6	0.4	4	0	2	38.24	2.354	6	0.3	3	2	3	46.92	1.937	6	0.2
1	3	0	29.17	3.062	6	0.7	1	4	1	38.69	2.327	6	0.2	3	3	2	47.30	1.922	6	0.6
3	1	0	29.17	3.062	6	0.4	5	-1	1	38.69	2.327	6	0.1	6	-3	2	47.30	1.922	6	0.5
0	0	3	29.73	3.005	2	0.3	5	-4	1	38.69	2.327	6	0.2	5	-1	3	48.43	1.880	6	0.4
4	-2	1	29.73	3.005	6	9.2	4	1	1	38.69	2.327	6	0.3	2	2	4	49.54	1.840	6	0.8
0	1	3	30.84	2.900	6	0.2	0	1	4	40.86	2.208	6	0.3	0	6	0	49.54	1.840	6	2.2
4	-3	1	30.84	2.899	6	2.1	5	-2	2	40.87	2.208	6	0.1							
4	-1	1	30.84	2.899	6	1.5	0	5	0	40.87	2.208	6	0.1							

Di-n-propylamine CoAPO–50 AFY



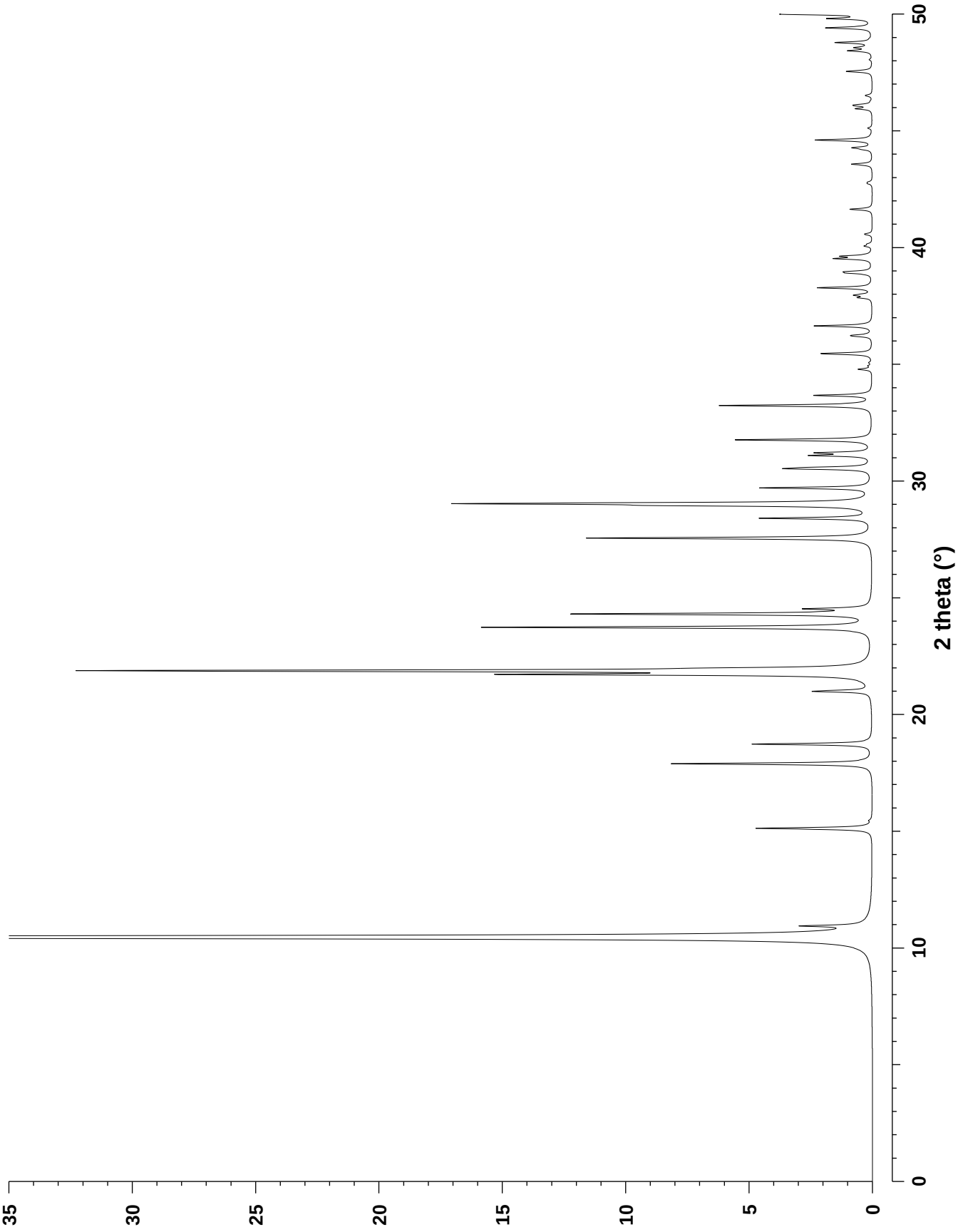
CHEMICAL COMPOSITION: $|(H_2O)_4|\ [Al_6P_6O_{24}]$

REFINED COMPOSITION: $|(H_2O)_4|\ [Al_6P_6O_{24}]$

CRYSTAL DATA: $P112_1$ (No. 4) unique axis **c**
$a = 9.486$ Å $b = 9.914$ Å $c = 8.126$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 121.49°$
X-ray Rietveld refinement, $R_{wp} = 0.127$

REFERENCE: J. B. Higgins, R. M. Dessau, H-X. Li, M. E. Davis and J.M. Newsam, *American Crystallographic Association Abstracts* **K005** 39 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	10.46	8.454	2	87.1	0	3	0	31.75	2.818	2	4.3	1	-3	3	43.56	2.078	4	1.0
1	-1	0	10.47	8.452	2	100.0	3	-3	0	31.76	2.817	2	6.0	2	-3	3	43.56	2.077	4	0.5
1	0	0	10.94	8.089	2	4.1	3	0	0	33.23	2.696	2	11.3	1	2	3	44.19	2.049	4	0.4
0	1	1	15.12	5.858	4	4.7	0	3	1	33.66	2.662	4	2.3	3	-2	3	44.20	2.049	4	0.1
1	-1	1	15.12	5.858	4	3.9	3	-3	1	33.67	2.662	4	2.1	2	2	2	44.26	2.046	4	0.4
1	0	1	15.46	5.733	4	0.2	0	1	3	34.78	2.579	4	0.4	4	-2	2	44.27	2.046	4	0.5
1	-2	0	17.89	4.957	2	14.8	1	-1	3	34.78	2.579	4	0.6	0	4	1	44.28	2.045	4	0.3
1	1	0	18.73	4.738	2	5.7	1	0	3	34.93	2.568	4	0.2	4	-4	1	44.29	2.045	4	0.1
2	-1	0	18.73	4.737	2	3.1	3	0	1	35.06	2.559	4	0.2	2	1	3	44.57	2.033	4	0.2
1	-2	1	20.99	4.232	4	3.8	1	-3	2	35.45	2.532	4	1.6	3	-1	3	44.57	2.033	4	0.3
0	2	0	21.02	4.227	2	0.5	2	-3	2	35.45	2.532	4	2.2	0	0	4	44.60	2.032	2	3.9
2	-2	0	21.02	4.226	2	0.2	1	2	2	36.20	2.482	4	0.3	1	3	2	45.11	2.010	4	0.3
1	1	1	21.71	4.093	4	13.4	3	-2	2	36.20	2.481	4	0.6	0	1	4	45.94	1.975	4	0.8
2	-1	1	21.72	4.092	4	11.4	2	-4	0	36.24	2.478	2	1.1	1	-1	4	45.94	1.975	4	0.3
0	0	2	21.87	4.063	2	56.5	2	1	2	36.64	2.453	4	1.5	1	0	4	46.07	1.970	4	0.8
2	0	0	21.98	4.045	2	6.1	3	-1	2	36.64	2.452	4	2.8	3	1	2	46.10	1.969	4	0.3
0	2	1	23.73	3.750	4	15.1	1	-2	3	37.85	2.377	4	0.9	4	-1	2	46.10	1.969	4	0.4
2	-2	1	23.73	3.749	4	13.6	2	-4	1	37.95	2.371	4	0.9	0	3	3	46.50	1.953	4	0.4
0	1	2	24.30	3.662	4	12.2	1	-4	0	37.97	2.370	2	0.2	3	-3	3	46.51	1.953	4	0.2
1	-1	2	24.31	3.662	4	10.3	4	-2	0	37.99	2.368	2	0.2	2	-5	1	47.53	1.913	4	1.0
1	0	2	24.52	3.631	4	4.3	1	1	3	38.27	2.351	4	3.2	3	-5	1	47.54	1.913	4	0.9
2	0	1	24.59	3.621	4	0.2	2	-1	3	38.28	2.351	4	0.9	3	0	3	47.58	1.911	4	0.2
1	-3	0	27.55	3.238	2	8.7	0	3	2	38.89	2.316	4	0.2	5	-3	0	48.04	1.894	2	0.2
2	-3	0	27.55	3.238	2	12.4	3	-3	2	38.90	2.315	4	1.2	1	-2	4	48.42	1.880	4	1.7
1	-2	2	28.40	3.142	4	8.1	1	3	0	38.95	2.312	2	0.7	0	4	2	48.55	1.875	4	0.3
3	-2	0	28.49	3.133	2	0.2	4	-3	0	38.96	2.312	2	1.0	4	-4	2	48.56	1.875	4	0.9
1	1	2	28.95	3.084	4	5.4	2	-2	3	39.52	2.280	4	2.6	1	1	4	48.77	1.867	4	1.3
2	-1	2	28.95	3.084	4	5.8	1	-4	1	39.61	2.275	4	0.4	2	-1	4	48.77	1.867	4	1.4
2	1	0	29.03	3.076	2	15.6	3	-4	1	39.62	2.275	4	0.6	2	3	1	49.40	1.845	4	2.9
3	-1	0	29.03	3.076	2	13.1	2	2	1	39.63	2.274	4	0.6	5	-3	1	49.42	1.844	4	0.6
1	-3	1	29.70	3.008	4	2.1	4	-2	1	39.64	2.274	4	0.6	0	2	4	49.80	1.831	4	1.8
2	-3	1	29.70	3.008	4	6.1	2	0	3	40.06	2.251	4	0.5	2	-2	4	49.80	1.831	4	1.2
0	2	2	30.52	2.929	4	2.8	3	0	2	40.14	2.247	4	0.3	2	-4	3	49.87	1.829	4	0.1
2	-2	2	30.52	2.929	4	2.5	1	3	1	40.56	2.224	4	0.3	1	4	0	49.98	1.825	2	2.4
1	2	1	30.57	2.924	4	1.7	4	-3	1	40.57	2.223	4	0.3	3	2	1	49.98	1.825	4	1.8
3	-2	1	30.58	2.924	4	1.5	3	1	1	41.63	2.169	4	1.1	5	-4	0	49.99	1.824	2	1.6
2	1	1	31.09	2.877	4	1.7	4	-1	1	41.64	2.169	4	0.6	5	-2	1	49.99	1.824	4	1.0
3	-1	1	31.09	2.877	4	2.5	2	-4	2	42.73	2.116	4	0.3							
2	0	2	31.20	2.866	4	3.7	4	-4	0	42.79	2.113	2	0.3							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ANA Analcime

CHEMICAL COMPOSITION: $|Na_{16}(H_2O)_{16}|\ [Si_{32}Al_{16}O_{96}]$
Cyclopean Islands, Greece

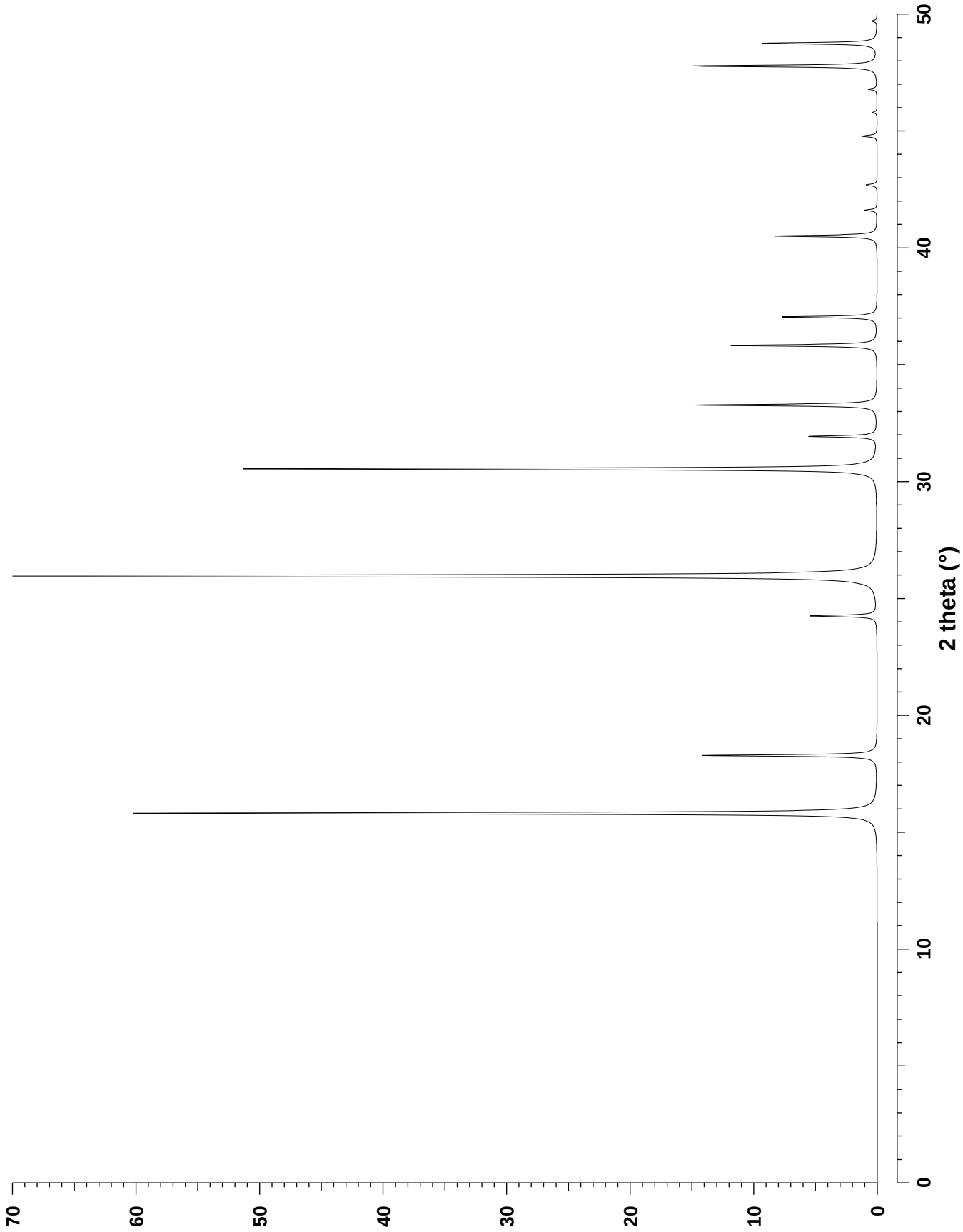
REFINED COMPOSITION: $|Na_{16}(H_2O)_{16}|\ [Si_{32}Al_{16}O_{96}]$

CRYSTAL DATA: $Ia\bar{3}d$ (No. 230)
$a = 13.73$ Å $b = 13.73$ Å $c = 13.73$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.04$

REFERENCE: G. Ferraris, D. W. Jones and J. Yerkess,
Z. Kristallogr. **135** 240–252 (1972).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	1	1	15.81	5.605	24	60.2	5	2	1	35.82	2.507	48	11.9	4	4	4	45.78	1.982	8	0.4
2	2	0	18.28	4.854	12	14.1	4	4	0	37.04	2.427	12	7.7	5	4	3	46.78	1.942	48	0.7
3	2	1	24.25	3.669	48	5.4	6	1	1	40.50	2.227	24	2.8	6	4	0	47.77	1.904	24	14.9
4	0	0	25.96	3.433	6	100.0	5	3	2	40.50	2.227	48	5.5	5	5	2	48.74	1.868	24	0.2
3	3	2	30.54	2.927	24	51.3	6	2	0	41.60	2.171	24	1.0	6	3	3	48.74	1.868	24	6.9
4	2	2	31.93	2.803	24	5.5	5	4	1	42.68	2.119	48	0.9	7	2	1	48.74	1.868	48	2.3
4	3	1	33.27	2.693	48	14.8	6	3	1	44.77	2.024	48	1.3	6	4	2	49.69	1.835	48	0.4

Analcime ANA



APC AlPO–C, Hydrated

CHEMICAL COMPOSITION: $|(H_2O)_{24}|\ [Al_{16}P_{16}O_{64}]$

REFINED COMPOSITION: $|(H_2O)_{16}O_8|\ [Al_{16}P_{16}O_{64}]$

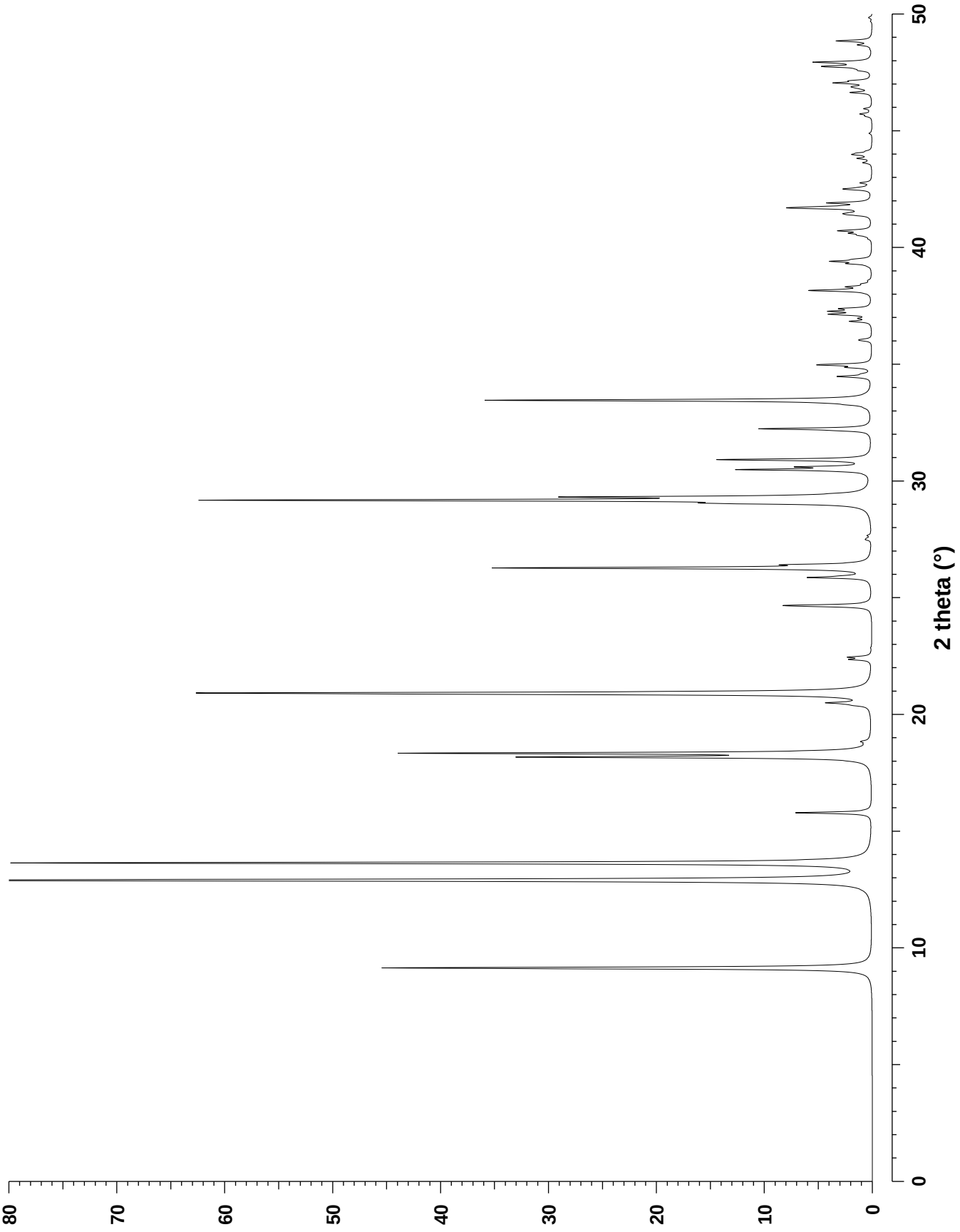
CRYSTAL DATA: *Pbca* (No. 61)
$a = 19.3525$ Å $b = 9.7272$ Å $c = 9.7621$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.033$

REFERENCE: J. J. Pluth and J. V. Smith,
Acta Cryst. **C42** 1118–1120 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	9.14	9.676	2	45.5	2	2	3	34.43	2.605	8	0.4	8	0	2	41.67	2.167	4	1.8
2	1	0	12.90	6.860	4	100.0	4	1	3	34.47	2.602	8	1.8	8	2	0	41.70	2.166	4	4.6
1	1	1	13.64	6.491	8	79.8	2	3	2	34.48	2.601	8	1.1	3	3	3	41.74	2.164	8	1.5
2	1	1	15.79	5.613	8	7.1	4	3	1	34.54	2.596	8	0.1	1	4	2	41.76	2.163	8	0.9
0	0	2	18.17	4.881	2	30.8	6	1	2	34.58	2.594	8	0.5	7	2	2	41.90	2.156	8	3.8
0	2	0	18.24	4.864	2	0.1	5	2	2	34.86	2.573	8	1.9	2	2	4	42.48	2.128	8	1.3
4	0	0	18.34	4.838	2	42.4	7	1	1	34.97	2.566	8	4.9	4	1	4	42.51	2.126	8	1.6
1	0	2	18.75	4.733	4	0.2	3	2	3	36.01	2.494	8	0.8	2	4	2	42.57	2.124	8	0.6
3	1	1	18.84	4.709	8	0.7	3	3	2	36.05	2.491	8	0.8	8	2	1	42.76	2.115	8	1.0
2	0	2	20.38	4.358	4	0.7	0	0	4	36.83	2.441	2	1.9	4	3	3	43.62	2.075	8	0.8
0	2	1	20.40	4.353	4	0.2	0	4	0	36.96	2.432	2	0.9	3	2	4	43.81	2.066	8	1.2
2	2	0	20.44	4.346	4	0.8	1	0	4	37.13	2.421	4	3.4	7	1	3	43.97	2.059	8	1.5
4	1	0	20.50	4.332	4	3.3	8	0	0	37.17	2.419	2	0.5	7	3	1	44.03	2.057	8	1.0
1	1	2	20.87	4.256	8	21.0	5	1	3	37.26	2.413	8	3.4	9	1	1	44.12	2.053	8	0.4
1	2	1	20.92	4.247	8	54.6	5	3	1	37.33	2.409	8	0.6	5	1	4	44.88	2.019	8	0.3
2	1	2	22.35	3.977	8	1.9	7	0	2	37.38	2.406	4	2.5	4	2	4	45.62	1.989	8	0.5
4	1	1	22.45	3.960	8	2.0	2	0	4	38.02	2.366	4	0.1	4	4	2	45.71	1.985	8	1.0
3	1	2	24.63	3.614	8	3.5	4	2	3	38.12	2.361	8	0.1	8	2	2	45.83	1.980	8	0.1
3	2	1	24.67	3.608	8	6.4	0	4	1	38.14	2.360	4	2.5	5	3	3	45.94	1.975	8	0.7
0	2	2	25.86	3.445	4	5.4	2	4	0	38.16	2.358	4	2.7	0	4	3	46.63	1.948	4	1.9
4	0	2	25.93	3.436	4	1.3	4	3	2	38.16	2.358	8	0.7	6	4	0	46.78	1.942	4	0.4
4	2	0	25.98	3.430	4	0.2	6	2	2	38.22	2.355	8	0.4	1	3	4	46.83	1.940	8	0.7
1	2	2	26.27	3.392	8	34.8	1	1	4	38.31	2.350	8	1.8	1	4	3	46.88	1.938	8	1.2
5	1	1	26.41	3.375	8	5.9	8	1	0	38.34	2.348	4	0.4	7	2	3	47.00	1.933	8	0.3
2	2	2	27.48	3.246	8	0.4	1	4	1	38.43	2.342	8	0.7	7	3	2	47.04	1.932	8	3.1
4	1	2	27.53	3.240	8	0.2	7	2	1	38.58	2.334	8	0.2	9	1	2	47.12	1.929	8	0.7
6	0	0	27.66	3.225	2	0.3	2	1	4	39.18	2.299	8	0.1	9	2	1	47.14	1.928	8	1.0
2	3	0	29.04	3.074	4	10.2	2	4	1	39.30	2.293	8	1.9	2	3	4	47.57	1.911	8	0.8
6	1	0	29.17	3.061	4	59.8	6	3	0	39.40	2.287	4	3.5	2	4	3	47.62	1.910	8	0.3
1	1	3	29.31	3.047	8	24.1	3	0	4	39.48	2.283	4	0.8	6	1	4	47.65	1.908	8	0.5
1	3	1	29.39	3.039	8	1.1	8	1	1	39.48	2.282	8	0.2	1	1	5	47.74	1.905	8	3.4
5	0	2	29.45	3.033	4	0.6	1	3	3	39.51	2.281	8	0.4	6	4	1	47.76	1.904	8	0.8
2	1	3	30.40	2.940	8	0.8	2	3	3	40.36	2.235	8	0.2	8	1	3	47.77	1.904	8	0.2
2	3	1	30.48	2.932	8	11.8	6	1	3	40.45	2.230	8	0.2	8	3	1	47.83	1.902	8	0.4
6	1	1	30.60	2.921	8	5.7	6	3	1	40.52	2.226	8	0.9	5	2	4	47.87	1.900	8	0.7
5	1	2	30.88	2.895	8	2.3	3	1	4	40.60	2.222	8	1.7	1	5	1	47.91	1.899	8	0.2
5	2	1	30.91	2.893	8	12.7	5	2	3	40.70	2.217	8	0.7	10	1	0	47.93	1.898	4	4.8
3	1	3	32.15	2.784	8	1.6	3	4	1	40.71	2.216	8	2.0	5	4	2	47.95	1.897	8	0.1
3	3	1	32.23	2.777	8	10.2	5	3	2	40.74	2.215	8	0.5	2	5	1	48.64	1.872	8	0.3
0	2	3	33.12	2.705	4	0.1	0	2	4	41.39	2.181	4	1.4	6	3	3	48.67	1.871	8	1.0
4	3	0	33.26	2.693	4	0.6	4	0	4	41.44	2.179	4	1.6	3	4	3	48.84	1.865	8	3.2
6	0	2	33.29	2.691	4	0.2	0	4	2	41.49	2.177	4	0.8	3	1	5	49.68	1.835	8	0.1
6	2	0	33.33	2.688	4	1.0	4	4	0	41.56	2.173	4	0.4	3	5	1	49.84	1.830	8	0.3
1	2	3	33.45	2.679	8	35.8	1	2	4	41.67	2.168	8	1.3							

AlPO–C, Hydrated

APC



APC AlPO–C, Dehydrated

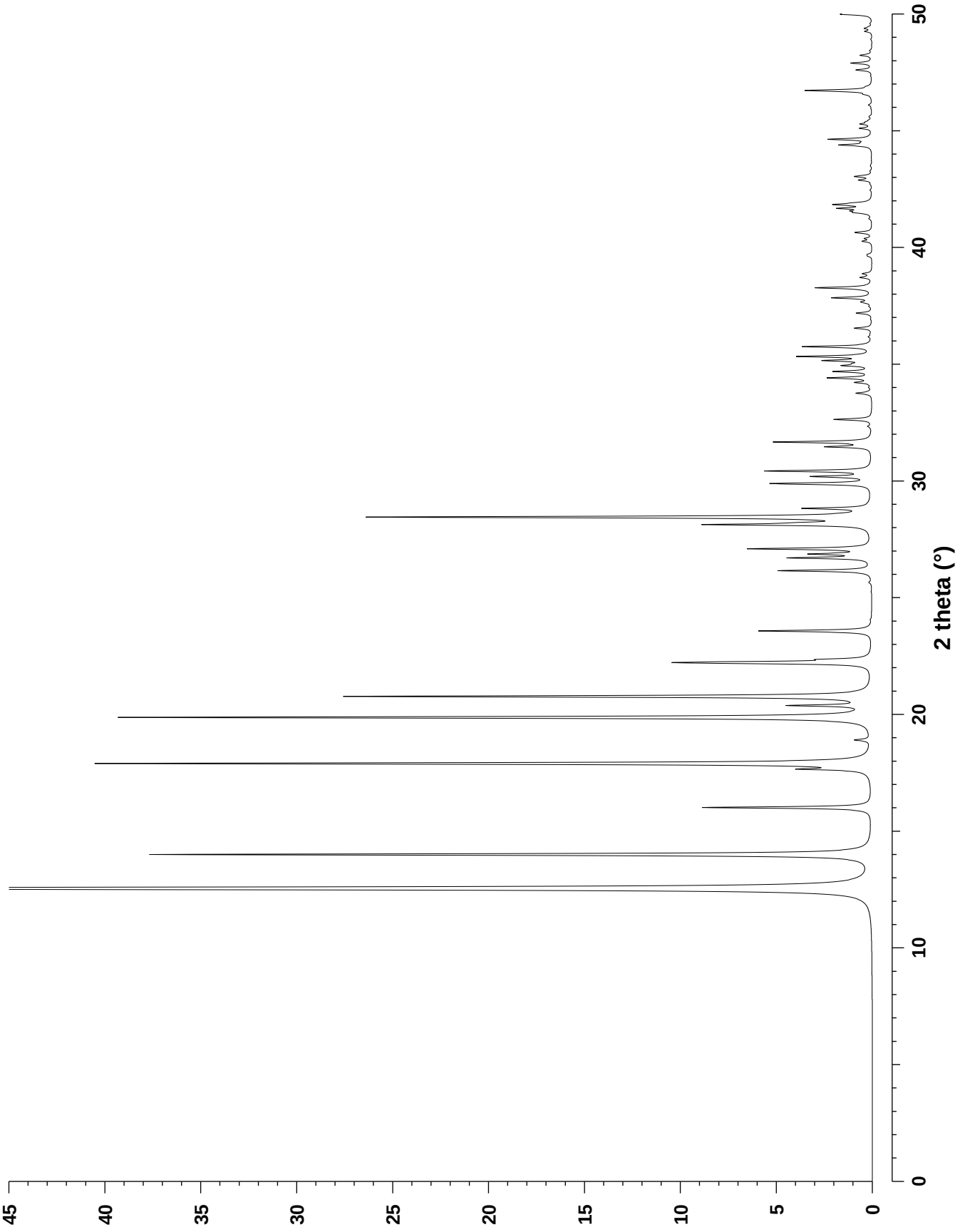
CHEMICAL COMPOSITION: $[Al_{16}P_{16}O_{64}]$

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: *Pbca* (No. 61)
$a = 19.816$ Å $b = 10.047$ Å $c = 8.935$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.17$, $R_F = 0.051$; At $T = 100$°C.

REFERENCE: E. B. Keller, W. M. Meier and R. M. Kirchner, *Solid State Ionics* **43** 93–102 (1990).

h	k	l	2θ	d	M	I_{rel}
2	1	0	12.55	7.055	4	100.0
1	1	1	14.00	6.327	8	37.6
2	1	1	16.01	5.537	8	8.8
0	2	0	17.65	5.023	2	3.0
4	0	0	17.90	4.954	2	40.4
3	1	1	18.90	4.696	8	0.8
0	0	2	19.87	4.468	2	39.2
1	0	2	20.38	4.358	4	4.0
1	2	1	20.77	4.276	8	27.4
2	2	1	22.19	4.005	8	4.2
1	1	2	22.23	3.998	8	8.0
4	1	1	22.35	3.978	8	1.9
2	1	2	23.57	3.774	8	5.9
3	1	2	25.65	3.473	8	0.1
5	1	1	26.15	3.408	8	4.9
0	2	2	26.70	3.338	4	4.2
4	0	2	26.87	3.318	4	2.9
1	2	2	27.09	3.292	8	6.3
4	2	1	27.18	3.281	8	0.2
2	3	0	28.13	3.173	4	8.1
2	2	2	28.21	3.164	8	1.6
4	1	2	28.33	3.150	8	0.3
6	1	0	28.45	3.137	4	26.1
1	3	1	28.82	3.097	8	3.3
2	3	1	29.88	2.990	8	5.2
5	0	2	30.14	2.965	4	0.4
6	1	1	30.19	2.960	8	2.8
5	2	1	30.42	2.938	8	5.5
5	1	2	31.46	2.844	8	2.3
1	1	3	31.66	2.826	8	5.1
4	2	2	32.34	2.768	8	0.2
2	1	3	32.63	2.744	8	2.0
1	3	2	33.75	2.655	8	0.8
6	2	1	34.00	2.637	8	0.1
3	1	3	34.21	2.621	8	0.8
7	1	1	34.41	2.606	8	2.3
2	3	2	34.68	2.587	8	1.9
6	1	2	34.94	2.568	8	1.4
0	2	3	35.02	2.562	4	0.5
5	2	2	35.15	2.553	8	2.3
1	2	3	35.33	2.541	8	3.8
0	4	0	35.75	2.512	2	3.6
3	3	2	36.17	2.483	8	0.1
5	3	1	36.54	2.459	8	0.9
0	4	1	37.18	2.418	4	0.8
7	0	2	37.61	2.391	4	0.1
3	2	3	37.66	2.389	8	0.4
7	2	1	37.84	2.377	8	2.1
4	3	2	38.18	2.357	8	0.2
6	3	0	38.27	2.352	4	2.9
7	1	2	38.71	2.326	8	0.6
5	1	3	38.87	2.317	8	0.5
6	3	1	39.63	2.274	8	0.2
3	4	1	39.69	2.271	8	0.2
4	4	0	40.26	2.240	4	0.5
0	0	4	40.38	2.234	2	0.3
8	2	0	40.61	2.222	4	0.3
5	3	2	40.64	2.220	8	0.5
1	0	4	40.64	2.220	4	0.2
0	4	2	41.23	2.189	4	0.1
2	0	4	41.44	2.179	4	0.1
1	4	2	41.49	2.176	8	0.7
4	4	1	41.56	2.173	8	0.8
1	1	4	41.67	2.167	8	1.5
8	0	2	41.69	2.166	4	0.2
6	1	3	41.82	2.160	8	1.2
7	2	2	41.84	2.159	8	0.8
8	2	1	41.90	2.156	8	0.6
3	3	3	42.88	2.109	8	0.7
7	3	1	43.04	2.101	8	0.9
0	2	4	44.38	2.041	4	1.7
4	0	4	44.49	2.036	4	0.3
1	2	4	44.63	2.030	8	2.2
7	1	3	45.10	2.010	8	0.6
4	4	2	45.28	2.003	8	0.6
2	2	4	45.37	1.999	8	0.2
4	1	4	45.45	1.996	8	0.1
8	2	2	45.60	1.989	8	0.1
2	5	0	46.09	1.969	4	0.2
1	5	1	46.55	1.951	8	0.2
7	3	2	46.67	1.946	8	0.3
10	1	0	46.72	1.944	4	3.2
9	1	2	46.88	1.938	8	0.2
1	4	3	47.58	1.911	8	0.1
5	1	4	47.60	1.910	8	0.7
10	1	1	47.88	1.900	8	0.1
7	2	3	47.89	1.900	8	1.0
4	2	4	48.22	1.887	8	0.6
3	5	1	48.43	1.879	8	0.1
1	3	4	49.25	1.850	8	0.3
6	3	3	49.38	1.846	8	0.4
1	5	2	49.98	1.825	8	1.6


0
10
20
30
40
50
2 theta (°)
45
40
35
30
25
20
15
10
5
0

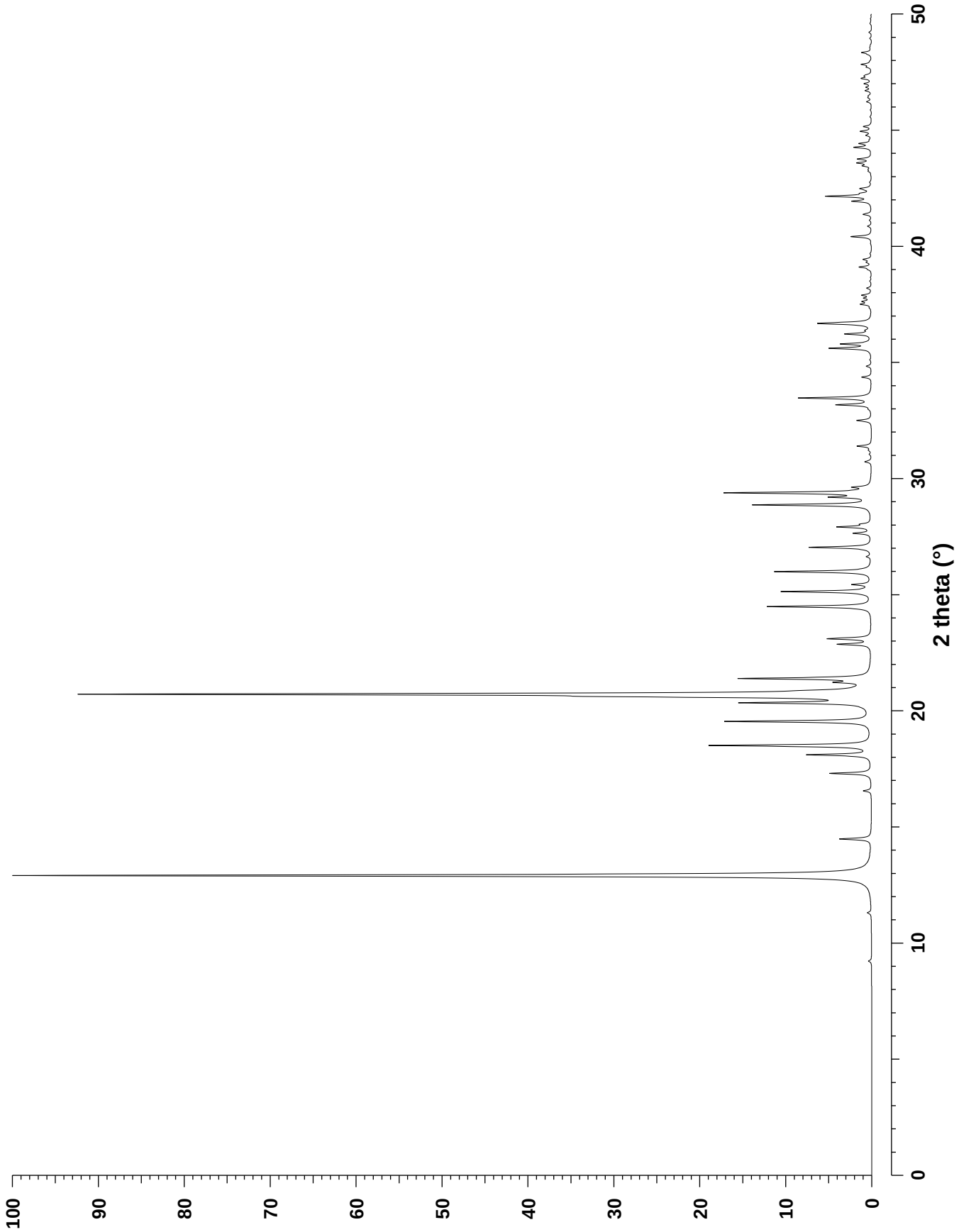
CHEMICAL COMPOSITION: $[Al_{16}P_{16}O_{64}]$

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: $Pca2_1$ (No. 29)
$a = 19.187$ Å $b = 8.576$ Å $c = 9.804$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.203$, $R_F = 0.115$; At $T = 100$°C.

REFERENCE: E. B. Keller, W. M. Meier and R. M. Kirchner,
Solid State Ionics **43** 93–102 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	9.22	9.594	2	0.4	3	1	3	32.49	2.756	8	1.7	0	2	4	42.48	2.128	4	1.2
1	1	0	11.30	7.829	4	0.4	1	3	1	32.97	2.717	8	0.2	8	2	0	43.22	2.093	4	0.3
2	0	1	12.91	6.857	4	100.0	4	0	3	33.17	2.701	4	4.0	8	1	2	43.30	2.089	8	0.1
1	1	1	14.48	6.118	8	3.7	6	0	2	33.46	2.678	4	5.0	7	2	2	43.31	2.089	8	0.1
2	1	1	16.55	5.355	8	1.0	4	2	2	33.46	2.678	8	3.4	6	3	1	43.45	2.083	8	0.1
3	1	0	17.30	5.127	4	4.9	7	1	0	34.35	2.611	4	0.1	1	4	1	43.46	2.082	8	0.8
0	0	2	18.10	4.902	2	7.4	3	3	0	34.36	2.610	4	1.0	2	2	4	43.57	2.077	8	0.4
4	0	0	18.50	4.797	2	18.8	4	1	3	34.83	2.576	8	0.3	5	3	2	43.58	2.077	8	1.2
3	1	1	19.54	4.543	8	17.0	1	2	3	34.83	2.576	8	0.3	9	1	0	43.75	2.069	4	1.6
2	0	2	20.34	4.365	4	13.9	6	1	2	35.10	2.557	8	0.1	8	2	1	44.25	2.047	8	1.2
4	0	1	20.61	4.309	4	20.9	3	3	1	35.60	2.522	8	4.7	2	4	1	44.26	2.046	8	0.8
0	2	0	20.71	4.288	2	89.1	2	2	3	35.79	2.509	8	3.4	7	1	3	44.41	2.040	8	1.0
0	1	2	20.87	4.256	4	2.6	6	2	1	36.22	2.480	8	3.0	3	3	3	44.42	2.039	8	0.4
4	1	0	21.22	4.186	4	2.8	5	2	2	36.37	2.470	8	0.2	3	4	0	44.57	2.033	4	0.1
1	2	0	21.23	4.185	4	0.3	0	3	2	36.38	2.469	4	0.3	9	1	1	44.77	2.024	8	0.6
1	1	2	21.39	4.155	8	15.0	4	3	0	36.59	2.456	4	0.3	6	2	3	44.94	2.017	8	1.3
2	1	2	22.86	3.890	8	3.8	0	0	4	36.66	2.451	2	3.3	5	1	4	45.15	2.008	8	0.9
4	1	1	23.10	3.850	8	3.7	1	3	2	36.69	2.449	8	3.8	3	4	1	45.57	1.990	8	0.2
1	2	1	23.11	3.849	8	1.4	3	2	3	37.34	2.408	8	0.2	7	3	0	45.86	1.978	4	0.1
2	2	1	24.48	3.636	8	12.1	8	0	0	37.50	2.398	2	1.2	0	4	2	46.21	1.964	4	0.5
3	2	0	25.00	3.562	4	0.2	2	3	2	37.61	2.391	8	0.9	4	4	0	46.39	1.957	4	0.3
3	1	2	25.13	3.543	8	10.4	4	3	1	37.76	2.382	8	0.8	1	4	2	46.47	1.954	8	0.3
5	1	0	25.43	3.503	4	2.1	2	0	4	37.89	2.375	4	1.1	6	0	4	46.69	1.945	4	0.5
4	0	2	25.99	3.428	4	11.3	0	1	4	38.19	2.357	4	0.5	4	2	4	46.70	1.945	8	0.2
3	2	1	26.63	3.348	8	0.5	1	1	4	38.49	2.339	8	0.2	7	3	1	46.84	1.939	8	0.6
5	1	1	27.03	3.299	8	7.3	8	1	0	38.99	2.310	4	0.2	8	0	3	46.99	1.934	4	0.8
0	2	2	27.64	3.227	4	2.0	3	3	2	39.10	2.304	8	1.3	8	2	2	47.21	1.925	8	0.6
6	0	0	27.90	3.198	2	0.2	5	3	0	39.30	2.292	4	0.5	2	4	2	47.23	1.924	8	0.6
4	2	0	27.91	3.197	4	3.7	6	0	3	39.42	2.286	4	0.2	2	0	5	47.32	1.921	4	0.5
4	1	2	28.03	3.183	8	0.4	4	2	3	39.43	2.285	8	0.7	4	4	1	47.36	1.919	8	0.3
1	2	2	28.03	3.183	8	0.6	6	2	2	39.68	2.272	8	0.1	9	1	2	47.71	1.906	8	0.5
2	0	3	28.86	3.093	4	13.7	5	3	1	40.41	2.232	8	2.4	1	1	5	47.82	1.902	8	1.1
2	2	2	29.19	3.059	8	4.2	6	1	3	40.86	2.209	8	0.4	6	1	4	47.95	1.897	8	0.1
6	0	1	29.38	3.040	4	13.7	4	3	2	41.11	2.196	8	0.2	8	1	3	48.25	1.886	8	0.2
4	2	1	29.39	3.039	8	3.4	4	0	4	41.37	2.183	4	1.0	10	0	1	48.33	1.883	4	1.1
1	1	3	29.62	3.016	8	1.8	8	0	2	41.93	2.154	4	2.1	2	1	5	48.56	1.875	8	0.1
2	1	3	30.72	2.910	8	0.8	5	2	3	41.98	2.152	8	0.1	0	3	4	48.95	1.861	4	0.1
3	2	2	31.04	2.881	8	0.2	0	4	0	42.15	2.144	2	5.2	1	3	4	49.20	1.852	8	0.3
6	1	1	31.21	2.865	8	0.3	1	3	3	42.27	2.138	8	0.8	3	1	5	49.79	1.831	8	0.1
5	1	2	31.39	2.850	8	1.7	1	4	0	42.42	2.131	4	0.4							


100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
2 theta (°)

AST Quinuclidine AlPO–16

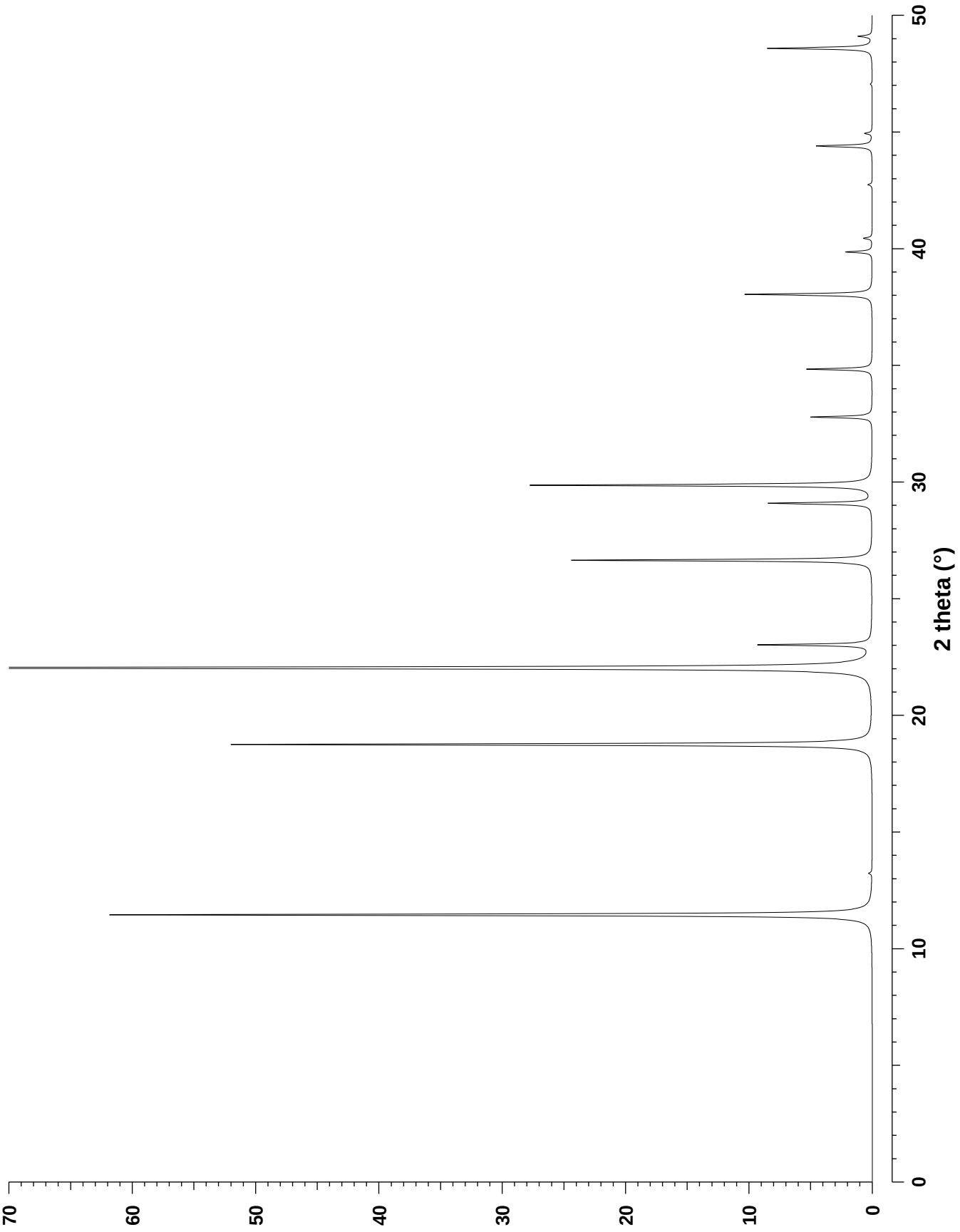
CHEMICAL COMPOSITION: $|(C_7H_{13}N)_4(H_2O)_{16}|\ [Al_{20}P_{20}O_{80}]$
$C_7H_{13}N$ = quinuclidine

REFINED COMPOSITION: $|(C_7H_{13}N)_4|\ [Al_{20}P_{20}O_{80}]$

CRYSTAL DATA: $F23$ (No. 196)
$a = 13.3832$ Å $b = 13.3832$ Å $c = 13.3832$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.192$, $R_F = 0.106$

REFERENCE: J. M. Bennett and R. M. Kirchner,
Zeolites **11** 502–506 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	11.45	7.727	8	61.9	4	0	2	29.86	2.993	12	18.6	6	0	2	42.73	2.116	12	0.2
2	0	0	13.23	6.692	6	0.3	4	2	2	32.78	2.732	24	5.0	6	2	0	42.73	2.116	12	0.2
2	2	0	18.75	4.732	12	52.0	3	3	3	34.83	2.576	8	0.3	5	3	3	44.39	2.041	24	4.6
3	1	1	22.03	4.035	24	100.0	5	1	1	34.83	2.576	24	5.1	6	2	2	44.93	2.018	24	0.6
2	2	2	23.02	3.863	8	9.2	4	4	0	38.03	2.366	12	10.3	4	4	4	47.04	1.932	8	0.2
4	0	0	26.64	3.346	6	24.4	5	3	1	39.85	2.262	24	2.1	7	1	1	48.58	1.874	24	4.8
3	3	1	29.08	3.070	24	8.4	4	4	2	40.44	2.231	24	0.3	5	5	1	48.58	1.874	24	3.7
4	2	0	29.86	2.993	12	9.2	6	0	0	40.44	2.231	6	0.5	6	0	4	49.09	1.856	12	1.1


0
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20
30
40
50
2 theta (°)
70
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0

AST Quinuclidinium fluoride octadecasil

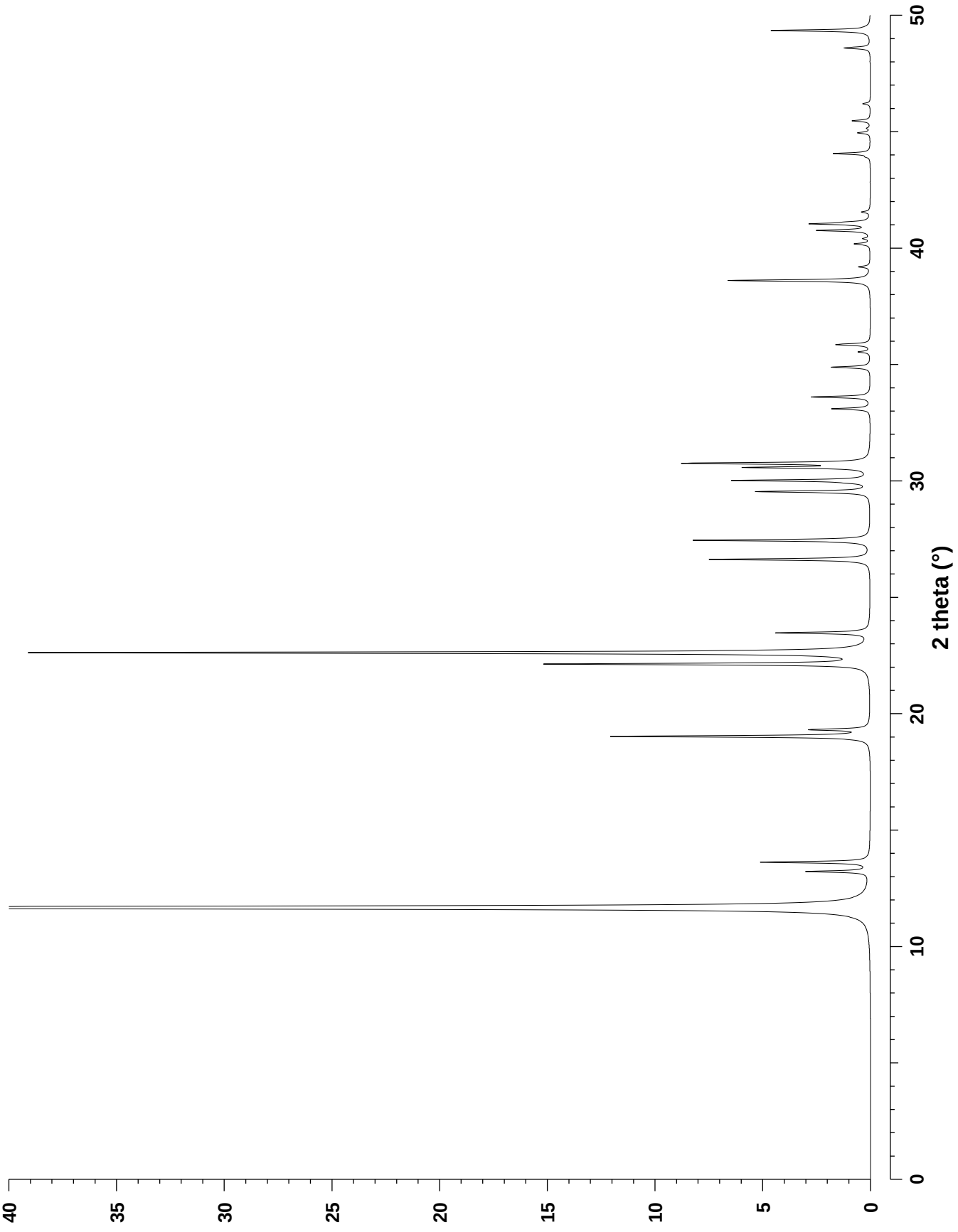
CHEMICAL COMPOSITION: $|(C_7H_{14}NF)_2|\ [Si_{20}O_{40}]$
$C_7H_{14}NF$ = quinuclidinium fluoride

REFINED COMPOSITION: $|C_{6.18}F_{0.07}|\ [Si_{20}O_{40}]$

CRYSTAL DATA: $I\,4/m$ (No. 87)
$a = 9.194$ Å $b = 9.194$ Å $c = 13.396$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.039$

REFERENCE: P. Caullet, J. L. Guth, J. Hazm, J. M. Lamblin and H. Gies, *Eur. J. Solid State Inorg. Chem.* **28** 345–361 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	11.67	7.580	8	100.0	1	1	4	30.01	2.977	8	6.3	3	2	3	40.75	2.214	8	1.8
0	0	2	13.22	6.698	2	2.9	2	2	2	30.57	2.924	8	5.5	2	3	3	40.75	2.214	8	0.7
1	1	0	13.62	6.501	4	5.1	1	3	0	30.75	2.907	4	8.5	4	1	1	41.03	2.200	8	2.4
1	1	2	19.02	4.665	8	12.0	2	0	4	33.09	2.707	8	1.8	1	4	1	41.03	2.200	8	0.3
2	0	0	19.31	4.597	4	2.7	1	3	2	33.60	2.667	8	0.1	1	3	4	41.11	2.195	8	0.7
1	0	3	22.13	4.017	8	14.9	3	1	2	33.60	2.667	8	2.6	4	0	2	41.54	2.174	8	0.4
2	1	1	22.62	3.931	8	3.6	1	0	5	34.88	2.572	8	1.8	3	3	2	43.91	2.062	8	0.1
1	2	1	22.62	3.931	8	35.4	3	0	3	35.53	2.527	8	0.5	2	4	0	44.05	2.056	4	1.7
2	0	2	23.47	3.790	8	4.3	2	3	1	35.85	2.505	8	0.4	3	0	5	44.94	2.017	8	0.6
0	0	4	26.62	3.349	2	7.5	3	2	1	35.85	2.505	8	1.2	2	0	6	45.14	2.008	8	0.2
2	2	0	27.44	3.251	4	8.2	2	2	4	38.60	2.333	8	6.6	1	4	3	45.46	1.995	8	0.8
2	1	3	29.53	3.025	8	0.3	4	0	0	39.19	2.299	4	0.5	2	4	2	46.19	1.965	8	0.4
1	2	3	29.53	3.025	8	5.0	2	1	5	40.17	2.245	8	0.7	1	0	7	48.59	1.874	8	1.2
3	0	1	29.91	2.987	8	0.4	0	0	6	40.40	2.233	2	0.3	2	3	5	49.34	1.847	8	4.6


0
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2 theta (°)
40
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10
5
0

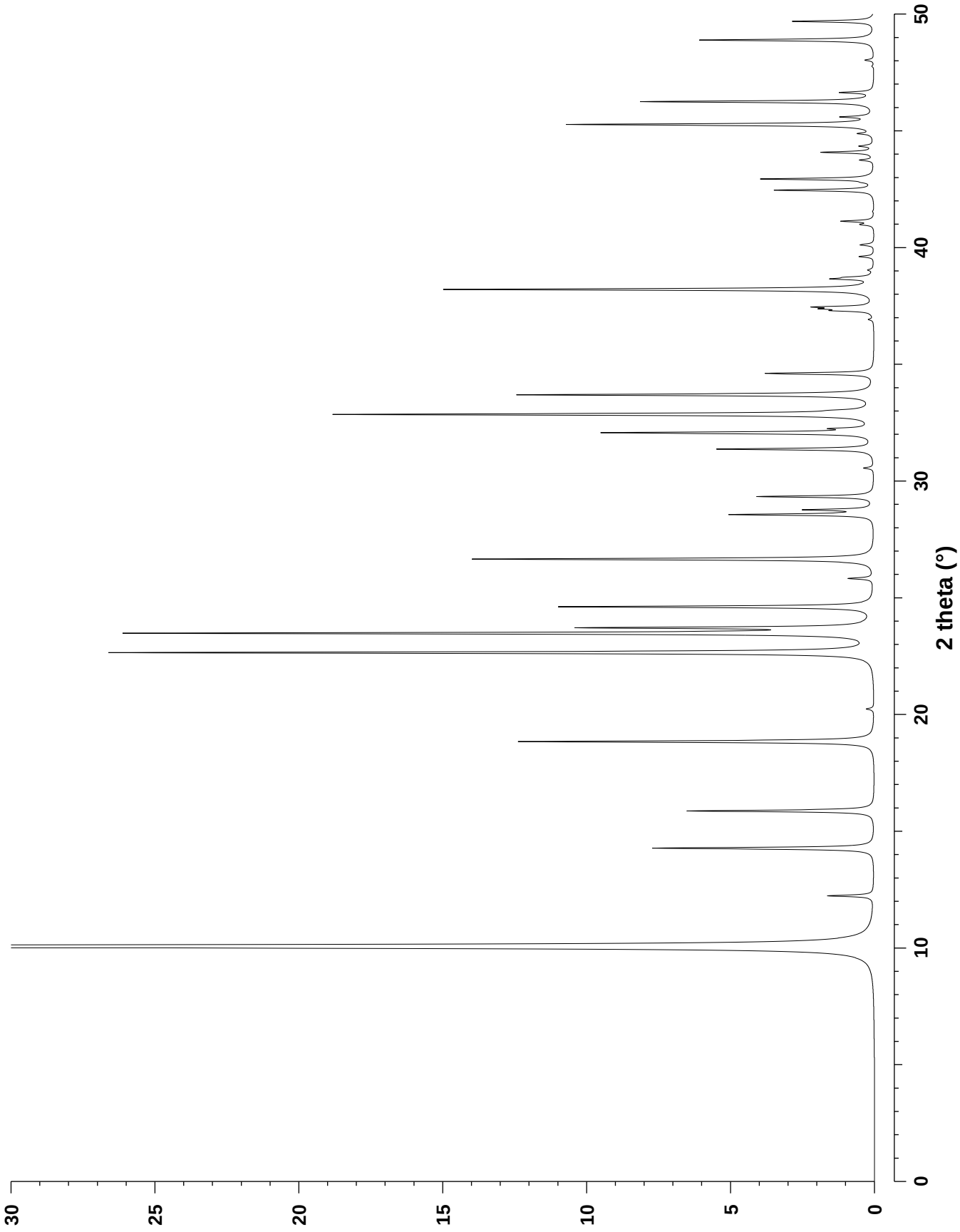
CHEMICAL COMPOSITION: $|((CH_3)_2NH)_2(H_2O)_2|\ [Ge_{20}O_{40}]$
$(CH_3)_2NH$ = dimethylamine

REFINED COMPOSITION: $|(C_4N_2)(H_2O)_2|\ [Ge_{20}O_{40}]$

CRYSTAL DATA: $P\,4/m\,cc$ (No. 124)
$a = 8.7795$ Å $b = 8.7795$ Å $c = 14.4696$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_F = 0.025$, $wR_{F2} = 0.053$; at -75 C.

REFERENCE: H. Li and O. M. Yaghi,
J. Am. Chem. Soc. **120** 10569–10570 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	10.07	8.780	4	100.0	2	0	4	32.06	2.792	8	9.4	4	0	0	41.12	2.195	4	1.1
0	0	2	12.23	7.235	2	1.6	3	1	0	32.24	2.776	8	1.1	4	1	0	42.45	2.129	8	3.5
1	1	0	14.27	6.208	4	7.7	3	1	1	32.85	2.727	16	18.7	2	0	6	42.78	2.114	8	0.2
1	0	2	15.87	5.583	8	6.5	3	0	2	33.02	2.713	8	0.6	4	1	1	42.93	2.107	16	3.9
1	1	2	18.84	4.711	8	12.4	2	1	4	33.69	2.660	16	12.4	3	3	0	43.74	2.069	4	0.5
2	0	0	20.23	4.390	4	0.3	3	1	2	34.60	2.592	16	3.8	2	1	6	44.07	2.055	16	1.8
2	1	0	22.65	3.926	8	26.5	3	2	0	36.91	2.435	8	0.2	4	1	2	44.34	2.043	16	0.5
2	1	1	23.48	3.789	16	25.8	0	0	6	37.29	2.412	2	1.2	3	2	4	44.87	2.020	16	0.5
2	0	2	23.71	3.753	8	9.6	3	1	3	37.37	2.406	16	1.3	3	1	5	45.26	2.003	16	10.7
0	0	4	24.61	3.617	2	10.9	3	2	1	37.45	2.401	16	1.8	3	3	2	45.59	1.990	8	1.0
2	1	2	25.82	3.451	16	0.9	2	2	4	38.20	2.356	8	15.0	4	2	0	46.24	1.963	8	8.1
1	0	4	26.65	3.345	8	14.0	2	1	5	38.65	2.330	16	1.3	4	1	3	46.63	1.948	16	1.1
1	1	4	28.56	3.126	8	5.0	1	0	6	38.72	2.325	8	0.7	4	2	2	48.02	1.895	16	0.3
2	2	0	28.76	3.104	4	2.3	3	2	2	39.03	2.308	16	0.2	3	2	5	48.88	1.863	16	6.1
2	1	3	29.33	3.045	16	4.1	3	0	4	39.61	2.275	8	0.5	4	1	4	49.68	1.835	16	2.8
3	0	0	30.55	2.926	4	0.3	1	1	6	40.11	2.248	8	0.5							
2	2	2	31.36	2.853	8	5.4	3	1	4	40.98	2.202	16	0.4							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2 theta (°)
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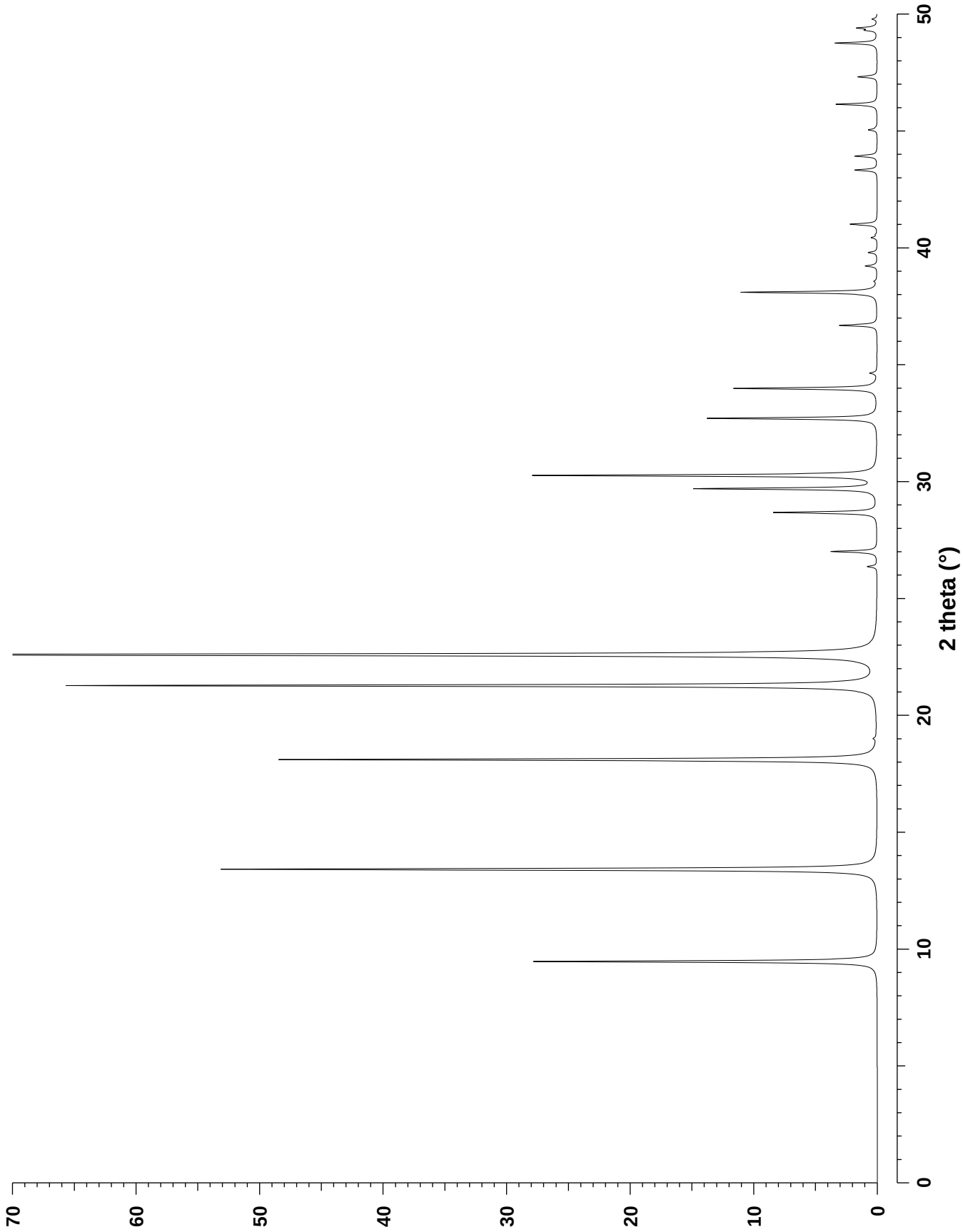
CHEMICAL COMPOSITION: $|((C_3H_7)_2NH)_x|\ [Al_7MgP_8O_{32}]$
$(C_3H_7)_2NH$ = di-n-propylamine

REFINED COMPOSITION: $|C_{13.16}O_{0.168}|\ [Al_{7.512}P_{7.504}O_{32}]$

CRYSTAL DATA: $I\,4/m$ (No. 87)
$a = 13.2088$ Å $b = 13.2088$ Å $c = 5.2771$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.02$, $R_F = 0.093$

REFERENCE: W. H. Baur, W. Joswig, D. Kassner, A. Bieniok, G. Finger and J. Kornatowski, *Z. Kristallogr.* **214** 154–159 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.47	9.340	4	39.6	1	4	1	32.70	2.738	8	9.1	4	0	2	43.92	2.061	8	2.6
2	0	0	13.41	6.604	4	75.6	0	0	2	33.98	2.639	2	16.5	3	3	2	45.04	2.013	8	1.0
1	0	1	18.10	4.900	8	69.0	5	1	0	34.63	2.590	4	0.8	6	1	1	45.15	2.008	8	0.1
2	2	0	19.00	4.670	4	0.3	2	0	2	36.68	2.450	8	4.4	4	2	2	46.13	1.968	8	3.1
1	3	0	21.27	4.177	4	20.8	3	4	1	38.09	2.362	8	1.7	2	4	2	46.13	1.968	8	1.6
3	1	0	21.27	4.177	4	72.5	5	0	1	38.09	2.362	8	9.7	5	4	1	47.31	1.921	8	1.3
2	1	1	22.59	3.935	8	42.3	4	3	1	38.09	2.362	8	4.3	4	5	1	47.31	1.921	8	0.9
1	2	1	22.59	3.935	8	100.0	4	4	0	38.56	2.335	4	0.3	5	5	0	48.75	1.868	4	4.6
3	0	1	26.36	3.381	8	1.1	2	2	2	39.22	2.297	8	1.4	1	7	0	48.75	1.868	4	0.2
4	0	0	27.00	3.302	4	5.3	3	5	0	39.79	2.265	4	0.4	5	1	2	49.30	1.848	8	0.8
3	3	0	28.67	3.113	4	11.9	5	3	0	39.79	2.265	4	0.6	1	5	2	49.30	1.848	8	0.4
2	3	1	29.69	3.009	8	6.4	1	3	2	40.43	2.231	8	0.6	3	6	1	49.40	1.845	8	1.2
3	2	1	29.69	3.009	8	14.6	2	5	1	40.56	2.224	8	0.1	6	3	1	49.40	1.845	8	1.1
2	4	0	30.26	2.954	4	23.9	6	0	0	41.00	2.201	4	3.1	4	6	0	49.78	1.832	4	0.3
4	2	0	30.26	2.954	4	15.7	6	2	0	43.32	2.088	4	1.1	6	4	0	49.78	1.832	4	0.2
4	1	1	32.70	2.738	8	10.5	2	6	0	43.32	2.088	4	1.5							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2 theta (°)
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70

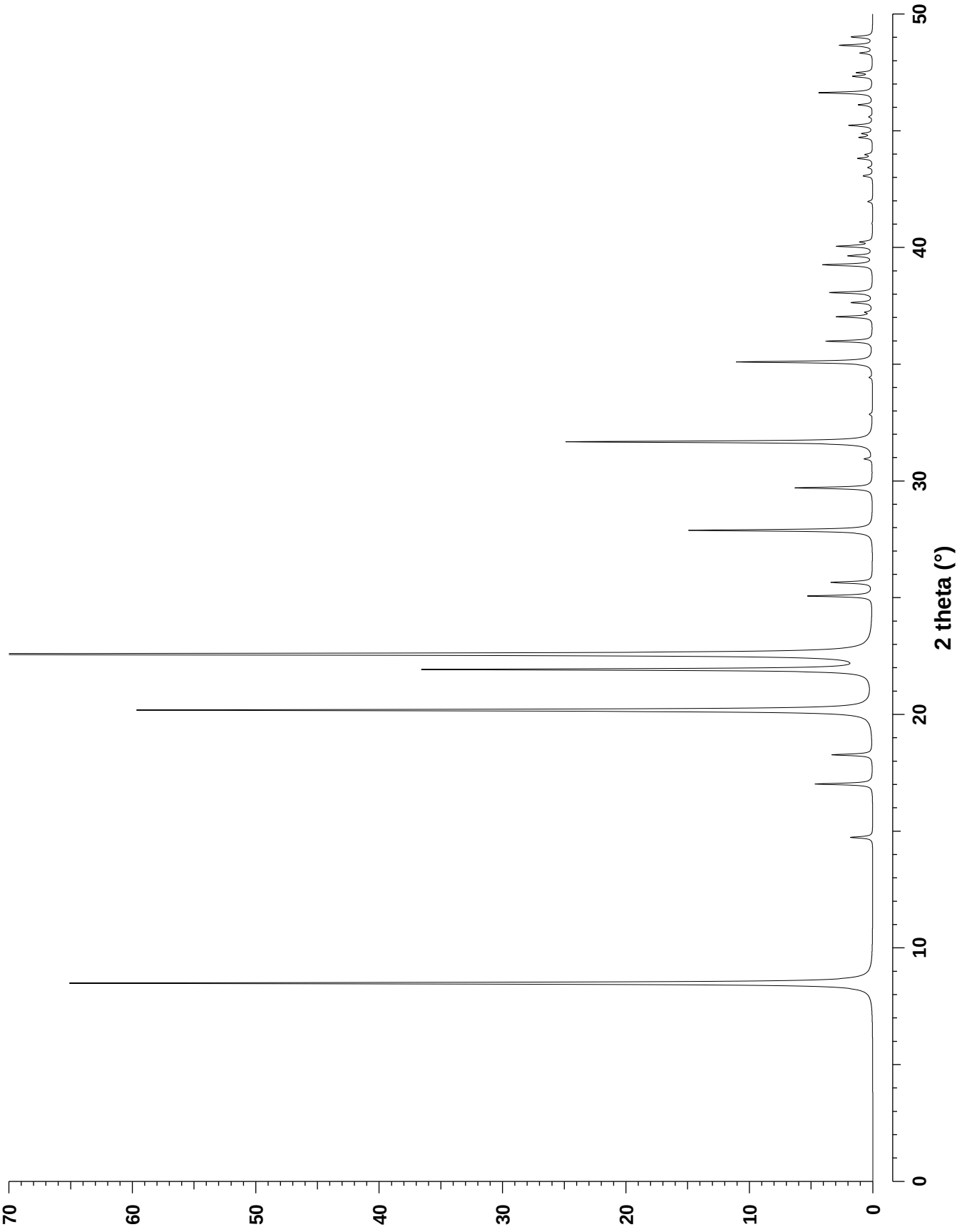
CHEMICAL COMPOSITION: $|((C_3H_7)_2NH)_2|\ [Al_{18}P_{17}SiO_{72}]$
$(C_3H_7)_2NH$ = di-n-propylamine

REFINED COMPOSITION: $|C_{14.76}|\ [Al_{17.71}P_{16.67}O_{72}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 20.839$ Å $b = 20.839$ Å $c = 5.041$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_{wF} = 0.018$, $R_F = 0.051$

REFERENCE: W. H. Baur, W. Joswig, D. Kassner and J. Kornatowski, *Acta Cryst.* **B50** 290–294 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.49	10.419	6	100.0	7	-3	1	35.09	2.557	6	11.6	0	8	1	43.97	2.059	6	0.9
0	3	0	14.73	6.016	6	2.8	0	1	2	35.98	2.496	6	5.8	4	2	2	44.71	2.027	6	1.1
2	2	0	17.02	5.210	6	7.2	2	0	2	37.03	2.428	6	4.5	6	-2	2	44.71	2.027	6	0.5
1	0	1	18.27	4.855	6	5.0	7	-6	1	37.22	2.416	6	0.8	9	-7	1	44.87	2.020	6	0.3
0	2	1	20.18	4.401	6	91.6	1	7	0	37.63	2.390	6	2.0	2	7	1	44.87	2.020	6	1.0
2	1	1	21.92	4.054	6	8.8	7	1	0	37.63	2.390	6	0.7	0	9	0	45.22	2.005	6	3.0
3	-1	1	21.92	4.054	6	46.8	3	-2	2	38.06	2.364	6	2.9	1	5	2	45.59	1.990	6	0.4
4	1	0	22.58	3.938	6	99.9	1	2	2	38.06	2.364	6	2.4	2	8	0	46.10	1.969	6	0.8
1	4	0	22.58	3.938	6	53.5	8	-5	1	39.25	2.295	6	2.6	8	2	0	46.10	1.969	6	1.0
4	-3	1	25.07	3.552	6	7.7	3	5	1	39.25	2.295	6	0.3	9	-1	1	46.62	1.948	6	0.2
1	3	1	25.07	3.552	6	0.4	7	0	1	39.25	2.295	6	3.3	8	1	1	46.62	1.948	6	6.5
3	3	0	25.65	3.473	6	5.2	6	3	0	39.64	2.274	6	1.0	3	4	2	47.32	1.921	6	2.3
5	-2	1	27.88	3.199	6	1.9	3	6	0	39.64	2.274	6	2.0	4	6	1	47.48	1.915	6	1.8
3	2	1	27.88	3.199	6	21.1	4	-1	2	40.05	2.251	6	0.6	10	-6	1	47.48	1.915	6	0.1
0	6	0	29.70	3.008	6	9.7	3	1	2	40.05	2.251	6	3.8	7	3	1	48.32	1.883	6	0.2
5	2	0	30.94	2.890	6	1.0	6	2	1	40.23	2.242	6	1.4	10	-3	1	48.32	1.883	6	1.4
6	-4	1	31.67	2.825	6	5.7	2	3	2	41.96	2.153	6	0.4	7	4	0	48.65	1.871	6	1.5
2	4	1	31.67	2.825	6	32.5	5	-3	2	41.96	2.153	6	0.2	4	7	0	48.65	1.871	6	2.6
6	-1	1	32.85	2.726	6	0.3	5	4	1	43.06	2.101	6	0.4	6	1	2	49.01	1.859	6	0.2
5	1	1	32.85	2.726	6	0.1	9	-4	1	43.06	2.101	6	0.8	7	-1	2	49.01	1.859	6	2.5
4	4	0	34.43	2.605	6	0.4	5	5	0	43.42	2.084	6	0.6							
4	3	1	35.09	2.557	6	5.4	5	0	2	43.81	2.067	6	1.9							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2 theta (°)
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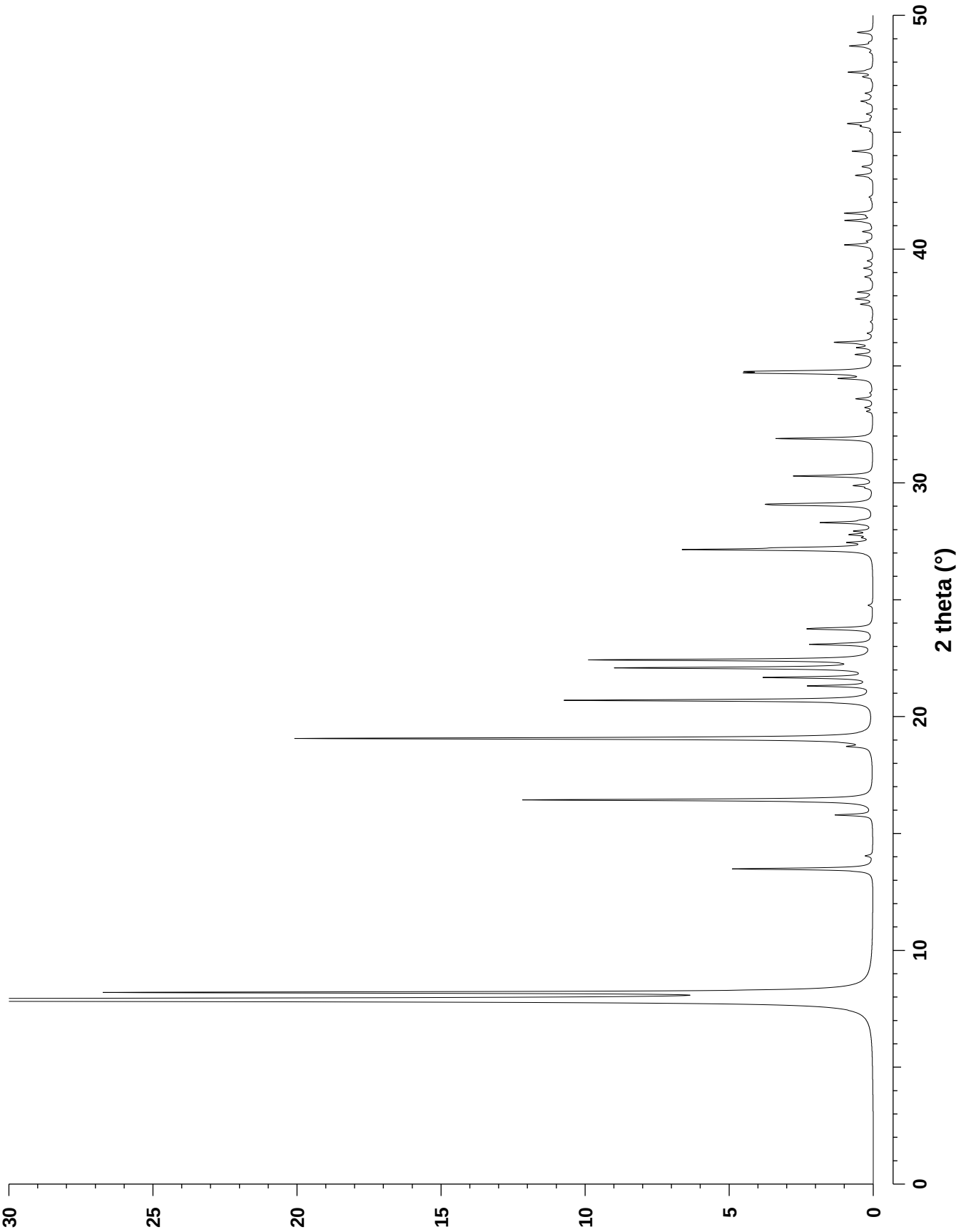
CHEMICAL COMPOSITION: $[(Al_{10.8}Mg)P_{12.2}O_{48}]$

REFINED COMPOSITION: $[Si_{24}O_{48}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 13.1483$ Å $b = 21.5771$ Å $c = 5.1639$ Å
$\alpha = 90°$ $\beta = 91.84°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.112$, $R_{wp} = 0.135$, $R_F = 0.058$

REFERENCE: J. V. Smith, J. J. Pluth and K. J. Andries,
Zeolites **13** 166–169 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	7.88	11.224	4	100.0	-3	3	1	29.09	3.069	4	2.4	-1	5	2	41.14	2.194	4	0.1
0	2	0	8.20	10.789	2	25.3	1	7	0	29.77	3.001	4	0.2	6	0	0	41.22	2.190	2	1.0
2	0	0	13.48	6.571	2	4.9	3	3	1	29.88	2.990	4	0.6	3	1	2	41.39	2.182	4	0.1
1	3	0	14.04	6.309	4	0.3	0	6	1	30.29	2.951	4	2.8	4	6	1	41.51	2.175	4	0.2
2	2	0	15.79	5.612	4	1.3	4	4	0	31.89	2.806	4	3.4	2	4	2	41.53	2.175	4	0.6
0	4	0	16.43	5.394	2	12.2	-2	6	1	33.05	2.710	4	0.2	1	5	2	41.53	2.174	4	0.3
-1	1	1	18.72	4.739	4	0.6	0	8	0	33.22	2.697	2	0.3	1	9	1	42.22	2.141	4	0.1
0	2	1	19.06	4.656	4	19.8	-3	5	1	33.59	2.668	4	0.6	3	3	2	43.13	2.098	4	0.2
1	1	1	19.12	4.641	4	1.0	-1	7	1	34.46	2.603	4	1.1	0	6	2	43.15	2.097	4	0.4
3	1	0	20.69	4.293	4	10.7	1	7	1	34.69	2.586	4	3.6	-5	5	1	43.52	2.079	4	0.4
2	4	0	21.31	4.169	4	2.2	0	0	2	34.76	2.581	2	3.6	2	10	0	44.18	2.050	4	0.7
1	5	0	21.67	4.100	4	3.7	-1	1	2	35.48	2.530	4	0.6	-6	2	1	45.24	2.004	4	0.3
-1	3	1	22.08	4.025	4	8.8	0	2	2	35.78	2.510	4	0.5	5	7	0	45.34	2.000	4	0.4
1	3	1	22.42	3.965	4	9.8	1	1	2	35.92	2.500	4	0.2	-3	5	2	45.37	1.999	4	0.6
-2	2	1	23.09	3.852	4	2.2	2	8	0	35.99	2.495	4	0.4	2	6	2	45.77	1.983	4	0.2
2	2	1	23.74	3.748	4	1.7	-4	4	1	36.01	2.494	4	1.0	-1	7	2	46.23	1.964	4	0.1
3	3	0	23.78	3.741	4	1.1	5	3	0	36.39	2.469	4	0.2	6	2	1	46.32	1.960	4	0.4
0	6	0	24.76	3.596	2	0.2	0	8	1	37.63	2.390	4	0.4	-4	8	1	46.66	1.947	4	0.3
4	0	0	27.14	3.285	2	6.2	2	0	2	37.86	2.376	2	0.3	4	8	1	47.36	1.919	4	0.3
-2	4	1	27.22	3.276	4	2.2	1	3	2	37.87	2.376	4	0.3	-2	10	1	47.56	1.912	4	0.8
3	1	1	27.44	3.251	4	0.7	-5	1	1	38.15	2.359	4	0.5	-6	4	1	47.66	1.908	4	0.1
-1	5	1	27.65	3.226	4	0.2	2	2	2	38.81	2.321	4	0.3	-5	7	1	48.41	1.880	4	0.1
2	4	1	27.78	3.211	4	0.7	5	1	1	39.18	2.299	4	0.3	6	6	0	48.67	1.871	4	0.3
1	5	1	27.93	3.195	4	0.6	-3	7	1	39.49	2.282	4	0.2	7	1	0	48.68	1.870	4	0.3
2	6	0	28.29	3.155	4	1.8	5	5	0	40.17	2.245	4	1.0	6	4	1	48.70	1.870	4	0.2
4	2	0	28.40	3.143	4	0.3	2	8	1	40.34	2.236	4	0.2	0	8	2	48.84	1.865	4	0.1
3	5	0	29.05	3.074	4	2.3	-2	4	2	40.74	2.215	4	0.4	5	7	1	49.26	1.850	4	0.5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ATT Tetramethylammonium hydroxide AlPO–12-TAMU

CHEMICAL COMPOSITION: $|((CH_3)_4NOH)_4|\ [Al_{12}P_{12}O_{48}]$
$(CH_3)_4NOH$ = tetramethylammonium hydroxide

REFINED COMPOSITION: $|(C_4NO)_4|\ [Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P2_12_12$ (No. 18)
$a = 10.3325$ Å $b = 14.6405$ Å $c = 9.5112$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.19$, $R_F = 0.17$

REFERENCE: P. R. Rudolf, C. Saldarriaga-Molina and A. Clearfield,
J. Phys. Chem. **90** 6122–6125 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	9.30	9.511	2	24.3	1	5	0	31.76	2.817	4	0.5	2	6	1	42.04	2.149	8	0.1
1	1	0	10.48	8.442	4	0.3	1	2	3	31.96	2.800	8	0.5	0	3	4	42.28	2.138	4	0.3
0	1	1	11.09	7.976	4	0.5	1	4	2	32.05	2.793	8	11.1	2	1	4	42.29	2.137	8	1.0
0	2	0	12.09	7.320	2	0.9	3	0	2	32.09	2.789	4	1.4	1	6	2	42.55	2.125	8	0.1
1	0	1	12.65	6.998	4	100.0	3	1	2	32.68	2.740	8	0.1	4	4	0	42.85	2.110	4	0.1
1	1	1	14.03	6.314	8	0.9	1	5	1	33.16	2.701	8	0.3	1	5	3	42.95	2.106	8	0.3
1	2	0	14.83	5.973	4	0.4	3	3	1	33.20	2.698	8	1.2	3	3	3	42.98	2.105	8	0.3
0	2	1	15.27	5.801	4	26.6	0	3	3	33.71	2.659	4	0.5	1	3	4	43.22	2.093	8	0.2
2	0	0	17.16	5.166	2	7.8	3	2	2	34.40	2.607	8	9.2	2	2	4	43.69	2.072	8	0.5
1	2	1	17.53	5.058	8	21.7	4	0	0	34.73	2.583	2	0.9	4	3	2	43.99	2.058	8	0.7
0	0	2	18.66	4.756	2	0.5	2	2	3	35.41	2.535	8	0.8	1	7	0	44.18	2.050	4	0.2
2	0	1	19.55	4.540	4	2.7	2	4	2	35.49	2.529	8	1.0	5	1	0	44.26	2.046	4	0.3
0	1	2	19.63	4.523	4	0.5	4	0	1	36.03	2.493	4	0.3	0	7	1	44.34	2.043	4	0.2
1	3	0	20.12	4.413	4	1.3	2	5	1	36.52	2.461	8	1.2	5	0	1	44.88	2.019	4	0.5
0	3	1	20.45	4.342	4	2.8	4	1	1	36.56	2.457	8	0.2	1	7	1	45.25	2.004	8	0.5
2	1	1	20.48	4.336	8	0.7	0	6	0	36.83	2.440	2	1.1	4	0	3	45.28	2.003	4	0.7
1	0	2	20.56	4.320	4	19.7	3	4	1	37.07	2.425	8	0.9	2	6	2	45.31	2.001	8	0.3
2	2	0	21.05	4.221	4	5.8	1	5	2	37.09	2.424	8	1.3	5	1	1	45.33	2.000	8	0.6
1	1	2	21.45	4.143	8	1.3	3	3	2	37.12	2.422	8	0.1	1	4	4	46.38	1.958	8	0.2
1	3	1	22.21	4.003	8	4.3	0	0	4	37.84	2.378	2	1.8	3	0	4	46.40	1.957	4	0.2
0	2	2	22.29	3.988	4	0.3	2	3	3	38.06	2.364	8	0.2	3	6	1	46.60	1.949	8	0.6
2	2	1	23.05	3.858	8	6.9	4	2	1	38.14	2.360	8	0.6	5	2	1	46.66	1.947	8	0.3
1	2	2	23.92	3.720	8	30.9	0	1	4	38.35	2.347	4	0.4	3	1	4	46.84	1.940	8	0.2
0	4	0	24.32	3.660	2	1.0	1	4	3	38.57	2.334	8	0.3	4	2	3	47.04	1.932	8	2.1
2	3	0	25.10	3.548	4	1.3	3	0	3	38.60	2.333	4	0.1	4	4	2	47.11	1.929	8	0.1
2	0	2	25.46	3.499	4	0.2	1	0	4	38.86	2.317	4	0.5	0	7	2	47.49	1.915	4	0.8
0	4	1	26.09	3.416	4	44.4	1	6	1	39.09	2.304	8	0.9	5	3	0	47.80	1.903	4	0.3
0	3	2	26.16	3.406	4	0.1	3	1	3	39.10	2.304	8	0.8	0	0	5	47.81	1.902	2	0.9
2	1	2	26.19	3.403	8	0.5	1	1	4	39.37	2.289	8	0.3	1	6	3	47.86	1.901	8	1.9
2	3	1	26.82	3.324	8	1.4	4	0	2	39.71	2.270	4	1.7	2	7	1	47.89	1.900	8	0.2
1	4	1	27.50	3.243	8	5.3	2	5	2	40.16	2.246	8	0.7	3	2	4	48.13	1.890	8	0.6
3	0	1	27.54	3.238	4	51.5	4	1	2	40.20	2.243	8	0.6	5	1	2	48.43	1.880	8	0.4
1	3	2	27.58	3.235	8	0.5	3	5	0	40.43	2.231	4	0.4	1	0	5	48.67	1.871	4	0.3
0	0	3	28.15	3.170	2	0.4	3	2	3	40.59	2.222	8	0.7	2	4	4	48.96	1.860	8	0.2
2	2	2	28.27	3.157	8	0.5	4	3	1	40.64	2.220	8	0.3	1	1	5	49.09	1.856	8	0.1
0	1	3	28.81	3.099	4	0.1	3	4	2	40.67	2.219	8	3.1	0	5	4	49.37	1.846	4	0.2
1	0	3	29.47	3.031	4	9.7	1	2	4	40.85	2.209	8	0.2	0	2	5	49.51	1.841	4	0.1
2	4	0	29.92	2.987	4	1.6	2	4	3	41.54	2.174	8	0.5	3	6	2	49.64	1.837	8	0.2
1	1	3	30.11	2.968	8	0.2	3	5	1	41.58	2.172	8	0.1	5	2	2	49.69	1.835	8	0.2
0	2	3	30.73	2.909	4	7.6	0	6	2	41.60	2.171	4	0.2	0	8	0	49.83	1.830	2	2.3
0	4	2	30.83	2.901	4	0.2	4	2	2	41.66	2.168	8	2.4	3	5	3	49.99	1.824	8	0.2
2	4	1	31.39	2.849	8	1.0	2	0	4	41.82	2.160	4	0.3							
2	3	2	31.46	2.844	8	1.0	0	5	3	42.00	2.151	4	1.3							

Tetramethylammonium hydroxide AlPO–12-TAMU **ATT**

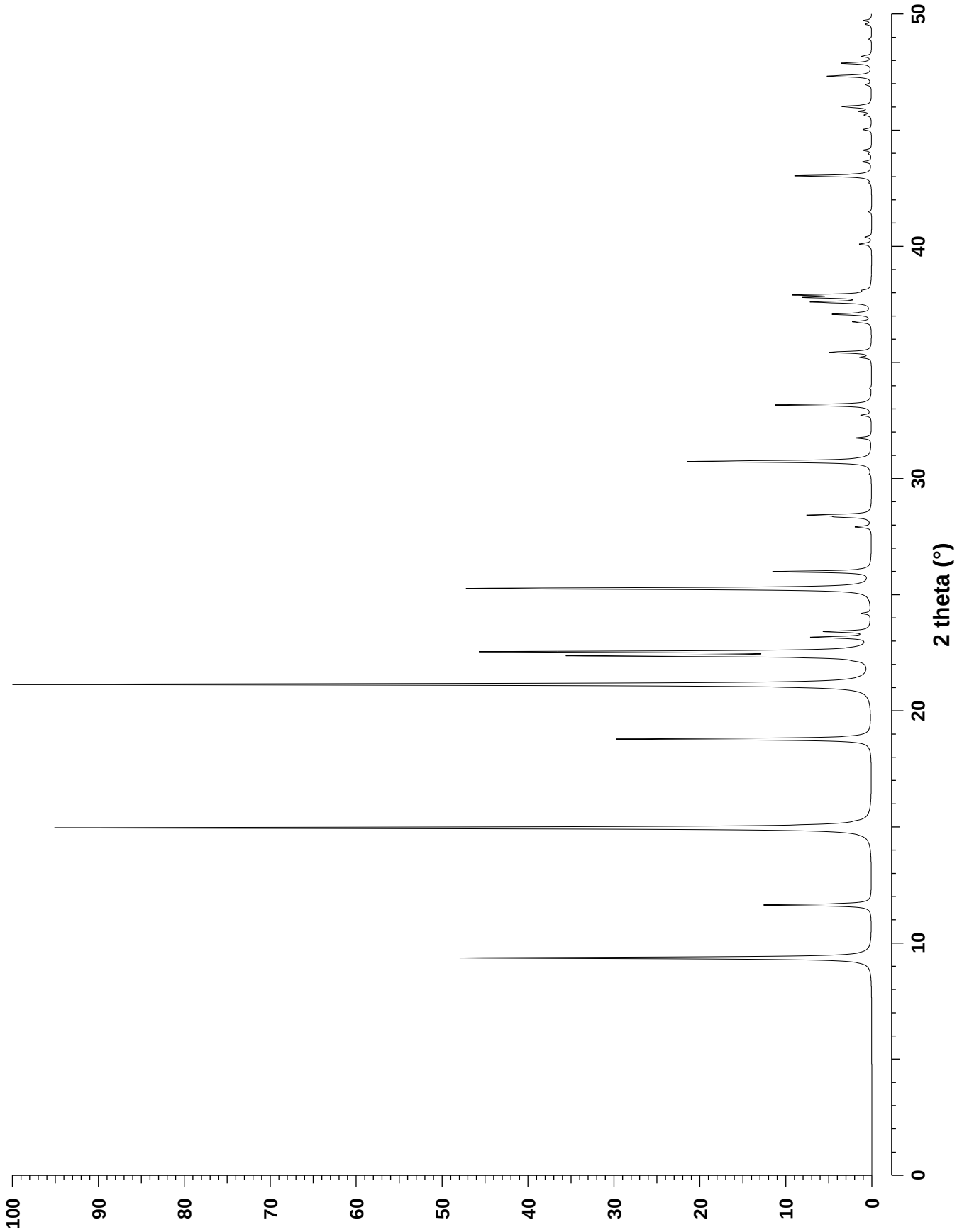
CHEMICAL COMPOSITION: $[Al_{12}P_{12}O_{48}]$

REFINED COMPOSITION: $[Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: *Acmm* (No. 67) $\bar{\mathbf{c}}\mathbf{ba}$ setting
$a = 9.4489$ Å $b = 15.2028$ Å $c = 8.4084$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.041$, $R_{F^2} = 0.133$; At $T = 593$ K.

REFERENCE: J. W. Richardson, Jr., J. V. Smith and J. J. Pluth,
J. Phys. Chem. **94** 3365–3367 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	9.36	9.449	2	48.0	3	1	1	30.88	2.896	8	0.3	0	0	4	43.03	2.102	2	9.0
0	2	0	11.64	7.601	2	12.6	0	4	2	31.74	2.819	4	1.8	4	3	1	43.62	2.075	8	0.8
1	2	0	14.96	5.923	4	95.2	1	5	1	32.72	2.737	8	1.2	3	1	3	43.64	2.074	8	0.3
1	1	1	15.26	5.805	8	0.3	1	4	2	33.16	2.702	8	11.3	4	0	2	43.97	2.059	4	0.3
2	0	0	18.78	4.724	2	29.7	1	1	3	33.88	2.646	8	0.2	1	7	1	44.12	2.053	8	0.3
0	0	2	21.13	4.204	2	100.0	3	3	1	35.21	2.549	8	1.3	1	0	4	44.13	2.052	4	0.7
2	2	0	22.15	4.013	4	0.5	0	6	0	35.43	2.534	2	4.9	1	5	3	45.02	2.013	8	1.0
2	1	1	22.36	3.976	8	33.4	2	5	1	36.74	2.446	8	2.2	4	2	2	45.64	1.988	8	0.8
1	3	1	22.54	3.944	8	44.0	3	4	0	37.07	2.425	4	4.4	1	2	4	45.80	1.981	8	1.4
1	0	2	23.16	3.841	4	6.7	2	4	2	37.13	2.421	8	0.5	3	6	0	45.97	1.974	4	1.1
0	4	0	23.41	3.801	2	5.3	3	2	2	37.59	2.393	8	6.8	2	6	2	46.02	1.972	8	3.0
0	2	2	24.19	3.679	4	1.1	2	1	3	37.79	2.381	8	6.9	3	3	3	46.95	1.935	8	0.7
1	4	0	25.26	3.526	4	47.2	1	3	3	37.90	2.374	8	8.3	2	7	1	47.32	1.921	8	4.4
1	2	2	25.99	3.428	8	11.4	4	0	0	38.09	2.362	2	0.7	2	0	4	47.33	1.921	4	0.9
2	3	1	27.91	3.196	8	1.9	4	2	0	39.97	2.256	4	0.1	0	8	0	47.87	1.900	2	3.6
3	0	0	28.34	3.150	2	3.0	4	1	1	40.09	2.249	8	1.4	2	5	3	48.17	1.889	8	1.1
2	0	2	28.42	3.141	4	7.0	2	6	0	40.39	2.233	4	0.8	2	2	4	48.91	1.862	8	0.3
2	4	0	30.18	2.961	4	0.2	2	3	3	41.48	2.177	8	0.4	0	4	4	49.55	1.839	4	0.7
3	2	0	30.73	2.910	4	21.5	3	5	1	42.71	2.117	8	0.2	5	2	0	49.71	1.834	4	0.9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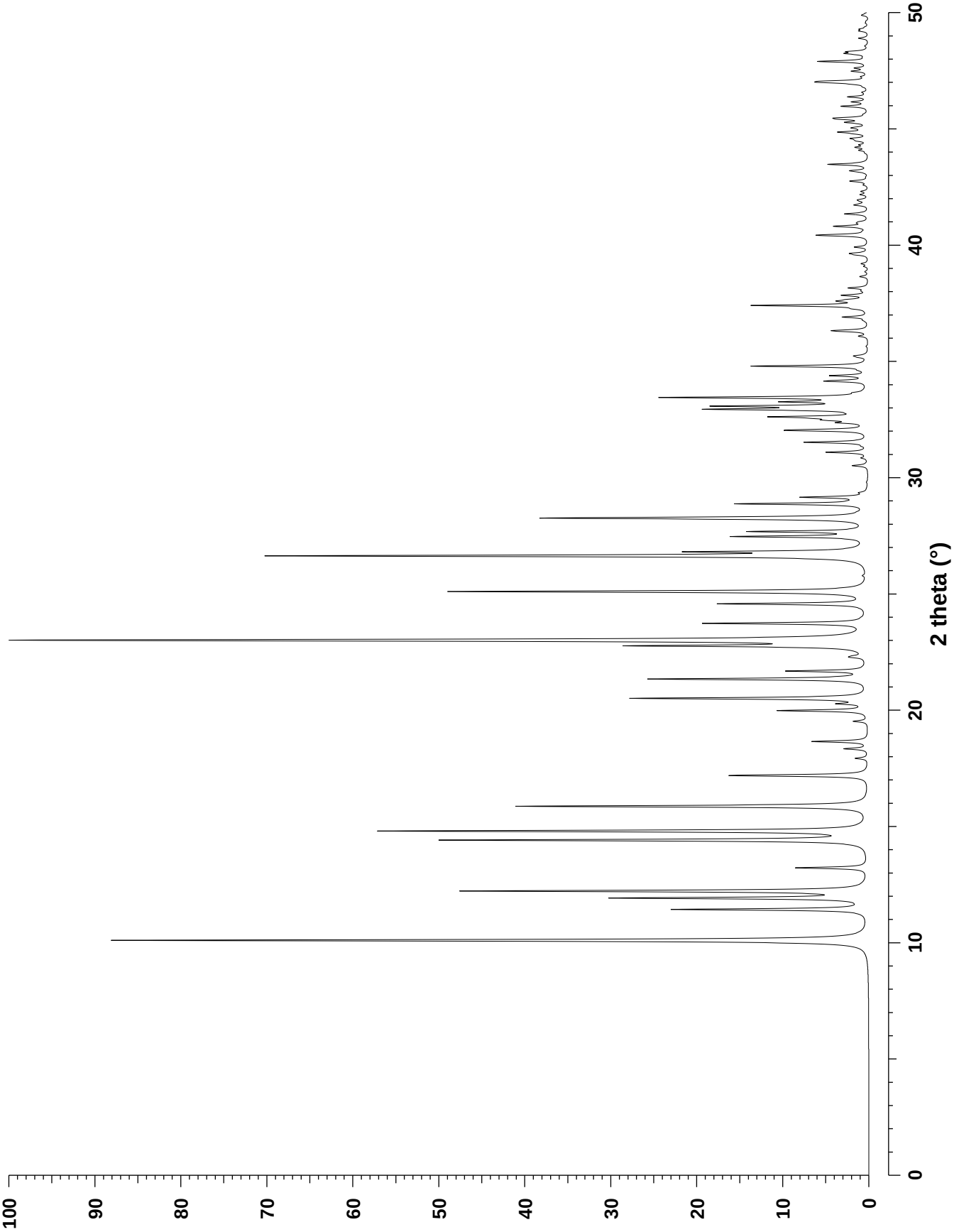
CHEMICAL COMPOSITION: $|(C_7H_{21}N_2)_{1.33}|\ [Al_{12}P_{12}O_{48}]$
$C_7H_{21}N_2 = N,N,N',N'$-tetramethyl-1,3-propanediamine

REFINED COMPOSITION: $|N_{2.84}C_{13.41}O_4H_4|\ [Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P1\,2_1/a\,1$ (No. 14) unique axis **b**, cell choice 3
$a = 10.3307$ Å $b = 17.5241$ Å $c = 8.6757$ Å
$\alpha = 90.0°$ $\beta = 123.369°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R = 0.046$, $R_w = 0.042$

REFERENCE: J. M. Bennett, J. M. Cohen, G. Artioli, J. J. Pluth and J. V. Smith, *Inorg. Chem.* **24** 188–193 (1985).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	10.10	8.762	2	100.0	0	4	2	32.06	2.792	4	2.2	2	7	0	41.71	2.165	4	0.6
1	1	0	11.43	7.740	4	25.7	1	6	0	32.36	2.766	4	3.1	2	2	2	41.72	2.165	4	0.7
-1	1	1	11.92	7.424	4	33.2	1	5	1	32.47	2.758	4	3.9	4	0	0	41.88	2.157	2	0.6
0	0	1	12.22	7.245	2	53.3	-1	6	1	32.54	2.751	4	3.2	-3	5	3	41.93	2.155	4	0.9
0	1	1	13.22	6.696	4	9.4	-2	2	3	32.61	2.746	4	11.5	-3	1	4	42.17	2.143	4	0.8
1	2	0	14.41	6.148	4	56.0	3	2	0	32.77	2.732	4	0.6	-2	7	2	42.30	2.136	4	0.9
-1	2	1	14.80	5.986	4	64.2	2	5	0	32.93	2.720	4	18.5	-1	8	1	42.73	2.116	4	1.1
0	2	1	15.87	5.584	4	46.5	-1	1	3	32.95	2.718	4	1.5	0	4	3	42.75	2.115	4	1.5
-2	0	1	17.19	5.158	2	18.4	-1	5	2	33.01	2.713	4	1.6	4	2	0	43.19	2.094	4	2.1
-2	1	1	17.93	4.948	4	1.7	0	6	1	33.07	2.709	4	18.0	-2	2	4	43.47	2.082	4	5.3
1	3	0	18.34	4.837	4	3.1	1	2	2	33.26	2.693	4	9.3	-2	6	3	44.07	2.055	4	1.1
-1	3	1	18.65	4.757	4	7.4	-3	4	1	33.44	2.680	4	26.8	3	6	0	44.20	2.049	4	1.4
0	3	1	19.52	4.548	4	1.9	-2	5	2	33.65	2.664	4	0.9	-5	1	2	44.31	2.044	4	0.9
-2	2	1	19.98	4.445	4	11.8	-1	2	3	34.15	2.625	4	5.6	1	1	3	44.47	2.037	4	1.0
0	4	0	20.27	4.381	2	3.2	-3	2	3	34.38	2.608	4	4.8	-4	1	4	44.52	2.035	4	0.8
1	1	1	20.51	4.330	4	31.3	-2	3	3	34.61	2.592	4	0.6	1	6	2	44.58	2.033	4	1.9
-1	1	2	21.34	4.163	4	28.9	-4	0	2	34.79	2.579	2	15.3	4	3	0	44.79	2.023	4	1.0
-2	0	2	21.68	4.098	2	10.4	-4	1	2	35.17	2.551	4	0.9	3	4	1	44.85	2.021	4	3.5
-2	1	2	22.28	3.991	4	1.6	1	3	2	35.23	2.547	4	1.5	-5	1	3	45.02	2.014	4	0.6
1	2	1	22.33	3.981	4	0.8	-1	3	3	36.08	2.489	4	1.2	-3	7	1	45.03	2.013	4	0.9
1	4	0	22.76	3.906	4	29.1	-3	3	3	36.30	2.475	4	1.3	-2	3	4	45.06	2.012	4	0.8
2	2	0	22.98	3.870	4	18.2	-4	2	2	36.31	2.474	4	3.2	-5	2	2	45.26	2.004	4	1.7
-2	3	1	23.00	3.866	4	37.8	-4	0	1	36.34	2.472	2	0.6	-1	6	3	45.28	2.003	4	1.2
-1	4	1	23.02	3.864	4	69.3	-3	5	1	36.90	2.436	4	3.3	1	2	3	45.41	1.997	4	2.7
-1	2	2	23.10	3.850	4	1.4	-1	6	2	37.25	2.414	4	0.6	-4	2	4	45.46	1.995	4	2.1
0	4	1	23.73	3.749	4	21.4	-3	5	2	37.40	2.405	4	0.6	-3	6	3	45.46	1.995	4	1.3
0	0	2	24.57	3.623	2	19.5	1	7	0	37.40	2.404	4	12.2	-5	2	3	45.95	1.975	4	0.6
1	3	1	25.09	3.549	4	3.9	3	4	0	37.40	2.404	4	2.5	-4	5	3	45.97	1.974	4	3.1
0	1	2	25.10	3.548	4	51.7	-1	7	1	37.57	2.394	4	1.3	1	8	1	46.15	1.967	4	2.0
0	2	2	26.63	3.348	4	77.9	0	1	3	37.59	2.393	4	2.0	-1	2	4	46.37	1.958	4	2.6
-2	4	1	26.70	3.339	4	2.8	-4	0	3	37.65	2.389	2	1.7	-1	8	2	46.56	1.951	4	0.6
-3	1	1	26.81	3.326	4	20.5	1	4	2	37.84	2.377	4	3.0	-4	3	4	46.99	1.934	4	3.6
-3	1	2	27.46	3.248	4	17.2	-4	3	2	38.15	2.359	4	2.6	-4	6	2	47.00	1.933	4	0.9
-1	5	1	27.68	3.223	4	15.2	-1	4	3	38.64	2.330	4	1.1	-2	8	2	47.04	1.932	4	4.4
-3	2	1	28.25	3.159	4	39.2	2	5	1	39.20	2.298	4	0.9	-5	1	1	47.24	1.924	4	0.6
0	5	1	28.29	3.155	4	8.0	-4	3	1	39.58	2.277	4	1.3	-5	3	3	47.47	1.915	4	2.0
-3	2	2	28.87	3.093	4	17.2	0	6	2	39.64	2.274	4	2.1	3	5	1	47.61	1.910	4	1.6
0	3	2	29.00	3.079	4	0.6	3	1	1	39.91	2.259	4	1.8	-1	3	4	47.89	1.900	4	1.7
-1	4	2	29.15	3.064	4	8.5	0	3	3	40.41	2.232	4	4.4	1	9	0	47.89	1.899	4	4.9
2	0	1	29.35	3.043	2	0.8	-2	5	3	40.44	2.231	4	3.4	-4	6	1	48.23	1.887	4	2.5
-3	3	1	30.51	2.930	4	2.1	-3	6	1	40.79	2.212	4	1.3	2	5	2	48.31	1.884	4	2.5
-2	5	1	30.84	2.899	4	0.8	-4	3	3	40.81	2.211	4	3.4	-5	4	2	48.89	1.863	4	1.3
-3	3	2	31.09	2.877	4	5.4	3	2	1	40.94	2.204	4	0.9	-1	7	3	49.20	1.852	4	1.1
3	1	0	31.52	2.838	4	8.4	1	5	2	40.99	2.202	4	0.8	-4	6	3	49.28	1.849	4	1.0
1	1	2	32.03	2.794	4	9.5	1	7	1	41.34	2.184	4	3.1	-2	5	4	49.88	1.828	4	0.9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2 theta (°)
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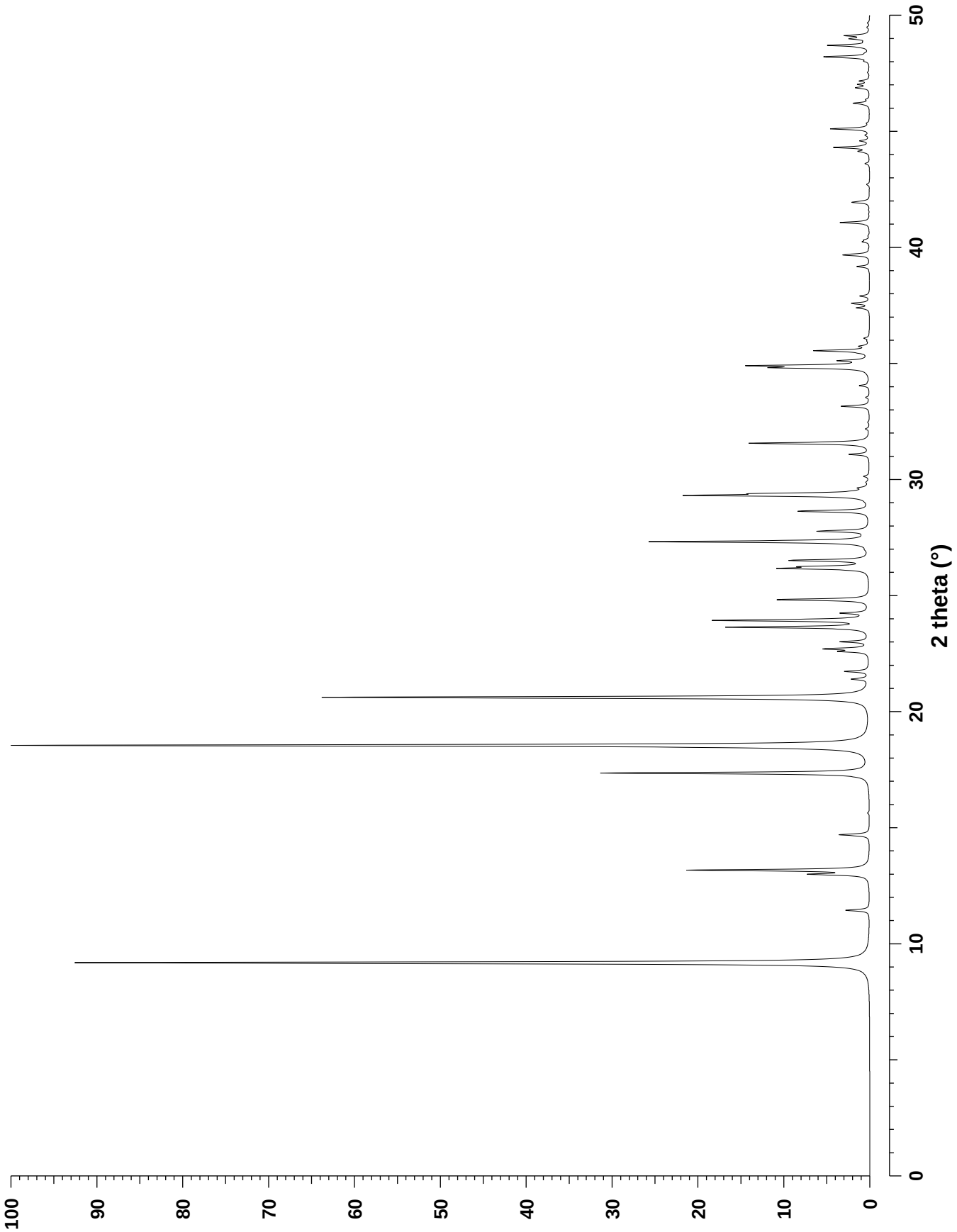
CHEMICAL COMPOSITION: $|(C_7H_{13}N)_4(PO_3OH)_2|\ [Al_{24}P_{24}O_{96}]$
$C_7H_{13}N$ = quinuclidine

REFINED COMPOSITION: $|P_2O_{8.48}(C_7N)_4|\ [Al_{24}P_{24}O_{96}]$

CRYSTAL DATA: $P\,4/n\,cc$ (No. 130) origin at centre $\overline{1}$
$a = 13.628$ Å $b = 13.628$ Å $c = 15.463$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.18$

REFERENCE: J. W. Richardson, Jr., J. J. Pluth and J. V. Smith,
Naturwiss. **76** 467–469 (1989).
And J. J. Pluth, Private communication (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.18	9.636	4	92.8	4	2	1	29.88	2.990	16	0.2	6	1	2	41.98	2.152	16	0.4
0	0	2	11.44	7.732	2	2.8	3	3	2	30.13	2.966	8	0.6	5	2	4	42.70	2.117	16	0.4
2	0	0	12.99	6.814	4	6.3	3	1	4	31.08	2.878	16	2.3	6	2	2	43.60	2.076	16	0.5
1	0	2	13.17	6.725	8	21.1	4	2	2	31.56	2.835	16	14.1	6	1	3	44.07	2.055	16	0.2
1	1	2	14.69	6.030	8	3.6	4	1	3	32.17	2.782	16	0.4	5	4	2	44.13	2.052	16	1.1
2	1	1	15.63	5.670	16	0.2	2	1	5	32.46	2.758	16	0.2	4	4	4	44.30	2.045	8	4.1
2	0	2	17.35	5.112	8	31.3	3	2	4	33.15	2.703	16	3.3	4	1	6	44.58	2.032	16	1.1
2	2	0	18.41	4.818	4	1.6	5	1	0	33.53	2.673	8	0.4	5	1	5	44.82	2.022	16	0.4
2	1	2	18.54	4.786	16	100.0	5	1	1	34.04	2.634	16	1.2	3	3	6	45.10	2.010	8	4.6
3	1	0	20.61	4.310	8	63.9	0	0	6	34.81	2.577	2	9.7	5	3	4	45.34	2.000	16	0.3
3	1	1	21.40	4.151	16	1.9	5	0	2	34.90	2.571	8	8.3	4	2	6	46.13	1.968	16	0.3
2	2	2	21.73	4.089	8	2.8	4	3	2	34.90	2.571	16	4.4	6	3	2	46.20	1.965	16	1.9
2	1	3	22.59	3.936	16	3.1	4	0	4	35.11	2.556	8	3.2	6	0	4	46.36	1.958	8	0.3
3	0	2	22.70	3.917	8	5.0	1	0	6	35.45	2.532	8	0.4	6	1	4	46.87	1.938	16	1.6
0	0	4	23.01	3.866	2	3.2	5	1	2	35.54	2.526	16	6.3	0	0	8	47.01	1.933	2	1.3
3	1	2	23.63	3.764	16	16.5	3	1	5	35.73	2.513	16	0.3	5	5	0	47.16	1.927	4	1.0
1	0	4	23.93	3.719	8	18.0	4	1	4	35.74	2.512	16	0.7	1	0	8	47.51	1.914	8	0.1
3	2	1	24.24	3.672	16	3.0	5	2	1	35.96	2.497	16	0.2	7	1	1	47.54	1.912	16	0.1
1	1	4	24.82	3.588	8	10.7	1	1	6	36.08	2.490	8	0.6	1	1	8	48.01	1.895	8	0.4
4	0	0	26.16	3.407	4	9.5	5	2	2	37.39	2.405	16	1.5	6	4	0	48.15	1.890	8	0.2
3	2	2	26.24	3.396	16	6.4	3	2	5	37.58	2.394	16	0.5	7	0	2	48.20	1.888	8	5.2
2	0	4	26.51	3.362	8	9.1	4	2	4	37.58	2.393	16	1.6	6	2	4	48.36	1.882	16	0.2
3	1	3	26.97	3.306	16	0.2	2	1	6	37.90	2.374	16	1.1	5	0	6	48.62	1.873	8	0.4
2	1	4	27.32	3.264	16	25.7	4	4	2	39.17	2.300	8	1.5	7	1	2	48.69	1.870	16	2.1
4	1	1	27.60	3.232	16	0.1	2	2	6	39.66	2.273	8	1.7	5	5	2	48.69	1.870	8	2.6
3	3	0	27.77	3.212	4	5.9	6	0	0	39.68	2.271	4	1.7	5	4	4	48.85	1.864	16	0.3
4	0	2	28.63	3.118	8	8.3	3	0	6	40.23	2.242	8	0.8	2	0	8	48.98	1.860	8	2.0
3	2	3	29.30	3.048	16	1.0	5	3	2	40.31	2.237	16	0.6	7	2	1	49.02	1.858	16	0.1
4	2	0	29.31	3.047	8	18.8	4	3	4	40.49	2.228	16	0.1	5	1	6	49.11	1.855	16	2.8
4	1	2	29.39	3.039	16	10.1	5	1	4	41.06	2.198	16	3.5	2	1	8	49.47	1.842	16	0.3
2	2	4	29.63	3.015	8	0.9	6	2	0	41.93	2.155	8	1.9	6	4	2	49.66	1.836	16	0.2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*BEA Beta, Polymorph A SiO_2 Framework

CHEMICAL COMPOSITION: $[Si_{64}O_{128}]$

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: $P4_122$ (No. 91)
$a = 12.661$ Å $b = 12.661$ Å $c = 26.406$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
DLS refinement.

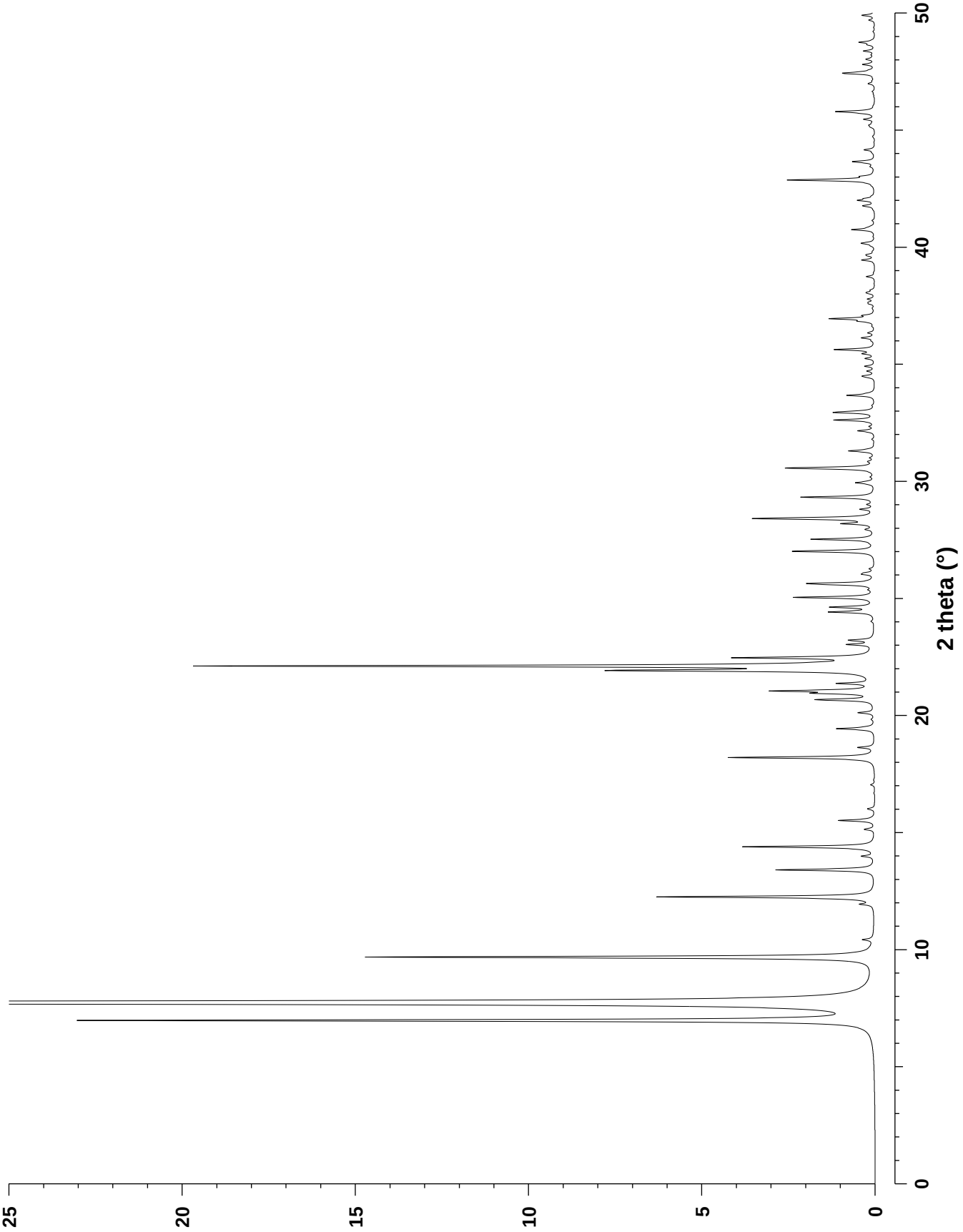
REFERENCE: J. M. Newsam, M. M. J. Treacy, W. T. Koetsier and C. B. deGruyter, *Proc. Roy. Soc.* (London) **A420** 375–405 (1988).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	6.98	12.661	4	22.8	3	2	2	26.26	3.394	16	0.1	2	1	10	37.58	2.393	16	0.1
1	0	1	7.74	11.417	8	100.0	0	0	8	27.01	3.301	2	2.4	5	1	3	37.64	2.390	16	0.1
1	0	2	9.68	9.138	8	14.7	2	0	7	27.52	3.241	8	1.8	4	2	6	37.78	2.381	16	0.2
1	1	1	10.43	8.479	8	0.3	1	0	8	27.93	3.194	8	0.2	3	1	9	38.02	2.367	16	0.1
1	1	2	11.94	7.410	8	0.3	4	0	0	28.19	3.165	4	0.9	5	0	4	38.06	2.364	8	0.1
1	0	3	12.25	7.227	8	6.3	4	0	1	28.40	3.143	8	2.9	1	0	11	38.16	2.359	8	0.1
0	0	4	13.41	6.602	2	2.9	2	1	7	28.43	3.139	16	0.5	5	1	4	38.74	2.324	16	0.2
2	0	0	13.99	6.331	4	0.3	2	2	6	28.44	3.138	8	0.6	4	0	8	39.44	2.285	8	0.3
2	0	1	14.39	6.156	8	3.8	3	2	4	28.80	3.100	16	0.4	2	2	10	39.63	2.274	8	0.1
1	0	4	15.14	5.854	8	0.3	4	0	2	29.01	3.078	8	0.2	5	2	3	39.68	2.271	16	0.2
2	0	2	15.52	5.708	8	1.0	3	0	6	29.32	3.046	8	2.1	2	0	11	40.17	2.245	8	0.4
2	1	1	16.01	5.536	16	0.2	3	3	0	29.94	2.984	4	0.5	5	2	4	40.74	2.215	16	0.6
2	1	2	17.04	5.204	16	0.1	2	0	8	30.54	2.927	8	1.0	2	1	11	40.83	2.210	16	0.1
1	0	5	18.20	4.874	8	4.2	3	2	5	30.57	2.924	16	1.9	5	3	1	41.74	2.164	16	0.1
2	1	3	18.63	4.762	16	0.5	4	1	3	30.84	2.899	16	0.1	5	1	6	41.77	2.163	16	0.3
2	0	4	19.43	4.569	8	1.1	2	2	7	31.00	2.885	8	0.1	4	0	9	41.99	2.152	8	0.4
1	1	5	19.51	4.549	8	0.1	1	0	9	31.29	2.858	8	0.7	5	2	5	42.07	2.148	16	0.2
2	2	1	20.12	4.413	8	0.5	4	1	4	32.15	2.784	16	0.5	3	2	10	42.85	2.110	16	0.3
2	1	4	20.67	4.298	16	1.7	4	2	2	32.34	2.768	16	0.1	6	0	0	42.86	2.110	4	2.1
2	2	2	20.95	4.239	8	1.4	3	1	7	32.61	2.746	16	1.1	5	3	3	42.90	2.108	16	0.2
3	0	0	21.05	4.220	4	2.8	3	3	4	32.94	2.719	8	1.1	5	0	7	43.02	2.102	8	0.3
1	0	6	21.37	4.157	8	1.0	4	0	5	32.99	2.715	8	0.2	6	1	1	43.62	2.075	16	0.2
2	0	5	21.92	4.055	8	6.9	2	0	9	33.67	2.662	8	0.8	5	2	6	43.65	2.074	16	0.4
3	0	2	22.11	4.020	8	19.2	4	1	5	33.76	2.655	16	0.1	2	1	12	44.15	2.051	16	0.3
3	1	0	22.20	4.004	8	0.7	2	1	9	34.43	2.605	16	0.1	1	0	13	45.21	2.006	8	0.1
2	2	3	22.28	3.990	8	0.3	4	2	4	34.47	2.602	16	0.1	5	2	7	45.46	1.995	16	0.2
3	1	1	22.46	3.959	16	3.7	3	0	8	34.50	2.600	8	0.2	5	1	8	45.72	1.984	16	0.2
1	1	6	22.51	3.950	8	0.4	1	0	10	34.70	2.585	8	0.2	3	2	11	45.78	1.982	16	1.1
2	1	5	23.03	3.862	16	0.7	3	2	7	34.91	2.570	16	0.3	2	0	13	46.98	1.934	8	0.2
3	1	2	23.21	3.831	16	0.7	3	1	8	35.24	2.547	16	0.3	5	0	9	47.42	1.917	8	0.9
3	1	3	24.42	3.644	16	1.3	5	0	0	35.45	2.532	4	0.2	5	2	8	47.48	1.915	16	0.2
1	0	7	24.62	3.615	8	1.0	4	3	1	35.62	2.521	16	0.7	6	0	6	47.80	1.903	8	0.3
2	0	6	24.64	3.614	8	0.3	5	0	1	35.62	2.521	8	0.4	5	1	9	48.00	1.895	16	0.1
3	0	4	25.04	3.556	8	2.3	4	3	2	36.12	2.487	16	0.3	5	4	4	48.03	1.894	16	0.2
3	2	0	25.36	3.512	8	0.1	5	1	1	36.34	2.472	16	0.2	5	3	7	48.37	1.882	16	0.3
3	2	1	25.59	3.481	16	0.8	5	1	2	36.83	2.440	16	0.4	6	2	5	48.64	1.872	16	0.2
2	1	6	25.64	3.475	16	1.6	4	3	3	36.94	2.434	16	0.7	6	3	2	48.74	1.868	16	0.4
3	1	4	26.03	3.423	16	0.3	5	0	3	36.94	2.434	8	0.6	5	2	9	49.69	1.835	16	0.2
2	2	5	26.09	3.415	8	0.2	4	0	7	37.08	2.425	8	0.3	5	0	10	49.90	1.828	8	0.4

Zeolite beta and its mineral analog tschernichite are intergrown materials and *BEA represents the framework of a hypothetical end member. Simulated powder patterns for intergrown variants are presented later in this book.

Beta, Polymorph A SiO_2 Framework

*BEA



BIK Bikitaite

CHEMICAL COMPOSITION: $|Li_2(H_2O)_2|\ [Si_4Al_2O_{12}]$
Bikita, Zimbabwe

REFINED COMPOSITION: $|Li_{1.86}(H_2O)_2|\ [Si_{3.89}Al_{2.13}O_{12}]$

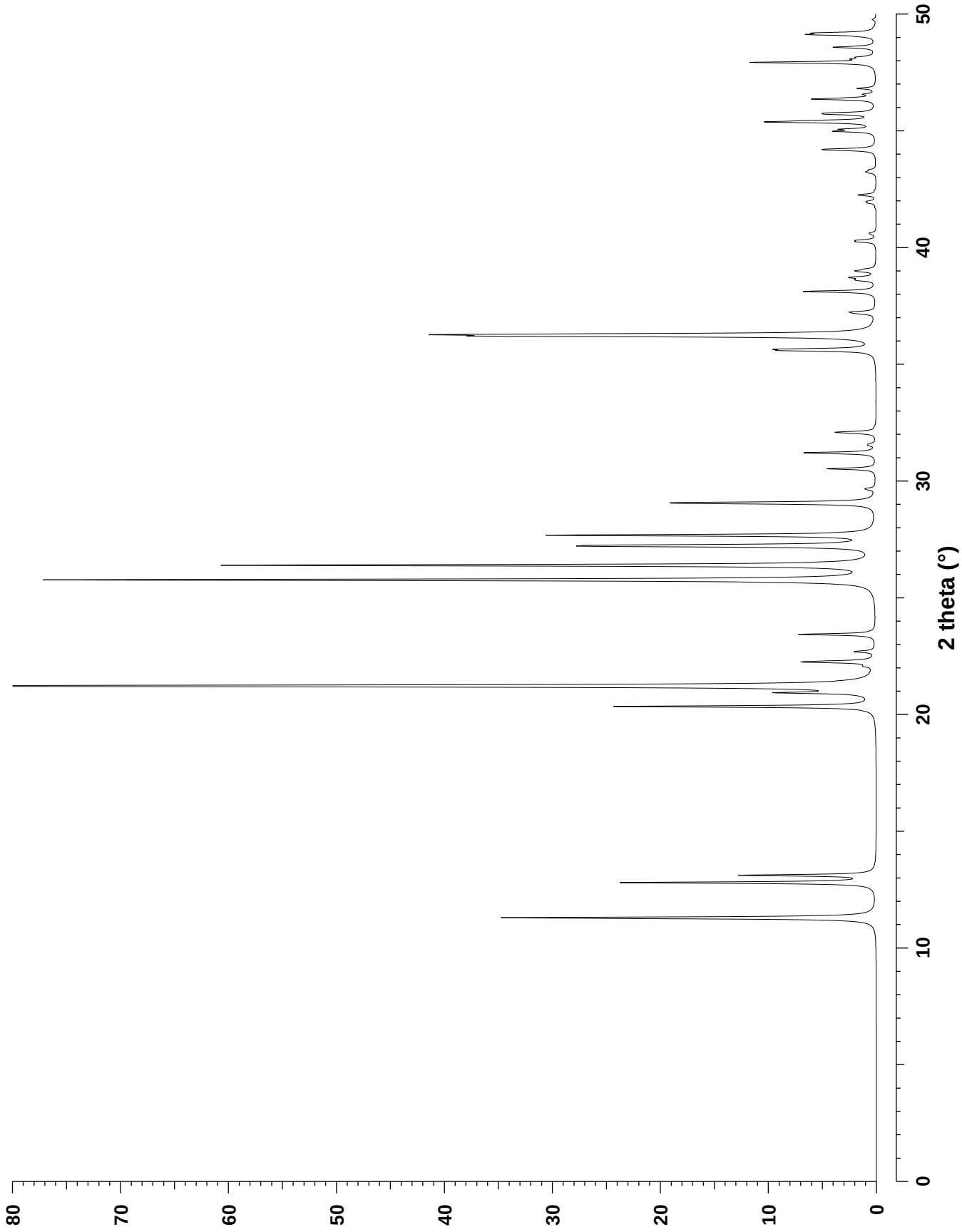
CRYSTAL DATA: $P1$ (No. 1)
$a = 8.6071$ Å $b = 4.9540$ Å $c = 7.5972$ Å
$\alpha = 89.900°$ $\beta = 114.437°$ $\gamma = 89.988°$
Neutron single crystal refinement, $R_w = 0.056$

REFERENCE: K. Ståhl, Å. Kvick and S. Ghose,
Zeolites **9** 303–311 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	11.29	7.836	2	45.2	2	1	1	35.58	2.523	2	8.8	2	-2	0	43.23	2.093	2	0.6
0	0	1	12.80	6.917	2	30.6	2	-1	1	35.64	2.519	2	9.3	0	1	3	43.25	2.092	2	0.4
-1	0	1	13.11	6.754	2	16.1	-1	0	3	35.76	2.511	2	0.3	0	-1	3	43.32	2.089	2	0.7
1	0	1	20.34	4.366	2	31.3	-3	-1	1	36.20	2.482	2	18.6	-3	1	3	44.17	2.050	2	4.0
-2	0	1	20.93	4.244	2	9.7	-3	1	1	36.21	2.481	2	18.4	-3	-1	3	44.21	2.049	2	4.1
1	1	0	21.21	4.189	2	69.7	0	2	0	36.27	2.477	2	43.5	0	2	2	44.97	2.016	2	4.5
1	-1	0	21.23	4.185	2	68.2	1	1	2	37.17	2.419	2	1.9	0	-2	2	45.06	2.012	2	3.6
0	1	1	22.05	4.031	2	0.6	1	-1	2	37.23	2.415	2	2.5	1	0	3	45.36	1.999	2	7.5
0	-1	1	22.09	4.024	2	0.5	1	2	0	38.09	2.363	2	0.5	-2	2	2	45.38	1.998	2	4.9
-1	1	1	22.24	3.997	2	5.4	-3	1	2	38.10	2.362	2	3.9	2	-1	2	45.43	1.996	2	0.4
-1	-1	1	22.27	3.993	2	4.6	1	-2	0	38.11	2.361	2	0.5	-2	-2	2	45.43	1.996	2	4.3
2	0	0	22.69	3.918	2	2.4	-3	-1	2	38.12	2.361	2	4.5	3	1	1	45.70	1.985	2	4.3
-1	0	2	23.43	3.797	2	9.3	0	2	1	38.58	2.333	2	1.5	3	-1	1	45.75	1.983	2	4.4
0	0	2	25.76	3.458	2	100.0	0	-2	1	38.63	2.330	2	1.3	4	0	0	46.35	1.959	2	7.0
-2	0	2	26.39	3.377	2	78.4	-1	2	1	38.70	2.326	2	1.5	-4	-1	1	46.39	1.957	2	0.9
1	1	1	27.20	3.279	2	25.4	-1	-2	1	38.73	2.325	2	1.7	-4	1	1	46.41	1.956	2	0.8
1	-1	1	27.25	3.273	2	23.3	3	1	0	38.96	2.312	2	1.1	-4	1	2	46.55	1.951	2	0.7
-2	1	1	27.67	3.223	2	20.0	3	-1	0	39.00	2.310	2	1.7	-4	-1	2	46.56	1.951	2	0.6
-2	-1	1	27.68	3.223	2	20.4	0	0	3	39.07	2.306	2	1.0	-4	0	3	46.81	1.941	2	2.2
2	1	0	29.04	3.075	2	13.5	-1	1	3	40.24	2.241	2	1.9	-2	0	4	47.92	1.898	2	15.0
2	-1	0	29.07	3.072	2	14.9	-1	-1	3	40.30	2.238	2	2.0	2	2	1	48.07	1.893	2	1.8
-1	1	2	29.62	3.016	2	0.6	-2	1	3	40.56	2.224	2	0.4	2	-2	1	48.15	1.890	2	1.7
-1	-1	2	29.67	3.011	2	1.0	-2	-1	3	40.61	2.221	2	0.6	-3	-2	1	48.57	1.875	2	2.7
2	0	1	30.52	2.929	2	5.9	3	0	1	41.71	2.165	2	0.1	-3	2	1	48.58	1.874	2	2.6
-3	0	1	31.20	2.867	2	8.7	1	2	1	41.90	2.156	2	0.9	-1	0	4	49.03	1.858	2	0.5
0	1	2	31.52	2.838	2	0.7	1	-2	1	41.97	2.153	2	1.0	1	1	3	49.11	1.855	2	6.9
0	-1	2	31.58	2.833	2	0.7	-2	2	1	42.24	2.139	2	1.0	1	-1	3	49.18	1.853	2	6.0
-2	1	2	32.06	2.792	2	2.7	-2	-2	1	42.25	2.139	2	1.3	1	-2	2	49.42	1.844	2	0.1
-2	-1	2	32.09	2.789	2	3.0	-4	0	1	42.44	2.130	2	0.1	-3	0	4	49.76	1.832	2	0.4
1	0	2	32.33	2.769	2	0.1	2	2	0	43.19	2.095	2	0.6							

Bikitaite

BIK



BOG Boggsite

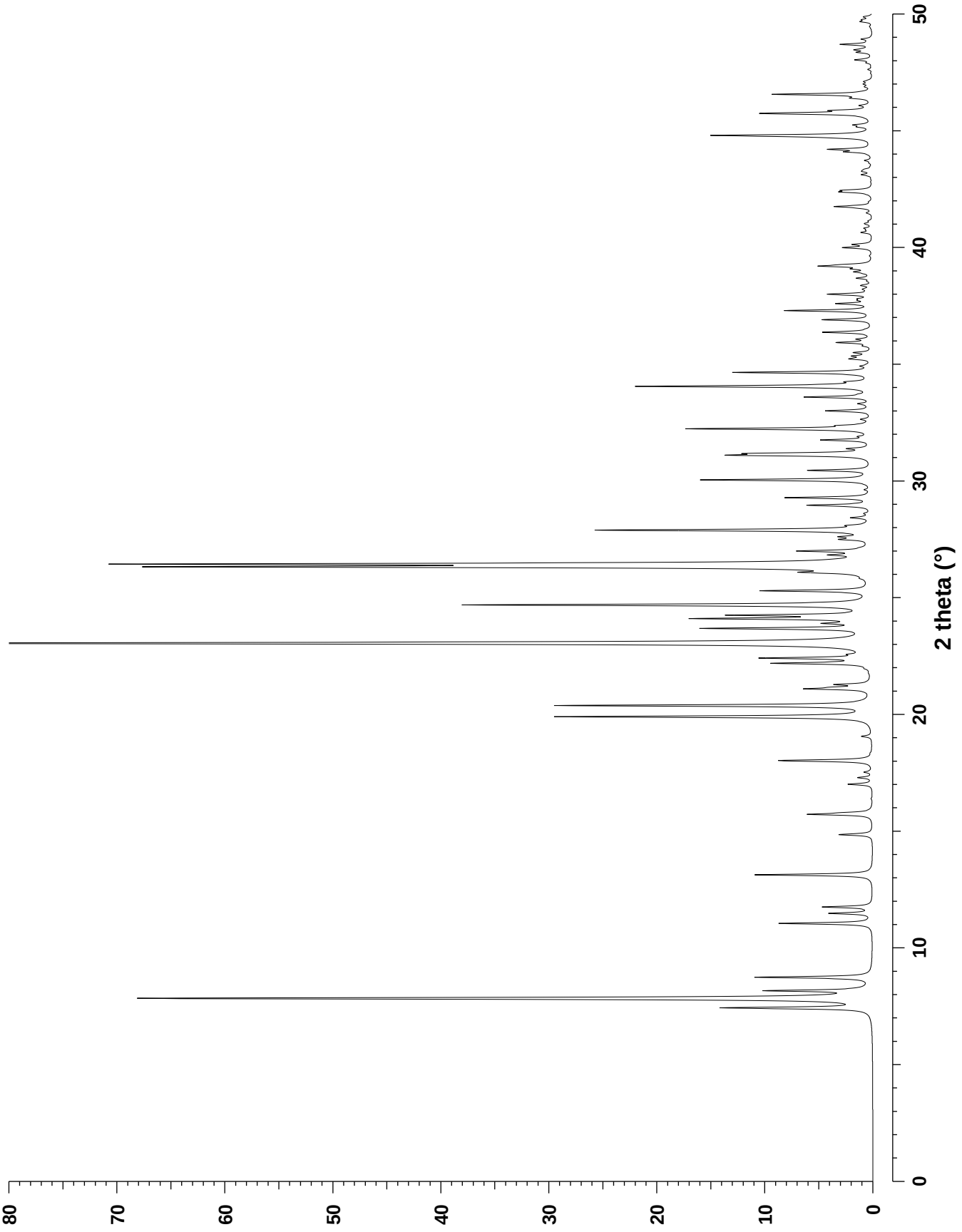
CHEMICAL COMPOSITION: $|Na_{2.9}Ca_{7.8}(H_2O)_{70}|\ [Si_{77.5}Al_{18.3}O_{192}]$
Goble area, Oregon, U.S.A.

REFINED COMPOSITION: $|(H_2O)_{137.04}|\ [Si_{77.76}Al_{18.24}O_{192}]$

CRYSTAL DATA: *Imma* (No. 74)
$a = 20.236$ Å $b = 23.798$ Å $c = 12.798$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.094$

REFERENCE: J. J. Pluth and J. V. Smith,
American Mineralogist **75** 501–507 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	7.43	11.899	2	13.6	2	6	2	27.89	3.198	8	19.0	3	2	5	38.37	2.346	8	0.5
0	1	1	7.84	11.271	4	68.2	0	5	3	28.09	3.177	4	1.5	8	4	0	38.68	2.328	4	1.3
1	0	1	8.17	10.816	4	9.2	5	3	2	28.42	3.141	8	1.7	6	5	3	38.95	2.312	8	1.3
2	0	0	8.74	10.118	2	10.8	4	6	0	28.60	3.121	4	0.5	7	5	2	39.08	2.305	8	1.1
1	2	1	11.05	8.004	8	8.7	0	2	4	28.90	3.090	4	0.7	7	6	1	39.20	2.298	8	4.4
2	2	0	11.48	7.708	4	3.9	3	4	3	28.96	3.083	8	5.7	3	8	3	39.26	2.295	8	1.5
2	1	1	11.75	7.529	8	4.6	2	0	4	29.28	3.051	4	8.0	0	5	5	39.99	2.254	4	2.7
0	3	1	13.13	6.742	4	11.0	0	8	0	30.04	2.975	2	15.8	0	9	3	40.12	2.247	4	1.7
3	0	1	14.85	5.967	4	3.0	5	0	3	30.44	2.936	4	1.6	3	4	5	40.63	2.220	8	0.4
0	2	2	15.72	5.636	4	5.7	1	3	4	30.45	2.936	8	4.4	5	5	4	40.64	2.220	8	0.5
2	3	1	15.79	5.611	8	1.8	1	6	3	31.10	2.875	8	11.4	3	10	1	40.82	2.210	8	0.7
1	4	1	17.01	5.213	8	2.3	3	1	4	31.17	2.870	8	9.1	8	1	3	41.68	2.167	8	0.6
2	4	0	17.29	5.129	4	1.3	5	2	3	31.38	2.851	8	1.8	5	0	5	41.75	2.163	4	3.2
4	0	0	17.53	5.059	2	0.7	0	4	4	31.75	2.818	4	4.2	0	11	1	42.37	2.133	4	2.5
2	2	2	18.02	4.924	8	8.8	4	6	2	31.90	2.805	8	0.8	2	8	4	42.44	2.130	8	2.3
4	2	0	19.06	4.656	4	1.0	5	5	2	32.23	2.778	8	17.2	8	3	3	43.11	2.098	8	0.9
0	5	1	19.90	4.461	4	29.4	5	6	1	32.37	2.766	8	2.1	5	9	2	43.25	2.092	8	0.7
0	4	2	20.38	4.357	4	29.4	7	2	1	32.63	2.744	8	0.5	7	3	4	43.72	2.071	8	0.6
3	4	1	21.09	4.213	8	5.6	3	3	4	32.98	2.716	8	1.0	4	9	3	44.09	2.054	8	2.1
0	1	3	21.16	4.199	4	2.3	2	4	4	33.00	2.715	8	3.5	1	3	6	44.20	2.049	8	1.7
1	0	3	21.28	4.174	4	3.0	4	5	3	33.30	2.690	8	0.8	3	6	5	44.20	2.049	8	2.0
3	3	2	22.19	4.007	8	8.4	3	6	3	33.59	2.668	8	5.5	1	9	4	44.68	2.028	8	1.0
2	4	2	22.21	4.002	8	0.6	6	4	2	33.60	2.667	8	0.6	3	1	6	44.72	2.026	8	0.9
4	0	2	22.40	3.969	4	0.8	5	4	3	34.05	2.633	8	21.0	5	10	1	44.74	2.026	8	1.0
0	6	0	22.41	3.966	2	9.0	1	5	4	34.05	2.633	8	0.7	10	0	0	44.79	2.024	2	14.2
1	2	3	22.57	3.939	8	1.0	6	1	3	34.10	2.630	8	0.6	0	4	6	45.16	2.008	4	1.0
5	0	1	23.05	3.859	4	100.0	7	1	2	34.24	2.618	8	1.6	2	7	5	45.24	2.004	8	1.3
4	4	0	23.08	3.854	4	0.5	0	9	1	34.64	2.590	4	12.9	8	0	4	45.72	1.984	4	6.4
0	3	3	23.68	3.757	4	15.1	6	6	0	34.92	2.569	4	0.7	0	12	0	45.75	1.983	2	5.2
1	6	1	23.90	3.724	8	3.2	7	4	1	35.22	2.548	8	1.7	8	5	3	45.86	1.979	8	3.0
2	6	0	24.10	3.693	4	15.7	0	1	5	35.27	2.545	4	0.6	3	3	6	46.07	1.970	8	0.8
5	2	1	24.25	3.671	8	12.1	1	0	5	35.35	2.539	4	1.5	8	2	4	46.39	1.957	8	1.4
3	0	3	24.69	3.605	4	37.9	8	0	0	35.49	2.530	2	1.6	3	9	4	46.55	1.951	8	8.9
2	3	3	25.29	3.522	8	10.1	6	3	3	35.78	2.510	8	0.6	9	6	1	46.99	1.934	8	0.6
1	4	3	26.08	3.417	8	4.4	7	3	2	35.92	2.500	8	3.2	10	0	2	47.10	1.929	4	0.5
5	1	2	26.32	3.386	8	61.3	0	6	4	36.07	2.490	4	1.2	5	6	5	47.90	1.899	8	0.5
0	6	2	26.44	3.371	4	64.6	3	5	4	36.36	2.471	8	4.4	0	12	2	48.03	1.894	4	1.5
3	5	2	26.83	3.323	8	2.7	0	3	5	36.90	2.436	4	4.6	8	4	4	48.35	1.882	8	1.1
3	6	1	26.99	3.303	8	5.5	5	7	2	37.29	2.411	8	8.1	0	6	6	48.46	1.879	4	1.4
4	4	2	27.01	3.301	8	1.0	7	0	3	37.58	2.393	4	0.8	3	5	6	48.69	1.870	8	2.7
6	2	0	27.49	3.245	4	2.4	5	3	4	37.59	2.393	8	2.2	2	12	2	48.92	1.862	8	0.9
5	4	1	27.55	3.237	8	0.5	6	6	2	37.73	2.384	8	0.8	5	3	6	49.66	1.836	8	0.5
6	1	1	27.61	3.231	8	1.5	0	10	0	37.80	2.380	2	0.9	10	4	2	49.67	1.835	8	0.5
4	1	3	27.61	3.231	8	0.6	2	3	5	37.99	2.368	8	3.7	8	7	3	49.75	1.833	8	0.8
0	0	4	27.88	3.200	2	7.0	5	8	1	38.20	2.356	8	0.5	5	11	2	49.87	1.828	8	0.7


0
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2 theta (°)
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80

BPH Beryllophosphate-H

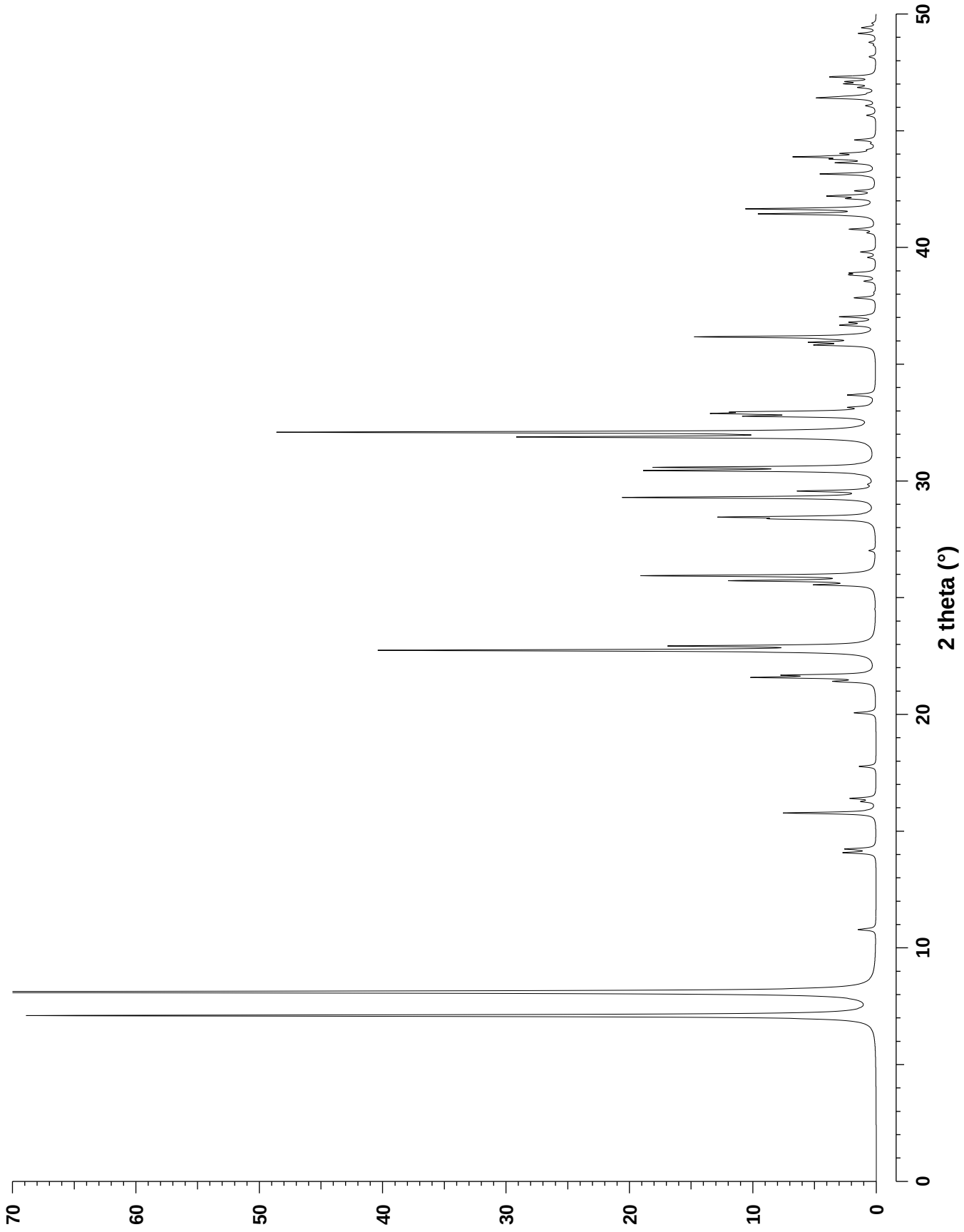
CHEMICAL COMPOSITION: $|Na_7K_7(H_2O)_{20}|\ [Be_{14}P_{14}O_{56}]$

REFINED COMPOSITION: $|Na_{8.36}K_{5.49}(H_2O)_{30.48}|\ [Be_{14}P_{14}O_{56}]$

CRYSTAL DATA: $P321$ (No. 150)
$a = 12.5815$ Å $b = 12.5815$ Å $c = 12.4508$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.192$, $R_F = 0.106$

REFERENCE: G. Harvey, Ch. Baerlocher and T. Wroblewski,
Z. Kristallogr. **201** 113–123 (1992).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	7.10	12.451	2	68.8	0	3	3	32.77	2.733	6	5.6	3	3	0	43.14	2.097	6	4.5
1	0	0	8.11	10.896	6	100.0	4	0	0	32.88	2.724	6	10.1	0	0	6	43.62	2.075	2	3.0
1	0	1	10.79	8.200	6	0.1	1	3	2	32.95	2.719	12	4.4	3	3	1	43.78	2.068	12	2.7
0	1	1	10.79	8.200	6	1.3	3	1	2	32.95	2.719	12	4.3	1	4	3	43.88	2.063	12	1.4
1	1	0	14.08	6.291	6	2.6	2	0	4	33.15	2.703	6	1.4	4	1	3	43.88	2.063	12	4.7
0	0	2	14.23	6.225	2	2.4	0	2	4	33.15	2.703	6	0.2	0	5	2	44.02	2.057	6	0.7
1	1	1	15.78	5.615	12	7.5	4	0	1	33.68	2.661	6	0.4	5	0	2	44.02	2.057	6	1.6
2	0	0	16.27	5.448	6	1.1	0	4	1	33.68	2.661	6	1.9	0	3	5	44.09	2.054	6	0.1
0	1	2	16.40	5.405	6	0.5	2	2	3	35.82	2.507	12	4.3	4	0	4	44.18	2.050	6	0.3
1	0	2	16.40	5.405	6	1.5	3	2	0	35.93	2.500	12	4.4	0	4	4	44.18	2.050	6	0.2
2	0	1	17.77	4.991	6	1.3	4	0	2	35.99	2.496	6	0.2	1	0	6	44.44	2.038	6	0.3
1	1	2	20.07	4.425	12	1.8	0	0	5	36.07	2.490	2	1.6	2	4	1	44.60	2.032	12	0.2
0	0	3	21.41	4.150	2	2.9	1	2	4	36.17	2.483	12	9.1	4	2	1	44.60	2.032	12	1.5
2	1	0	21.58	4.118	12	9.1	2	1	4	36.17	2.483	12	5.2	3	3	2	45.65	1.987	12	0.7
2	0	2	21.68	4.100	6	2.6	3	2	1	36.67	2.451	12	1.9	1	1	6	46.06	1.971	12	0.8
0	2	2	21.68	4.100	6	3.8	2	3	1	36.67	2.451	12	0.8	5	1	0	46.40	1.957	12	4.1
2	1	1	22.74	3.910	12	15.5	3	1	3	36.79	2.443	12	1.5	2	4	2	46.45	1.955	12	0.3
1	2	1	22.74	3.910	12	24.3	1	3	3	36.79	2.443	12	0.4	4	2	2	46.45	1.955	12	1.4
1	0	3	22.93	3.878	6	14.3	0	1	5	37.03	2.428	6	2.9	2	2	5	46.51	1.952	12	0.4
0	1	3	22.93	3.878	6	0.9	4	1	0	37.84	2.378	12	1.8	3	2	4	46.60	1.949	12	0.2
3	0	1	25.55	3.487	6	4.3	0	3	4	38.07	2.363	6	0.1	2	3	4	46.60	1.949	12	0.2
1	1	3	25.72	3.464	12	11.2	1	4	1	38.55	2.335	12	0.4	2	0	6	46.85	1.939	6	1.1
2	1	2	25.94	3.435	12	12.6	4	1	1	38.55	2.335	12	0.6	0	2	6	46.85	1.939	6	0.2
1	2	2	25.94	3.435	12	6.1	2	3	2	38.82	2.320	12	0.3	5	1	1	47.00	1.933	12	0.6
0	2	3	27.01	3.301	6	0.1	3	2	2	38.82	2.320	12	1.5	1	5	1	47.00	1.933	12	1.7
2	0	3	27.01	3.301	6	0.4	1	1	5	38.90	2.315	12	1.8	0	5	3	47.10	1.929	6	1.7
2	2	0	28.37	3.145	6	6.3	0	4	3	39.57	2.277	6	0.6	5	0	3	47.10	1.929	6	0.4
0	3	2	28.45	3.137	6	9.4	2	0	5	39.80	2.265	6	0.5	3	1	5	47.30	1.922	12	1.8
3	0	2	28.45	3.137	6	2.1	0	2	5	39.80	2.265	6	0.7	1	3	5	47.30	1.922	12	1.8
2	2	1	29.29	3.050	12	20.4	1	4	2	40.62	2.221	12	0.6	4	1	4	48.16	1.889	12	0.5
3	1	0	29.56	3.022	12	5.9	2	2	4	40.78	2.212	12	2.1	3	3	3	48.65	1.872	12	0.2
1	0	4	29.85	2.993	6	0.2	5	0	0	41.43	2.179	6	9.2	1	5	2	48.78	1.867	12	0.3
0	1	4	29.85	2.993	6	0.1	3	1	4	41.65	2.168	12	3.7	5	1	2	48.78	1.867	12	0.2
1	3	1	30.44	2.937	12	1.4	1	3	4	41.65	2.168	12	6.6	2	1	6	49.16	1.853	12	0.6
3	1	1	30.44	2.937	12	16.1	0	5	1	42.09	2.147	6	0.6	1	2	6	49.16	1.853	12	0.9
2	1	3	30.58	2.923	12	10.8	5	0	1	42.09	2.147	6	1.3	4	2	3	49.41	1.845	12	1.0
1	2	3	30.58	2.923	12	5.9	2	3	3	42.20	2.141	12	2.1	2	4	3	49.41	1.845	12	0.2
2	2	2	31.88	2.807	12	27.3	3	2	3	42.20	2.141	12	1.5	4	0	5	49.60	1.838	6	0.1
1	1	4	32.08	2.790	12	47.5	1	2	5	42.42	2.131	12	0.5	0	4	5	49.60	1.838	6	0.2
3	0	3	32.77	2.733	6	3.4	2	1	5	42.42	2.131	12	1.0							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2 theta (°)
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70

BRE Brewsterite

CHEMICAL COMPOSITION: $|K_{0.02}Ba_{0.48}Sr_{1.42}(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$
Strontian, Argyll, Scotland

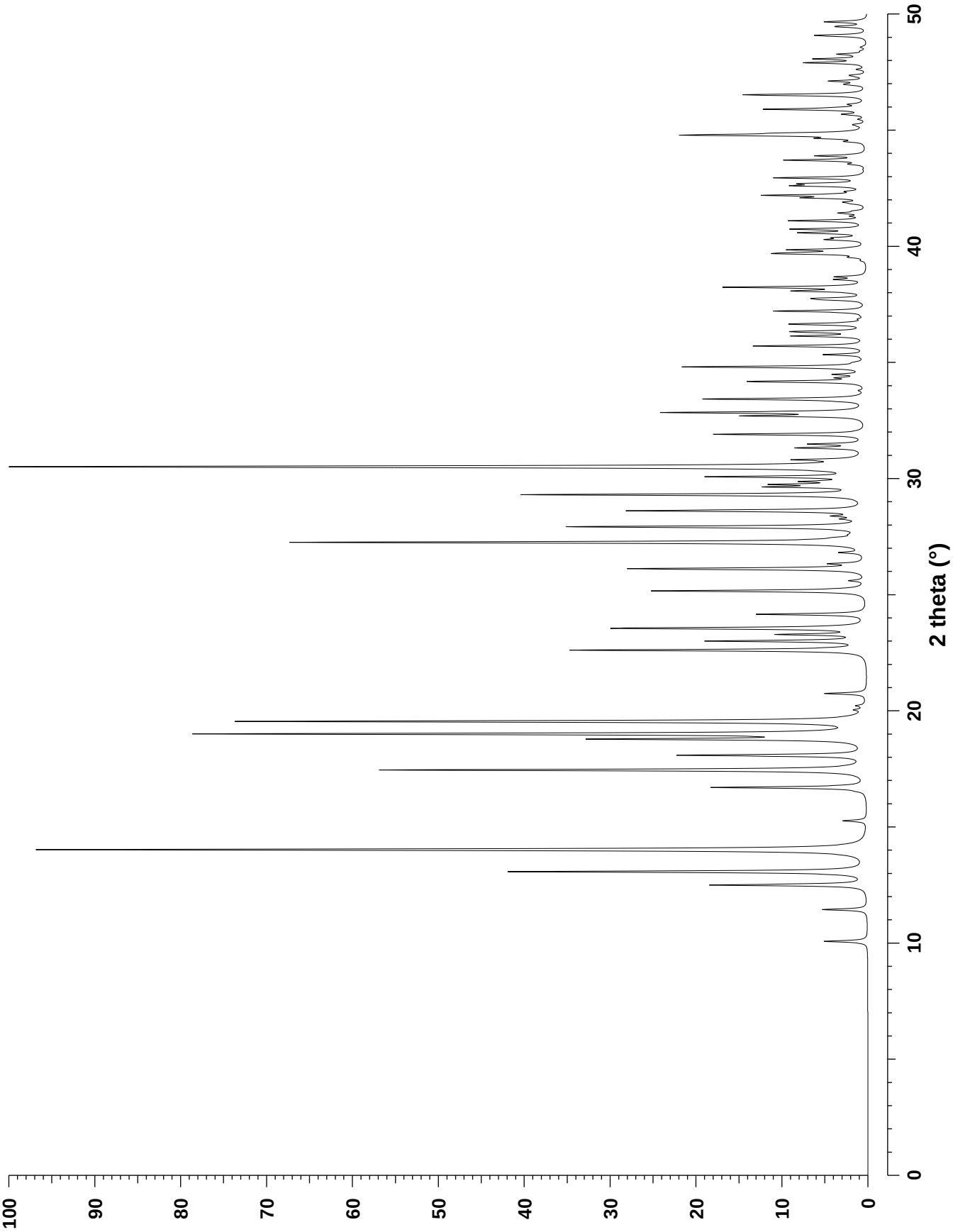
REFINED COMPOSITION: $|Ba_{0.52}Sr_{1.48}(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 6.793$ Å $b = 17.573$ Å $c = 7.759$ Å
$\alpha = 90°$ $\beta = 94.54°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: J. L. Schlenker, J. J. Pluth and J. V. Smith,
Acta Cryst. **B33** 2907–2910 (1977).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	10.07	8.786	2	5.3	1	5	1	31.31	2.857	4	7.9	3	2	0	41.29	2.186	4	1.4
0	0	1	11.44	7.735	2	5.4	1	3	2	31.48	2.841	4	6.4	1	3	3	41.42	2.180	4	3.0
0	1	1	12.50	7.079	4	18.8	-2	3	1	31.90	2.806	4	18.3	1	6	2	41.51	2.176	4	1.1
1	0	0	13.07	6.772	2	43.0	0	6	1	32.69	2.739	4	13.7	-2	6	1	41.83	2.159	4	1.2
1	1	0	14.02	6.319	4	100.0	-1	4	2	32.84	2.727	4	23.8	-1	4	3	41.89	2.157	4	2.0
0	2	1	15.26	5.806	4	2.9	1	6	0	33.33	2.688	4	1.1	-3	2	1	42.08	2.147	4	6.5
-1	0	1	16.70	5.307	2	18.6	2	4	0	33.41	2.682	4	9.9	2	4	2	42.19	2.142	4	11.7
-1	1	1	17.45	5.081	4	58.5	2	3	1	33.42	2.681	4	10.1	-2	0	3	42.35	2.134	2	1.6
1	0	1	18.08	4.906	2	22.5	-2	0	2	33.78	2.654	2	0.6	3	0	1	42.60	2.122	2	7.7
1	1	1	18.78	4.725	4	31.1	-2	1	2	34.17	2.624	4	14.1	-2	1	3	42.67	2.119	4	2.3
0	3	1	19.00	4.670	4	79.8	1	4	2	34.33	2.612	4	2.8	-2	5	2	42.69	2.118	4	4.6
-1	2	1	19.54	4.543	4	75.6	0	5	2	34.48	2.601	4	3.5	3	3	0	42.94	2.106	4	10.3
1	3	0	20.04	4.430	4	1.1	0	0	3	34.80	2.578	2	22.0	0	5	3	43.53	2.079	4	1.7
0	4	0	20.21	4.393	2	1.0	-1	6	1	34.99	2.564	4	0.8	-3	3	1	43.70	2.071	4	1.9
1	2	1	20.74	4.284	4	5.0	-2	2	2	35.33	2.540	4	5.0	1	4	3	43.70	2.071	4	7.7
-1	3	1	22.61	3.933	4	35.6	1	6	1	35.70	2.515	4	13.5	3	2	1	43.89	2.063	4	5.9
0	0	2	23.00	3.867	2	18.9	2	4	1	36.13	2.486	4	8.6	-1	7	2	44.50	2.036	4	2.0
0	4	1	23.28	3.820	4	10.0	-1	0	3	36.29	2.476	2	1.4	-1	8	1	44.64	2.030	4	4.4
0	1	2	23.55	3.777	4	30.4	0	2	3	36.31	2.474	4	4.9	-1	5	3	44.78	2.024	4	20.8
1	3	1	23.65	3.761	4	0.7	-1	5	2	36.33	2.472	4	3.4	-3	0	2	44.86	2.020	2	7.3
1	4	0	24.15	3.686	4	13.2	2	0	2	36.63	2.453	2	5.0	1	8	1	45.23	2.005	4	1.1
0	2	2	25.16	3.540	4	25.9	-1	1	3	36.66	2.451	4	5.5	3	3	1	45.46	1.995	4	0.8
-1	0	2	25.60	3.479	2	1.9	2	5	0	36.86	2.438	4	0.6	1	7	2	45.67	1.987	4	2.6
-1	1	2	26.11	3.413	4	28.6	-2	3	2	37.20	2.417	4	11.2	-3	4	1	45.89	1.977	4	10.6
2	0	0	26.32	3.386	2	0.6	0	7	1	37.67	2.388	4	1.4	2	0	3	45.90	1.977	2	1.5
-1	4	1	26.33	3.384	4	3.2	1	5	2	37.70	2.386	4	3.1	-2	7	1	45.97	1.974	4	1.6
2	1	0	26.81	3.325	4	2.7	-1	2	3	37.75	2.383	4	4.9	-3	2	2	46.10	1.969	4	1.7
1	4	1	27.25	3.273	4	69.2	-2	5	1	38.06	2.365	4	7.0	1	5	3	46.51	1.953	4	14.9
1	0	2	27.45	3.249	2	1.3	2	2	2	38.09	2.363	4	1.8	0	6	3	46.95	1.935	4	1.8
-1	2	2	27.58	3.235	4	0.6	1	7	0	38.23	2.354	4	16.8	0	0	4	46.99	1.934	2	1.1
0	5	1	27.88	3.200	4	5.7	0	6	2	38.56	2.335	4	3.4	2	7	1	47.10	1.929	4	2.4
-2	0	1	27.92	3.196	2	10.0	1	1	3	38.68	2.328	4	3.5	2	2	3	47.11	1.929	4	2.0
1	1	2	27.92	3.195	4	23.0	-1	3	3	39.52	2.280	4	1.6	0	1	4	47.29	1.922	4	0.6
2	2	0	28.25	3.159	4	2.1	-2	4	2	39.68	2.271	4	9.5	-2	4	3	47.35	1.920	4	1.8
-2	1	1	28.38	3.144	4	3.0	-1	7	1	39.72	2.269	4	1.4	-3	3	2	47.61	1.910	4	0.8
1	5	0	28.61	3.119	4	28.6	1	2	3	39.73	2.269	4	1.9	-1	0	4	47.89	1.899	2	4.8
1	2	2	29.30	3.048	4	41.2	2	3	2	39.84	2.263	4	8.6	3	5	0	47.89	1.899	4	2.6
2	0	1	29.63	3.015	2	10.4	3	0	0	39.94	2.257	2	0.7	0	9	1	48.06	1.893	4	6.0
-2	2	1	29.74	3.003	4	9.3	-1	6	2	40.25	2.241	4	0.7	3	0	2	48.26	1.886	2	3.2
-1	3	2	29.87	2.991	4	5.9	3	1	0	40.28	2.239	4	3.8	-1	8	2	49.04	1.857	4	1.4
2	1	1	30.07	2.972	4	18.0	1	7	1	40.36	2.235	4	3.1	-1	2	4	49.07	1.857	4	5.5
2	3	0	30.49	2.931	4	56.5	0	4	3	40.57	2.224	4	7.6	3	2	2	49.44	1.844	4	1.5
-1	5	1	30.51	2.930	4	41.1	2	6	0	40.73	2.215	4	8.6	2	8	0	49.46	1.843	4	2.5
0	6	0	30.52	2.929	2	13.8	-3	1	1	41.08	2.197	4	0.8	0	3	4	49.65	1.836	4	4.2
0	4	2	30.80	2.903	4	7.1	0	8	0	41.09	2.197	2	8.5	-3	4	2	49.67	1.836	4	1.0

Brewsterite BRE



CAN Cancrinite

CHEMICAL COMPOSITION: $|Na_7Ca_{0.9}(CO_3)_{1.4}(H_2O)_{2.1}|\ [Si_6Al_6O_{24}]$
Synthetic crystal.

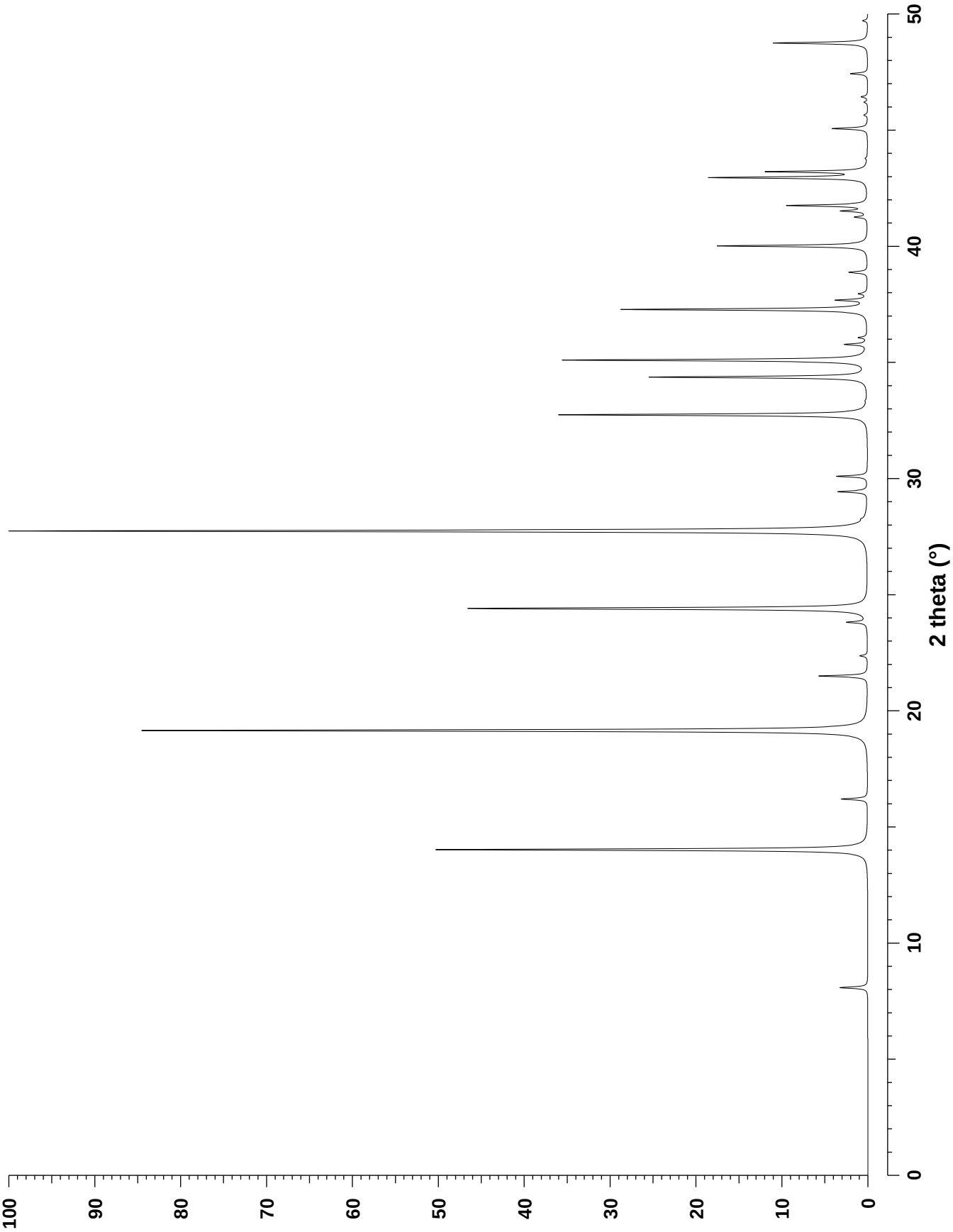
REFINED COMPOSITION: $|Na_8(CO_3)_{1.2}(H_2O)_2|\ [Si_6Al_6O_{24}]$

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 12.635$ Å $b = 12.635$ Å $c = 5.115$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.04$

REFERENCE: Y. I. Smolin, Y. F. Shepelev, I. K. Butikova and I. B. Kobyakov, *Kristallografiya* **26** 63–66 (1981).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	8.08	10.942	6	3.9	2	2	1	33.34	2.688	12	0.1	2	1	2	41.51	2.175	12	1.9
1	1	0	14.02	6.317	6	59.5	3	1	1	34.36	2.610	12	10.2	1	4	1	41.75	2.164	12	6.7
2	0	0	16.20	5.471	6	3.7	1	3	1	34.36	2.610	12	19.8	4	1	1	41.75	2.164	12	4.4
1	0	1	19.15	4.634	12	100.0	0	0	2	35.09	2.557	2	42.0	3	3	0	42.95	2.106	6	21.6
1	2	0	21.49	4.136	6	0.6	3	2	0	35.77	2.510	6	1.3	3	0	2	43.20	2.094	12	13.6
2	1	0	21.49	4.136	6	6.1	2	3	0	35.77	2.510	6	1.7	2	4	0	43.78	2.068	6	0.2
1	1	1	22.36	3.975	12	1.0	1	0	2	36.06	2.490	12	1.2	5	0	1	45.06	2.012	12	4.9
2	0	1	23.81	3.736	12	2.7	4	0	1	37.27	2.412	12	34.0	2	2	2	45.64	1.988	12	0.5
3	0	0	24.40	3.647	6	55.1	1	4	0	37.67	2.388	6	3.4	5	1	0	46.19	1.965	6	0.5
1	2	1	27.74	3.216	12	56.9	4	1	0	37.67	2.388	6	0.7	3	1	2	46.43	1.956	12	0.4
2	1	1	27.74	3.216	12	61.4	1	1	2	37.95	2.371	12	1.1	1	3	2	46.43	1.956	12	0.5
2	2	0	28.25	3.159	6	0.3	2	0	2	38.87	2.317	12	2.6	2	4	1	47.42	1.917	12	1.3
3	1	0	29.43	3.035	6	0.9	2	3	1	40.01	2.254	12	10.4	4	2	1	47.42	1.917	12	1.1
1	3	0	29.43	3.035	6	3.2	3	2	1	40.01	2.254	12	10.4	4	0	2	48.74	1.868	12	13.1
3	0	1	30.09	2.970	12	4.3	5	0	0	41.25	2.188	6	1.7	1	5	1	49.70	1.835	12	0.5
4	0	0	32.74	2.736	6	42.6	1	2	2	41.51	2.175	12	1.5	5	1	1	49.70	1.835	12	0.3

Cancrinite CAN



Tiptopite

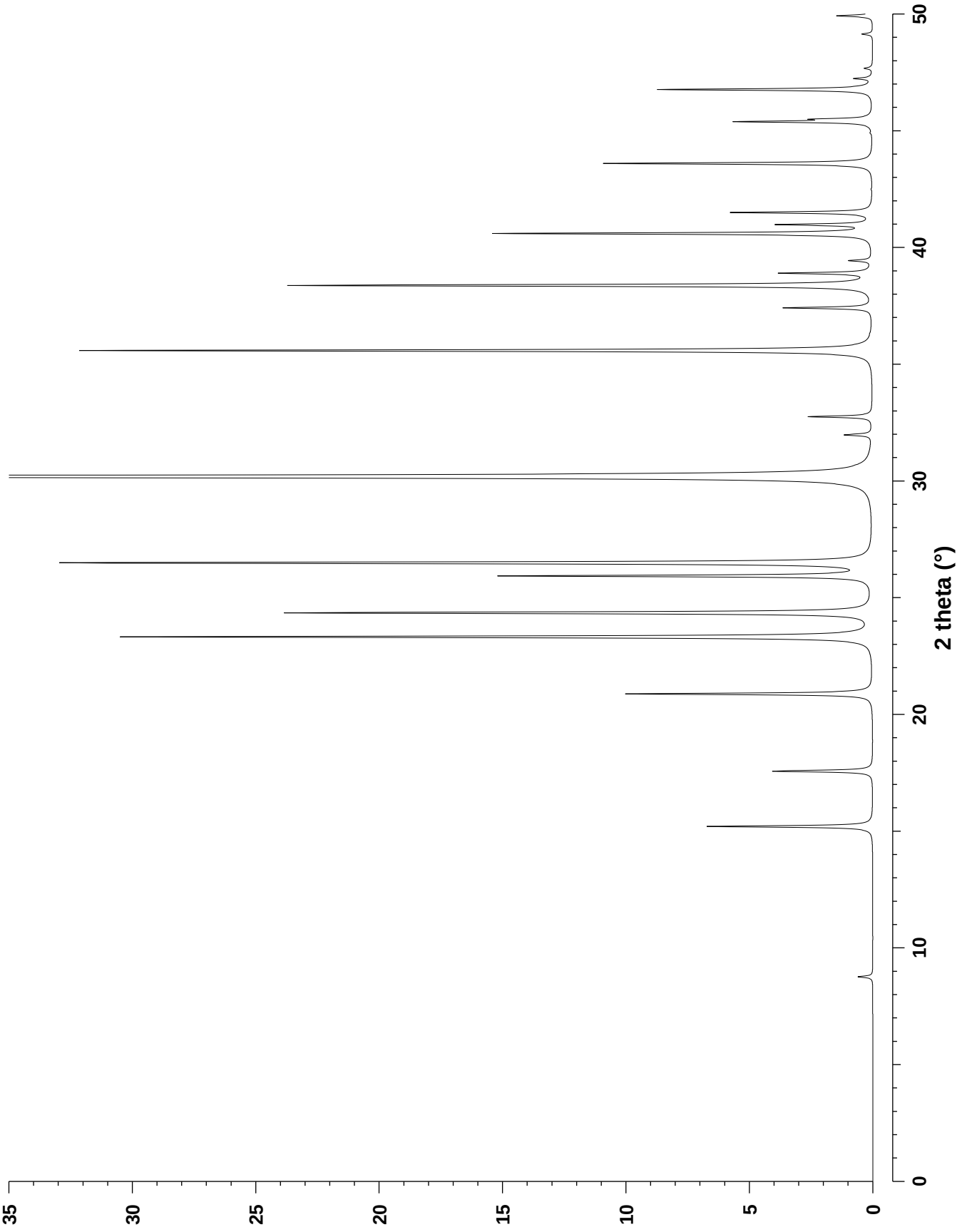
CHEMICAL COMPOSITION: $|K_2Li_{2.9}Na_{1.7}Ca_{0.7}(H_2O)_{1.3}(OH)_2\square_{0.7}|\ [Be_6P_6O_{24}]$
$\square$ = cation vacancy
Tip Top Mine, Custer, S. Dakota, U.S.A.

REFINED COMPOSITION: $|Li_{2.9}Na_{1.7}K_2Ca_{0.7}O_6|\ [Be_6P_6O_{24}]$

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 11.655$ Å $b = 11.655$ Å $c = 4.692$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.048$

REFERENCE: D. R. Peacor, R. C. Rouse and J. H. Ahn,
American Mineralogist **72** 816–820 (1987).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	8.76	10.094	6	0.8	3	0	1	32.75	2.734	12	3.5	3	2	1	43.59	2.076	12	4.2
1	1	0	15.20	5.827	6	9.0	4	0	0	35.58	2.523	6	43.2	2	1	2	45.38	1.998	12	4.1
2	0	0	17.57	5.047	6	5.5	3	1	1	37.41	2.404	12	3.1	1	2	2	45.38	1.998	12	3.2
1	0	1	20.88	4.255	12	13.4	1	3	1	37.41	2.404	12	1.7	1	4	1	45.49	1.994	12	0.9
2	1	0	23.32	3.815	6	2.0	0	0	2	38.37	2.346	2	31.8	4	1	1	45.49	1.994	12	1.7
1	2	0	23.32	3.815	6	38.8	2	3	0	38.89	2.316	6	1.3	3	3	0	46.76	1.942	6	11.7
1	1	1	24.35	3.655	12	31.9	3	2	0	38.89	2.316	6	3.7	3	0	2	47.23	1.924	12	1.0
2	0	1	25.93	3.436	12	20.2	1	0	2	39.43	2.285	12	1.2	2	4	0	47.67	1.907	6	0.3
3	0	0	26.49	3.365	6	44.1	4	0	1	40.59	2.222	12	20.6	4	2	0	47.67	1.907	6	0.1
2	1	1	30.19	2.960	12	100.0	4	1	0	40.97	2.203	6	2.7	5	0	1	49.13	1.854	12	0.6
1	2	1	30.19	2.960	12	34.2	1	4	0	40.97	2.203	6	2.4	2	2	2	49.91	1.827	12	2.0
3	1	0	31.97	2.799	6	0.8	1	1	2	41.49	2.176	12	7.7							
1	3	0	31.97	2.799	6	0.7	2	3	1	43.59	2.076	12	10.5							


0
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2 theta (°)
35
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0

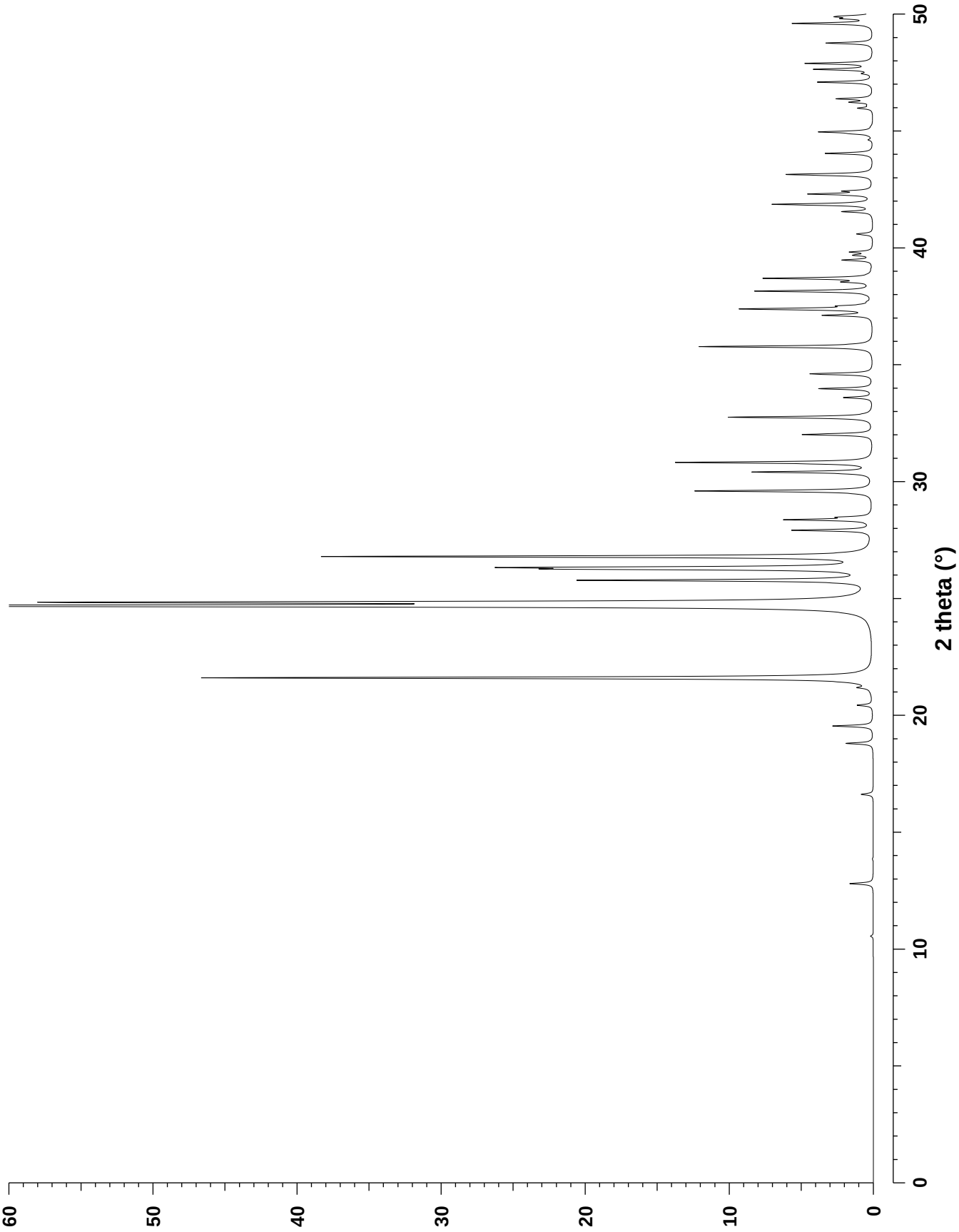
CHEMICAL COMPOSITION: $|Cs_4|\ [Si_{24}O_{48}]$

REFINED COMPOSITION: $|Cs_{3.26}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: *Ama*2 (No. 40)
$a = 16.776$ Å $b = 13.828$ Å $c = 5.021$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.0549$

REFERENCE: T. Araki,
Z. Kristallogr. **152** 207–213 (1980).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	10.55	8.388	2	0.2	4	4	0	33.59	2.668	4	2.1	7	1	1	42.29	2.137	8	4.5
0	2	0	12.80	6.914	2	1.7	4	3	1	33.97	2.639	8	3.9	3	6	0	42.42	2.131	4	1.8
2	2	0	16.62	5.335	4	0.9	6	2	0	34.60	2.592	4	4.5	4	5	1	43.12	2.098	8	4.3
0	1	1	18.80	4.720	4	2.0	0	0	2	35.77	2.510	2	12.5	8	0	0	43.14	2.097	2	2.4
1	1	1	19.54	4.543	8	2.9	0	5	1	37.11	2.422	4	3.4	4	2	2	44.03	2.057	8	3.4
3	2	0	20.43	4.348	4	1.1	5	4	0	37.35	2.408	4	1.8	0	4	2	44.61	2.031	4	0.3
4	0	0	21.18	4.194	2	0.7	6	1	1	37.38	2.406	8	6.7	4	6	0	44.87	2.020	4	1.0
2	1	1	21.60	4.113	8	48.3	2	0	2	37.39	2.405	4	1.7	1	4	2	44.95	2.017	8	3.7
3	1	1	24.68	3.607	8	100.0	1	5	1	37.51	2.398	8	1.8	2	4	2	45.97	1.974	8	1.0
4	2	0	24.83	3.586	4	53.4	5	3	1	37.69	2.387	8	0.1	7	4	0	46.08	1.970	4	0.2
0	4	0	25.77	3.457	2	20.8	0	2	2	38.14	2.360	4	8.4	5	5	1	46.22	1.964	8	1.5
0	3	1	26.25	3.396	4	17.8	1	2	2	38.53	2.337	8	1.8	7	3	1	46.37	1.958	8	2.6
1	4	0	26.32	3.386	4	22.3	2	5	1	38.69	2.327	8	7.8	5	2	2	47.08	1.930	8	4.0
1	3	1	26.79	3.328	8	39.4	1	6	0	39.47	2.283	4	2.2	8	1	1	47.44	1.916	8	0.6
2	4	0	27.91	3.196	4	5.7	2	2	2	39.68	2.272	8	1.3	3	4	2	47.63	1.909	8	4.1
2	3	1	28.36	3.147	8	6.1	7	2	0	39.81	2.264	4	1.6	5	6	0	47.88	1.900	4	4.8
4	1	1	28.47	3.135	8	1.9	3	5	1	40.58	2.223	8	1.0	6	0	2	48.75	1.868	4	3.4
5	2	0	29.59	3.019	4	12.8	2	6	0	40.59	2.222	4	0.2	0	7	1	49.59	1.838	4	5.7
3	4	0	30.40	2.940	4	8.6	3	2	2	41.54	2.174	8	1.7	6	5	1	49.80	1.831	8	1.8
3	3	1	30.81	2.902	8	14.1	6	4	0	41.54	2.174	4	0.4	4	4	2	49.88	1.828	8	1.9
6	0	0	32.01	2.796	2	5.1	6	3	1	41.85	2.158	8	7.2	1	7	1	49.91	1.827	8	0.7
5	1	1	32.75	2.735	8	10.4	4	0	2	41.94	2.154	4	0.2							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2 theta (°)
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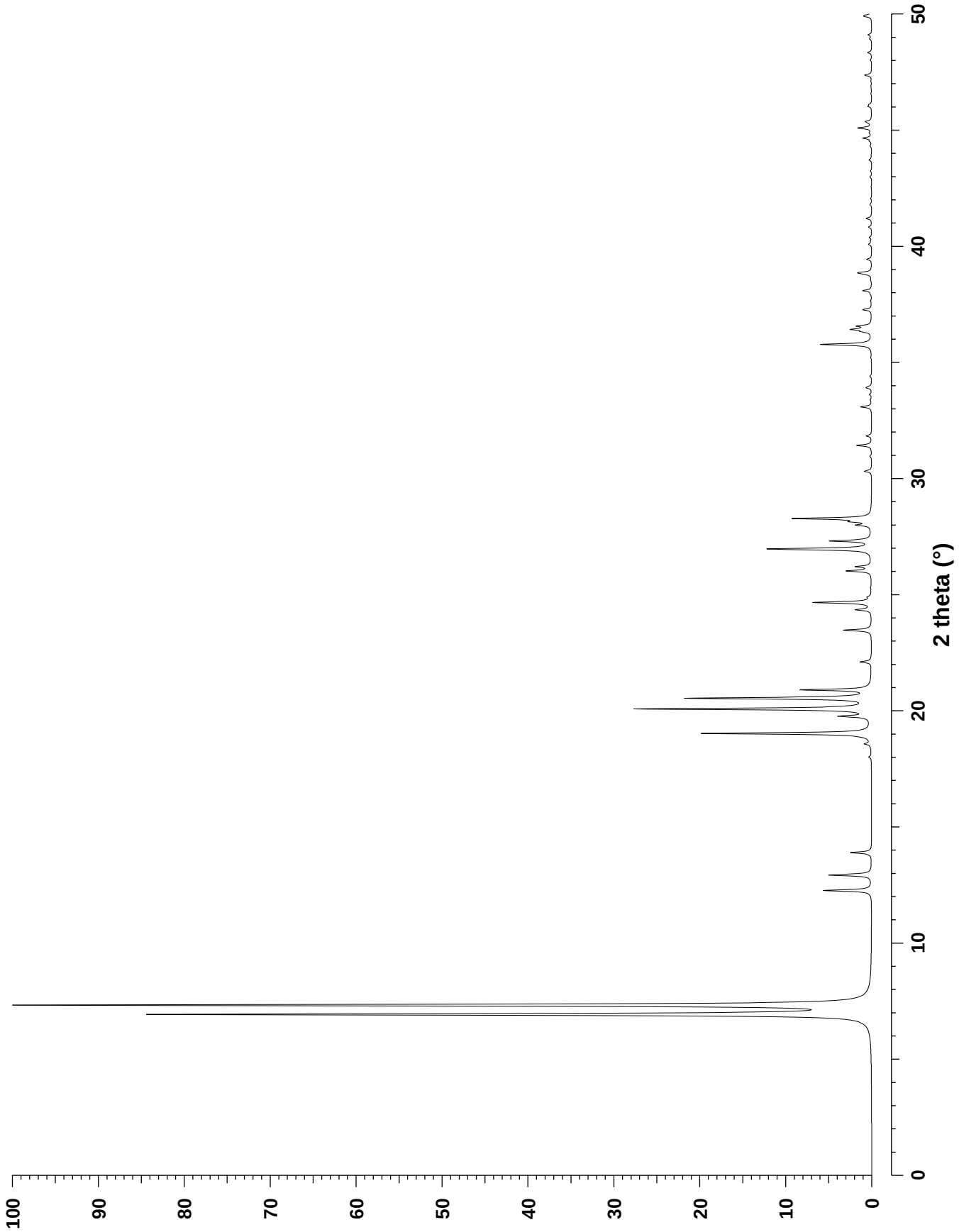
CHEMICAL COMPOSITION: $[Si_{32}O_{64}]$

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: *Imma* (No. 74)
$a = 13.695$ Å $b = 5.021$ Å $c = 25.497$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0875$, $R_{wp} = 0.1143$

REFERENCE: P. Wagner, M. Yoshikawa, M. Lavallo, K. Tsuji, M. Tsapatsis and M. E. Davis, *J. Chem. Soc., Chem. Commun.* 2179–2180 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	6.93	12.748	2	84.1	0	1	7	30.31	2.948	4	0.9	2	2	4	40.82	2.211	8	0.4
1	0	1	7.33	12.065	4	100.0	2	0	8	30.95	2.889	4	0.2	3	2	1	41.19	2.192	8	0.6
1	0	3	12.26	7.221	4	5.7	3	0	7	31.42	2.847	4	1.8	0	2	6	41.79	2.161	4	0.2
2	0	0	12.93	6.847	2	5.1	4	1	1	31.83	2.811	8	0.6	6	0	4	42.05	2.149	4	0.1
0	0	4	13.89	6.374	2	2.5	2	1	7	33.08	2.708	8	1.3	0	1	11	42.98	2.104	4	0.2
0	1	1	18.01	4.926	4	0.3	4	1	3	33.38	2.684	8	0.1	5	1	6	43.23	2.093	8	0.1
1	0	5	18.57	4.779	4	0.7	4	0	6	33.61	2.666	4	0.2	6	1	1	43.71	2.071	8	0.3
2	0	4	19.02	4.666	4	19.9	3	1	6	33.90	2.644	8	0.6	1	2	7	44.32	2.044	8	0.2
3	0	1	19.76	4.494	4	3.5	1	1	8	33.95	2.640	8	0.3	3	1	10	44.52	2.035	8	0.2
1	1	2	20.08	4.422	8	27.7	5	0	3	34.40	2.607	4	0.2	2	0	12	44.65	2.029	4	1.0
0	1	3	20.54	4.323	4	21.7	0	2	0	35.77	2.510	2	6.0	3	2	5	44.87	2.020	8	0.2
0	0	6	20.90	4.249	2	8.1	4	1	5	36.32	2.474	8	0.9	2	1	11	45.07	2.012	8	0.4
3	0	3	22.10	4.022	4	1.3	0	1	9	36.41	2.467	4	2.2	6	0	6	45.09	2.011	4	1.3
1	1	4	23.47	3.790	8	3.3	0	2	2	36.48	2.463	4	0.4	4	1	9	45.30	2.002	8	0.2
2	1	3	24.35	3.655	8	1.8	1	2	1	36.56	2.458	8	1.6	4	2	2	45.36	1.999	8	0.6
2	0	6	24.66	3.611	4	6.9	5	0	5	37.26	2.413	4	1.0	0	2	8	46.02	1.972	4	0.4
0	1	5	24.89	3.578	4	0.3	2	0	10	37.64	2.389	4	0.1	5	0	9	46.09	1.969	4	0.2
4	0	0	26.02	3.424	2	2.9	5	1	2	38.08	2.363	8	1.0	5	1	8	47.36	1.920	8	0.8
3	0	5	26.20	3.401	4	1.8	2	1	9	38.79	2.321	8	0.5	2	2	8	48.01	1.895	8	0.2
4	0	2	26.96	3.307	4	12.2	3	1	8	38.85	2.318	8	1.5	3	2	7	48.33	1.883	8	0.5
3	1	2	27.31	3.265	8	4.8	1	0	11	39.43	2.285	4	0.6	1	2	9	48.93	1.861	8	0.3
0	0	8	27.99	3.187	2	1.6	5	1	4	40.08	2.250	8	0.4	6	0	8	49.09	1.856	4	0.4
2	1	5	28.14	3.171	8	1.9	1	1	10	40.21	2.243	8	0.1	4	2	6	49.89	1.828	8	0.6
1	1	6	28.27	3.156	8	9.1	4	1	7	40.37	2.234	8	0.3	7	0	5	49.93	1.827	4	0.5


100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
2 theta (°)

CGF Cobalt Gallium Phosphate-5

CHEMICAL COMPOSITION: $|(C_6H_{14}N_2)_8|$ $[(Co_{16}Ga_{20}P_{36}O_{144}]$
$C_6H_{12}N_2$ = 1,4-diazabicyclo[2.2.2]-octane (DABCO)

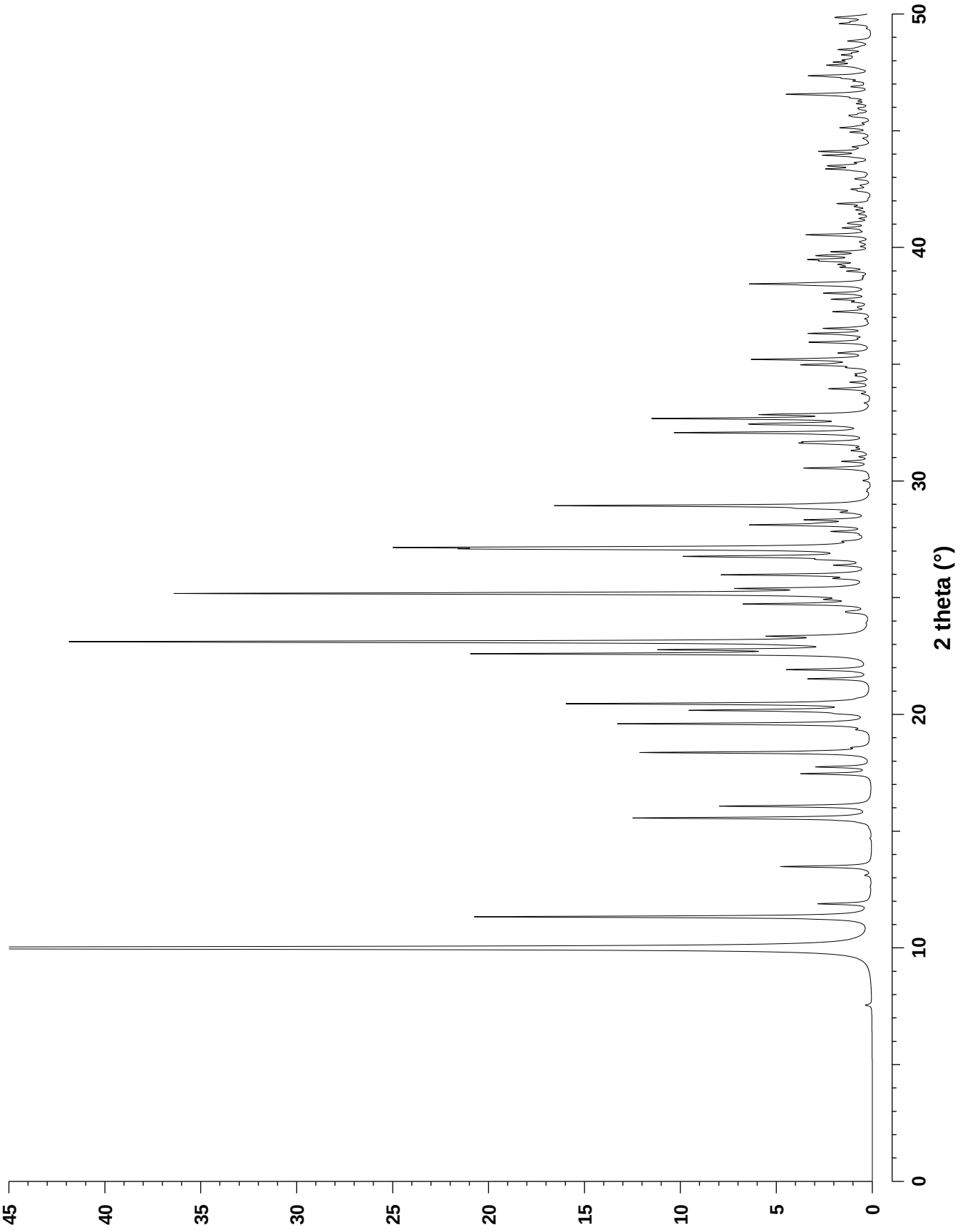
REFINED COMPOSITION: $|C_{48}N_{16}|$ $[Co_{16}Ga_{20}P_{36}O_{144}]$

CRYSTAL DATA: $I1\,2/a\,1$ (No. 15) unique axis **b**, cell choice 3
$a = 15.002$ Å $b = 17.688$ Å $c = 15.751$ Å
$\alpha = 90°$ $\beta = 97.24°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.0704$, $R_w = 0.0850$

REFERENCE: A. M. Chippindale and A. R. Cowley,
Zeolites **18** 176–181 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	10.00	8.844	2	100.0	-2	5	1	28.20	3.164	4	1.0	-4	0	6	39.66	2.272	2	1.3
0	0	2	11.33	7.813	2	20.7	-4	3	1	28.33	3.150	4	3.1	-4	6	2	39.81	2.264	4	1.9
2	0	0	11.89	7.441	2	2.7	1	5	2	28.64	3.116	4	0.8	6	3	1	40.53	2.225	4	2.8
-2	1	1	13.48	6.568	4	4.8	2	5	1	28.82	3.097	4	2.2	4	5	3	40.55	2.225	4	0.5
2	2	0	15.56	5.694	4	12.4	2	2	4	28.94	3.085	4	16.3	6	2	2	40.83	2.210	4	1.2
0	3	1	16.07	5.516	4	7.9	0	5	3	30.55	2.926	4	3.1	-4	2	6	41.01	2.201	4	0.6
2	0	2	17.46	5.078	2	3.6	-3	4	3	30.83	2.900	4	1.5	-2	1	7	41.04	2.199	4	0.5
0	1	3	17.75	4.996	4	2.8	3	1	4	31.29	2.859	4	0.8	-6	3	3	41.24	2.189	4	0.5
-2	2	2	18.37	4.828	4	12.0	1	6	1	31.60	2.831	4	0.8	6	4	0	41.75	2.163	4	0.7
3	1	0	18.58	4.776	4	0.7	-4	3	3	31.61	2.830	4	2.1	-6	2	4	41.87	2.157	4	1.7
-1	3	2	19.34	4.588	4	0.5	4	1	3	31.67	2.825	4	2.6	3	7	2	42.41	2.131	4	0.5
-2	3	1	19.60	4.529	4	13.2	-2	5	3	32.06	2.792	4	10.1	0	8	2	42.49	2.127	4	0.9
-1	2	3	20.03	4.432	4	0.8	0	3	5	32.42	2.761	4	4.3	2	4	6	43.36	2.087	4	2.0
-2	1	3	20.17	4.402	4	8.7	0	6	2	32.46	2.758	4	2.7	1	7	4	43.49	2.081	4	0.6
1	3	2	20.22	4.392	4	0.9	2	6	0	32.67	2.741	4	10.3	-5	1	6	43.49	2.081	4	1.2
2	3	1	20.46	4.340	4	15.7	-4	2	4	32.68	2.740	4	0.6	-2	3	7	43.63	2.075	4	0.6
-1	4	1	21.52	4.129	4	3.2	2	1	5	32.84	2.727	4	5.2	-4	6	4	43.94	2.061	4	2.2
3	2	1	21.91	4.057	4	2.6	5	1	2	33.93	2.642	4	0.8	2	1	7	44.10	2.054	4	1.1
1	4	1	21.92	4.054	4	1.8	2	4	4	33.95	2.641	4	1.5	4	7	1	44.11	2.053	4	1.4
2	1	3	22.60	3.934	4	20.1	-1	5	4	34.22	2.621	4	1.0	-5	4	5	44.31	2.044	4	0.8
0	0	4	22.76	3.906	2	6.3	3	3	4	34.50	2.600	4	0.6	4	0	6	44.93	2.017	2	0.7
0	3	3	22.78	3.903	4	3.8	-1	1	6	34.58	2.594	4	0.6	6	3	3	45.12	2.009	4	1.4
3	1	2	22.97	3.872	4	0.8	4	3	3	34.85	2.574	4	0.9	-4	7	3	45.60	1.989	4	0.7
0	4	2	23.11	3.848	4	41.4	-4	5	1	34.97	2.566	4	3.2	-6	4	4	45.65	1.987	4	0.8
-1	1	4	23.35	3.809	4	4.2	-2	0	6	35.04	2.561	2	0.6	-5	3	6	45.97	1.974	4	0.5
-2	0	4	24.36	3.653	2	0.8	2	6	2	35.20	2.550	4	5.9	4	2	6	46.15	1.967	4	0.6
-4	1	1	24.41	3.647	4	0.8	-4	1	5	35.47	2.531	4	1.4	0	0	8	46.49	1.953	2	0.7
-2	3	3	24.73	3.599	4	6.3	2	3	5	35.93	2.500	4	2.6	2	3	7	46.55	1.951	4	3.1
0	2	4	24.92	3.573	4	1.3	0	2	6	35.95	2.498	4	0.7	0	9	1	46.57	1.950	4	0.6
-4	0	2	25.18	3.537	2	36.0	-6	1	1	36.31	2.474	4	3.0	-2	7	5	46.88	1.938	4	0.9
-2	4	2	25.39	3.508	4	5.8	-2	2	6	36.53	2.460	4	2.4	-7	4	1	47.12	1.928	4	0.7
0	5	1	25.82	3.450	4	1.3	-4	4	4	37.24	2.414	4	1.8	0	8	4	47.24	1.924	4	0.9
4	2	0	25.98	3.429	4	7.6	6	2	0	37.66	2.388	4	0.8	-6	0	6	47.32	1.921	2	1.0
-2	2	4	26.39	3.377	4	1.6	6	1	1	37.78	2.381	4	1.9	-4	3	7	47.35	1.920	4	2.4
-1	4	3	26.63	3.347	4	1.6	2	0	6	38.02	2.367	2	0.7	4	5	5	47.80	1.903	4	1.8
2	4	2	26.73	3.335	4	2.4	-6	2	2	38.04	2.366	4	1.7	6	6	0	47.93	1.898	4	1.0
2	3	3	26.77	3.330	4	8.0	-4	3	5	38.37	2.346	4	1.2	-1	9	2	47.93	1.898	4	0.6
2	0	4	27.08	3.292	2	14.8	0	5	5	38.43	2.342	4	5.6	4	7	3	48.03	1.894	4	0.5
3	3	2	27.09	3.292	4	1.0	-3	6	3	38.49	2.339	4	1.1	-6	6	2	48.24	1.887	4	1.1
-3	4	1	27.14	3.286	4	0.5	4	6	0	38.98	2.311	4	1.1	1	9	2	48.33	1.883	4	0.6
-4	2	2	27.15	3.284	4	20.4	-6	3	1	39.15	2.301	4	1.3	-2	5	7	48.47	1.878	4	1.5
-1	3	4	27.41	3.253	4	0.7	-2	6	4	39.27	2.294	4	1.2	3	5	6	48.83	1.865	4	0.7
4	0	2	27.83	3.206	2	1.8	2	2	6	39.41	2.286	4	1.8	0	9	3	49.57	1.839	4	1.2
3	4	1	28.09	3.176	4	1.0	6	0	2	39.48	2.283	2	2.6	5	1	6	49.60	1.838	4	0.5
-4	1	3	28.12	3.174	4	5.2	0	7	3	39.64	2.273	4	1.5	6	5	3	49.85	1.829	4	1.5

Cobalt Gallium Phosphate-5 CGF



CGS Cobalt Gallium Phosphate-6

CHEMICAL COMPOSITION: $|(C_7H_{14}N)_4|\ [Co_4Ga_{12}P_{16}O_{64}]$
$C_7H_{13}N$ = quinuclidine

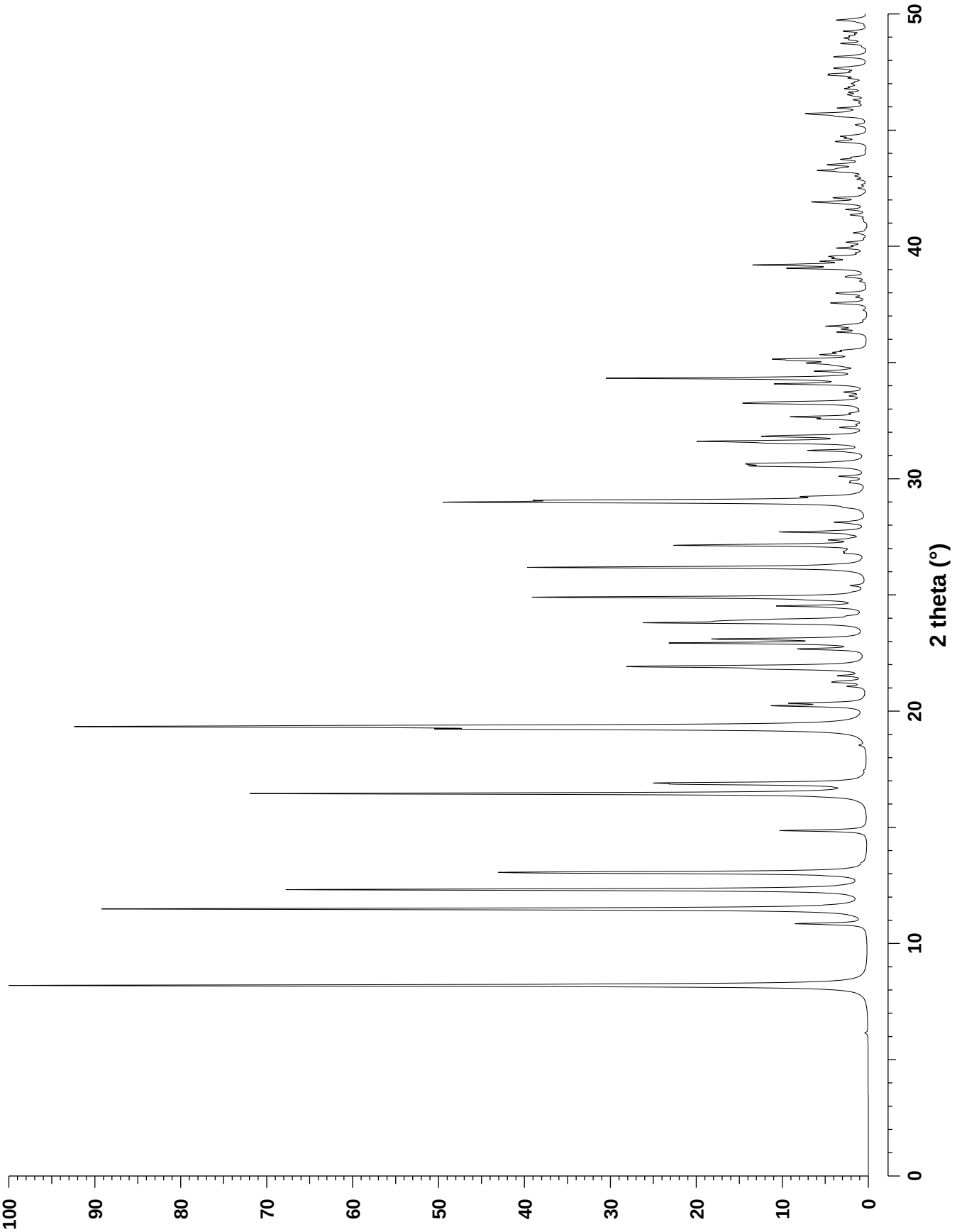
REFINED COMPOSITION: $|C_{28}N_4|\ [Co_4Ga_{12}P_{16}O_{64}]$

CRYSTAL DATA: $P1\,2_1/c\,1$ (No. 14) unique axis **b**, cell choice 1
$a = 14.365$ Å $b = 16.305$ Å $c = 8.734$ Å
$\alpha = 90°$ $\beta = 90.243°$ $\gamma = 90°$
X-ray single crystal refinement. $R = 0.0310$, $R_w = 0.0365$

REFERENCE: A. R. Cowley and A. M. Chippindale,
Microporous and Mesoporous Materials **28** 163–172 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.20	10.779	4	100.0	-4	1	1	27.36	3.259	4	3.5	4	3	2	36.43	2.467	4	2.3
0	2	0	10.85	8.153	2	8.1	3	0	2	27.71	3.220	2	10.0	-2	5	2	36.56	2.457	4	4.2
0	1	1	11.49	7.699	4	89.0	-3	1	2	28.13	3.172	4	3.5	2	5	2	36.63	2.453	4	1.4
2	0	0	12.32	7.182	2	67.4	-2	3	2	28.99	3.080	4	23.1	5	0	2	37.55	2.395	2	3.5
-1	1	1	13.03	6.796	4	22.9	-4	2	1	28.99	3.080	4	19.7	5	1	2	37.96	2.370	4	1.7
1	1	1	13.07	6.775	4	29.9	2	3	2	29.06	3.072	4	13.9	6	1	0	37.99	2.369	4	2.4
0	2	1	14.86	5.960	4	10.2	4	2	1	29.07	3.072	4	15.1	-4	5	1	38.67	2.329	4	1.8
2	2	0	16.45	5.389	4	71.6	0	5	1	29.23	3.055	4	5.1	4	5	1	38.72	2.325	4	1.4
-2	1	1	16.85	5.262	4	15.8	2	5	0	30.10	2.969	4	3.0	-5	2	2	39.05	2.307	4	8.3
2	1	1	16.91	5.242	4	19.4	-3	4	1	30.54	2.927	4	10.4	1	7	0	39.18	2.299	4	2.8
0	3	1	19.23	4.614	4	36.5	3	4	1	30.59	2.922	4	3.4	5	2	2	39.20	2.298	4	10.1
3	1	0	19.32	4.594	4	29.7	-1	4	2	30.62	2.919	4	5.3	4	4	2	39.35	2.290	4	4.0
-2	2	1	19.33	4.593	4	47.0	1	4	2	30.66	2.916	4	8.8	-3	6	1	39.48	2.283	4	1.8
2	2	1	19.38	4.580	4	31.7	0	1	3	31.21	2.866	4	6.4	1	6	2	39.57	2.277	4	3.2
-1	3	1	20.20	4.396	4	2.5	-4	3	1	31.53	2.837	4	7.3	3	3	3	39.92	2.258	4	3.3
1	3	1	20.23	4.391	4	8.5	4	3	1	31.60	2.831	4	13.7	-2	4	3	40.03	2.252	4	1.3
0	0	2	20.34	4.367	2	7.8	5	1	0	31.62	2.829	4	4.8	-4	1	3	40.17	2.245	4	2.3
0	1	2	21.06	4.218	4	2.0	-1	1	3	31.81	2.813	4	3.2	0	5	3	41.58	2.172	4	2.3
-1	0	2	21.24	4.183	2	3.0	-2	5	1	31.81	2.813	4	5.3	1	0	4	41.87	2.157	2	2.2
1	0	2	21.29	4.173	2	1.9	2	5	1	31.85	2.810	4	3.5	5	5	0	41.91	2.156	4	5.0
3	2	0	21.52	4.129	4	2.9	1	1	3	31.86	2.808	4	2.7	2	7	1	42.09	2.147	4	3.1
0	4	0	21.80	4.076	2	2.4	-4	0	2	32.20	2.780	2	2.8	5	5	1	43.26	2.091	4	2.7
-3	1	1	21.82	4.073	4	6.1	2	4	2	32.57	2.750	4	4.3	-1	2	4	43.33	2.088	4	1.4
3	1	1	21.90	4.059	4	18.1	0	2	3	32.66	2.742	4	6.7	-3	6	2	43.50	2.080	4	2.4
-1	1	2	21.94	4.052	4	14.9	-4	1	2	32.68	2.740	4	1.6	2	1	4	43.74	2.070	4	2.5
1	4	0	22.67	3.921	4	7.4	4	1	2	32.82	2.729	4	1.3	5	4	2	43.83	2.065	4	1.4
2	3	1	22.93	3.878	4	21.6	3	5	0	33.24	2.695	4	5.6	6	2	2	44.65	2.030	4	1.9
0	2	2	23.10	3.849	4	16.8	-5	1	1	33.24	2.695	4	3.6	-2	2	4	44.73	2.026	4	2.1
-2	0	2	23.80	3.738	2	4.7	4	4	0	33.25	2.695	4	1.7	0	6	3	45.67	1.987	4	2.6
-3	2	1	23.80	3.738	4	18.3	1	2	3	33.29	2.691	4	7.4	0	8	1	45.71	1.985	4	4.8
3	2	1	23.87	3.727	4	7.8	1	6	0	33.56	2.670	4	1.5	-2	3	4	46.52	1.952	4	1.6
-1	2	2	23.91	3.722	4	6.5	2	1	3	33.72	2.658	4	2.3	2	3	4	46.62	1.948	4	1.7
1	2	2	23.95	3.715	4	4.5	-4	2	2	34.08	2.631	4	9.9	-7	2	1	46.78	1.942	4	2.1
-2	1	2	24.43	3.644	4	1.4	0	5	2	34.32	2.613	4	29.9	7	2	1	46.86	1.939	4	1.4
2	1	2	24.52	3.631	4	9.7	-5	2	1	34.62	2.591	4	5.1	5	6	1	47.23	1.924	4	1.6
4	0	0	24.79	3.591	2	1.6	4	4	1	34.87	2.573	4	1.4	7	3	0	47.35	1.920	4	3.3
-1	4	1	24.88	3.579	4	8.1	0	3	3	34.96	2.566	4	2.3	-5	3	3	47.41	1.917	4	3.1
1	4	1	24.90	3.576	4	32.1	-2	2	3	34.98	2.565	4	3.1	-4	7	1	47.66	1.908	4	2.2
4	1	0	25.40	3.507	4	1.6	2	2	3	35.08	2.558	4	5.6	4	7	1	47.71	1.906	4	1.3
0	3	2	26.18	3.404	4	38.6	-1	6	1	35.14	2.554	4	5.9	-3	7	2	48.15	1.890	4	3.8
-2	2	2	26.22	3.398	4	1.7	1	6	1	35.15	2.553	4	3.0	-6	4	2	48.72	1.869	4	1.8
-3	3	1	26.80	3.326	4	1.7	5	3	0	35.34	2.540	4	4.0	-7	0	2	48.96	1.860	2	1.9
-2	4	1	27.13	3.287	4	1.7	-3	4	2	35.43	2.533	4	2.6	2	4	4	49.04	1.857	4	1.3
4	2	0	27.13	3.286	4	18.2	-1	3	3	35.51	2.528	4	1.9	4	1	4	49.25	1.850	4	2.6
2	4	1	27.17	3.282	4	4.8	-4	3	2	36.30	2.475	4	3.3	6	1	3	49.72	1.834	4	2.1

Cobalt Gallium Phosphate-6 CGS



CHA Chabazite

CHEMICAL COMPOSITION: $|K_{3.2}Na_{0.75}(H_2O)_{8.4}|\ [Si_{8.2}Al_{3.8}O_{24}]$
North East Azerbaijan, Iran

REFINED COMPOSITION: $|K_{4.16}(H_2O)_{7.23}|\ [Si_{8.16}Al_{3.84}O_{24}]$

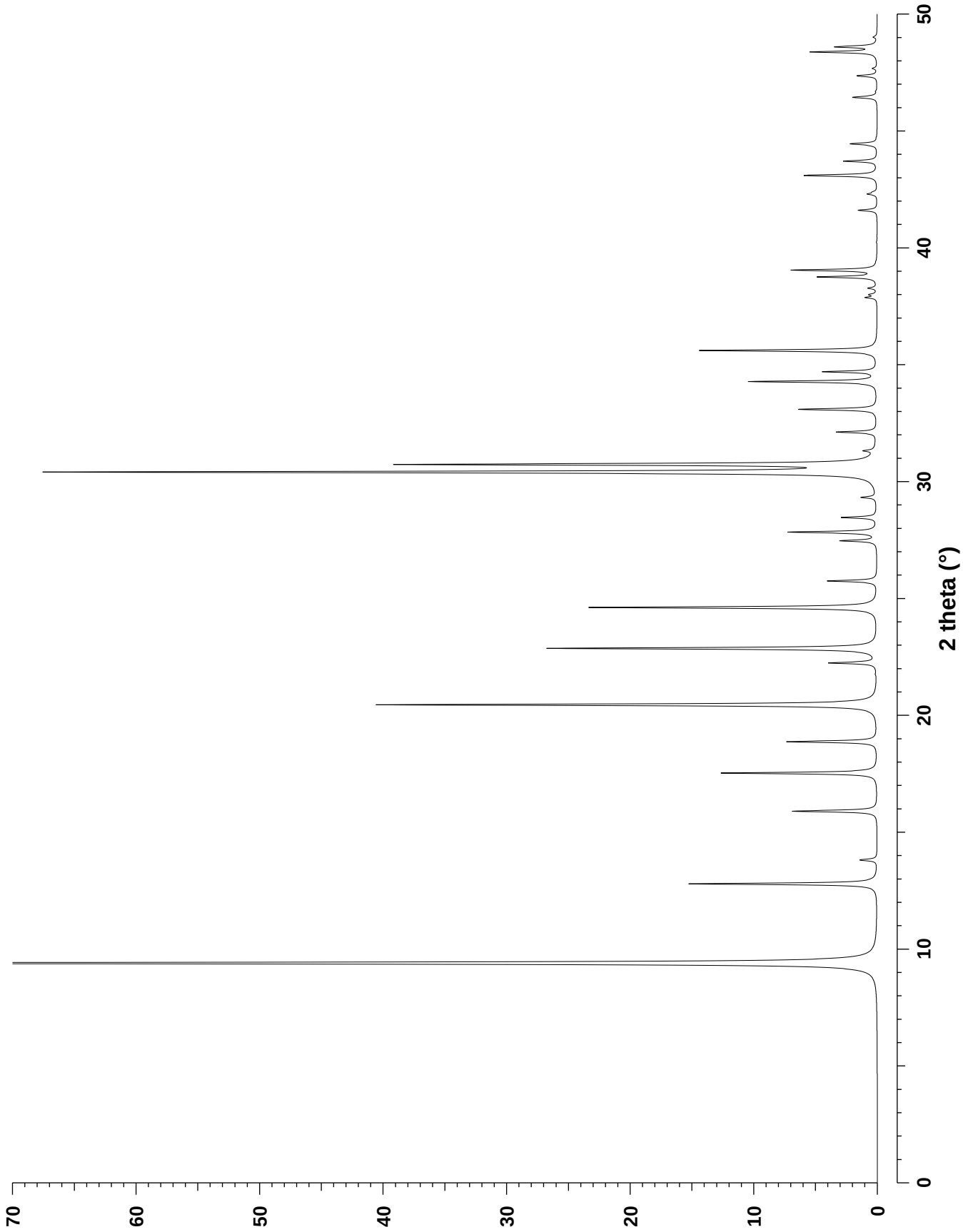
CRYSTAL DATA: $R\bar{3}m$ (No. 166) rhombohedral setting
$a = 9.459$ Å $b = 9.459$ Å $c = 9.459$ Å
$\alpha = 94.07°$ $\beta = 94.07°$ $\gamma = 94.07°$
X-ray single crystal refinement, $R = 0.05$

REFERENCE: M. Calligaris, G. Nardin and L. Randaccio,
Zeolites **3** 205–208 (1983).

h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$
1	0	0	9.40	9.408	6	100.0	3	-1	-1	30.40	2.940	6	63.6	3	3	0	42.29	2.137	6	0.1
1	0	-1	12.79	6.922	6	15.3	3	1	0	30.73	2.909	12	38.2	3	2	2	42.37	2.133	6	0.2
1	1	0	13.81	6.412	6	1.4	3	1	-1	31.31	2.856	12	0.9	4	1	-2	43.09	2.099	12	5.9
1	1	-1	15.90	5.575	6	6.9	2	2	-2	32.11	2.788	6	3.2	3	2	-3	43.70	2.071	12	2.7
1	1	1	17.53	5.059	2	12.6	3	1	1	33.08	2.708	6	5.0	4	2	0	44.36	2.042	12	0.1
2	0	0	18.87	4.704	6	7.3	3	0	-2	33.10	2.706	12	1.7	3	3	1	44.43	2.039	6	1.3
2	0	-1	20.45	4.342	12	40.6	3	-1	-2	34.27	2.616	12	10.4	4	2	-1	44.45	2.038	12	1.0
2	-1	-1	22.24	3.996	6	3.8	3	1	-2	34.69	2.586	12	4.3	4	2	1	46.43	1.956	12	1.7
2	1	-1	22.86	3.890	12	26.7	3	2	0	35.60	2.522	12	14.4	4	0	-3	46.46	1.955	12	0.5
2	1	1	24.61	3.617	6	23.3	3	2	1	37.87	2.376	12	0.9	4	-1	-3	47.35	1.920	12	1.6
2	0	-2	25.74	3.461	6	4.0	2	2	-3	37.99	2.368	6	0.6	4	1	-3	47.67	1.908	12	0.4
2	1	-2	27.46	3.248	12	3.0	4	0	0	38.27	2.352	6	0.7	5	0	0	48.37	1.882	6	5.4
2	2	0	27.83	3.206	6	7.2	4	0	-1	38.75	2.324	12	0.1	3	3	2	48.59	1.874	6	3.1
3	0	0	28.46	3.136	6	2.4	3	2	-2	38.75	2.324	12	4.6	5	0	-1	48.62	1.873	12	0.3
2	2	-1	28.46	3.136	6	0.5	3	0	-3	39.04	2.307	6	6.9	3	3	-3	49.01	1.858	6	0.3
3	0	-1	29.32	3.046	12	1.2	4	0	-2	41.60	2.171	12	1.5							
2	2	1	30.38	2.942	6	4.3	4	1	1	42.29	2.137	6	0.6							

Chabazite

CHA



CHA Methylbutylamine SAPO–47

CHEMICAL COMPOSITION: $|(C_5H_{12}NH_2)_{1.4}(H_2O)_{2.5}|$ $[Al_{6.0}Si_{1.4}P_{4.6}O_{24}]$
$C_5H_{12}NH_2$ = methylbutylamine

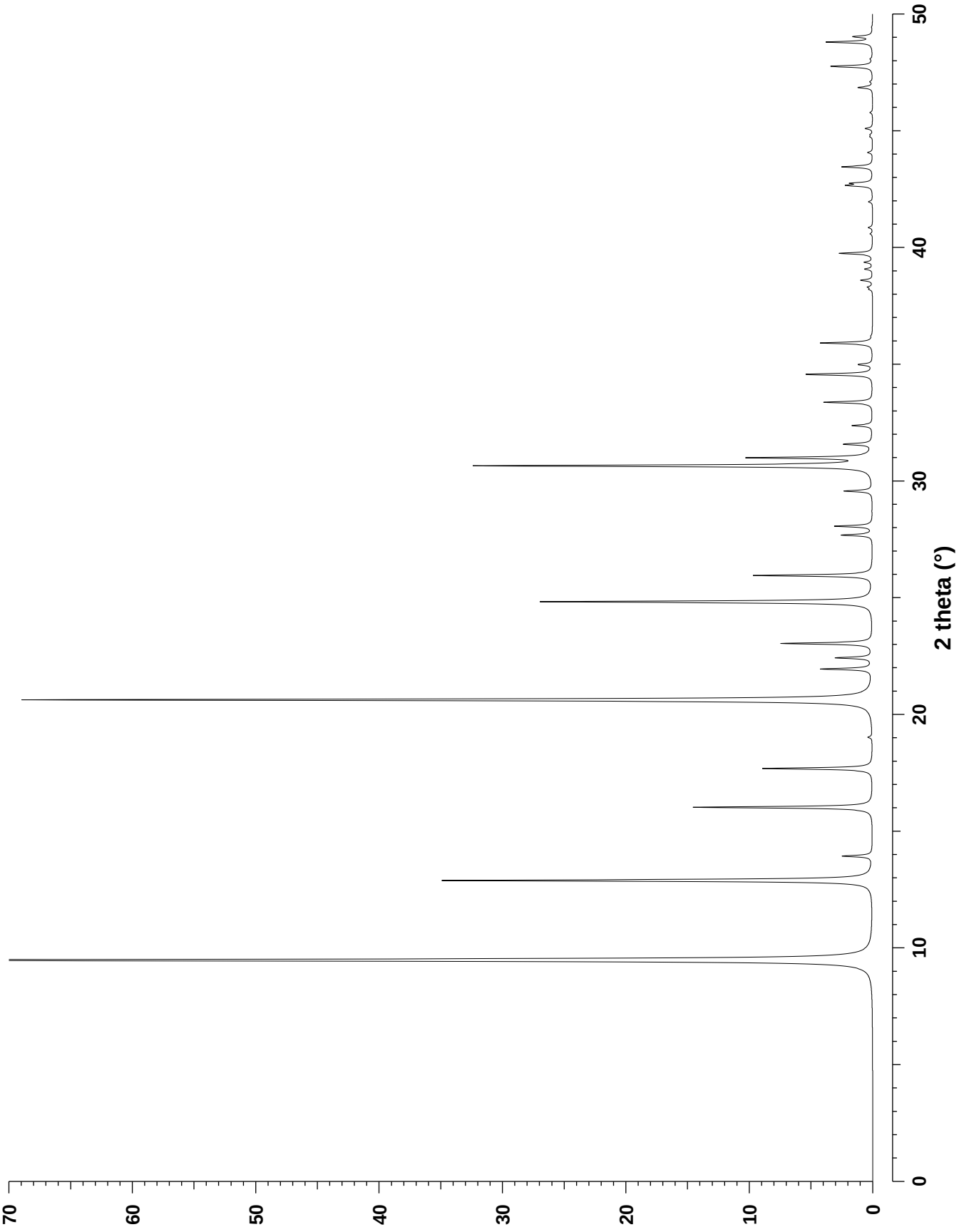
REFINED COMPOSITION: $|(C_5N)_{2.06}|$ $[Al_{5.47}P_{5.37}O_{24}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) rhombohedral setting
$a = 9.3834$ Å $b = 9.3834$ Å $c = 9.3834$ Å
$\alpha = 94.085°$ $\beta = 94.085°$ $\gamma = 94.085°$
X-ray single crystal refinement, $R_w = 0.068$

REFERENCE: J. J. Pluth and J. V. Smith,
J. Phys. Chem. **93** 6516–6520 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	9.48	9.332	6	100.0	3	1	-1	31.57	2.834	6	1.5	4	0	-2	41.95	2.154	6	0.1
1	0	-1	12.89	6.867	6	34.9	3	-1	1	31.57	2.834	6	0.8	3	0	3	42.65	2.120	6	1.1
1	0	1	13.93	6.359	6	2.4	2	-2	2	32.37	2.766	6	1.6	4	1	1	42.65	2.120	6	0.9
1	-1	1	16.02	5.531	6	14.6	3	1	1	33.36	2.686	6	2.9	3	2	2	42.74	2.116	6	0.3
1	1	1	17.68	5.017	2	8.9	3	-2	0	33.37	2.685	6	0.4	3	-1	3	42.74	2.115	6	0.9
2	0	0	19.02	4.666	6	0.3	3	0	-2	33.37	2.685	6	0.8	4	-2	-1	42.75	2.115	6	0.3
2	0	-1	20.62	4.308	6	23.7	3	-1	-2	34.56	2.596	6	3.3	4	-1	-2	42.75	2.115	6	0.1
2	-1	0	20.62	4.308	6	45.3	3	-2	-1	34.56	2.596	6	2.1	4	1	-2	43.45	2.083	6	1.5
2	0	1	21.94	4.051	6	0.4	3	-2	1	34.98	2.565	6	0.3	4	-2	1	43.45	2.083	6	1.0
2	1	0	21.94	4.051	6	3.7	1	-2	3	34.98	2.565	6	0.9	3	-3	2	44.06	2.055	6	0.3
2	-1	-1	22.42	3.965	6	3.0	2	0	3	35.90	2.501	6	1.8	2	-3	3	44.06	2.055	6	0.1
1	-1	2	23.04	3.859	6	0.4	3	0	2	35.90	2.501	6	2.5	4	0	2	44.74	2.025	6	0.2
2	-1	1	23.04	3.859	6	7.0	3	2	1	38.20	2.356	6	0.2	3	1	3	44.82	2.022	6	0.1
2	1	1	24.82	3.587	6	26.9	3	1	2	38.20	2.356	6	0.1	3	-2	3	45.09	2.011	6	0.6
2	0	-2	25.95	3.434	6	9.7	2	-3	2	38.30	2.350	6	0.4	4	-2	-2	45.77	1.982	6	0.2
1	-2	2	27.68	3.222	6	0.8	4	0	0	38.59	2.333	6	1.0	4	1	2	46.84	1.940	6	0.2
2	-2	1	27.68	3.222	6	1.7	2	-2	3	39.07	2.305	6	0.2	4	0	-3	46.85	1.939	6	0.3
2	0	2	28.06	3.180	6	3.1	4	0	-1	39.07	2.305	6	0.2	4	-3	0	46.85	1.939	6	0.6
3	0	-1	29.56	3.021	6	1.7	3	-2	2	39.07	2.305	6	0.2	2	-2	4	47.09	1.930	6	0.1
3	-1	0	29.56	3.021	6	0.6	3	0	-3	39.36	2.289	6	0.7	4	-1	-3	47.75	1.905	6	2.2
2	1	2	30.64	2.918	6	7.9	4	-1	-1	39.74	2.268	6	2.7	4	-3	-1	47.75	1.905	6	1.2
3	-1	-1	30.65	2.917	6	24.9	4	-1	1	40.85	2.209	6	0.1	1	-3	4	48.07	1.893	6	0.1
3	1	0	30.99	2.885	6	5.3	4	1	-1	40.85	2.209	6	0.2	5	0	0	48.79	1.866	6	3.8
3	0	1	30.99	2.885	6	4.6	4	-2	0	41.95	2.154	6	0.2	3	2	3	49.02	1.858	6	1.5

Methylbutylamine SAPO–47 CHA



CHEMICAL COMPOSITION: $|Ca_4Mn_4(H_2O)_8|\ [Si_{20}(BeOH)_8O_{52}]$
Val di San Giacomo, Chiavenna, Italy

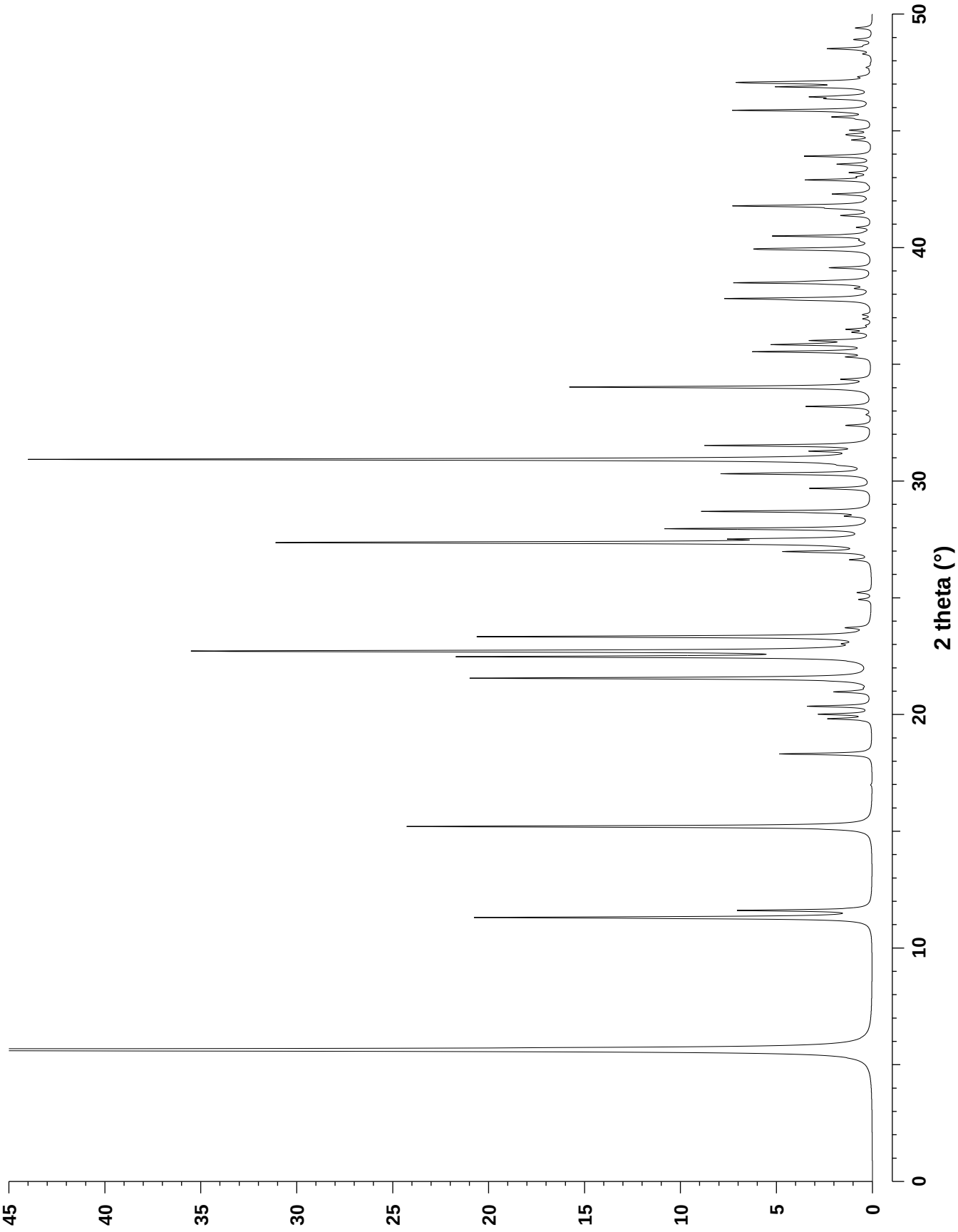
REFINED COMPOSITION: $|Ca_4Mn_4(H_2O)_8|\ [Si_{20}(BeOH)_8O_{52}]$

CRYSTAL DATA: *Pnab* (No. 60) **c̄ba** setting
$a = 8.729$ Å $b = 31.326$ Å $c = 4.903$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.041$

REFERENCE: V. Tazzoli, M. C. Domeneghetti, F. Mazzi and E. Cannillo
Eur. J. Mineral. **7** 1339–1344 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	5.64	15.663	2	100.0	1	9	1	33.19	2.699	8	3.4	3	8	1	42.89	2.108	8	3.4
0	4	0	11.30	7.832	2	20.6	2	7	1	34.02	2.635	8	15.7	4	4	0	43.03	2.102	4	0.5
1	2	0	11.61	7.625	4	6.7	0	12	0	34.35	2.610	2	1.4	2	3	2	43.20	2.094	8	1.1
1	4	0	15.20	5.829	4	24.3	3	6	0	35.31	2.542	4	1.1	0	8	2	43.56	2.078	4	1.8
0	1	1	18.31	4.844	4	4.8	1	10	1	35.53	2.527	8	6.1	2	4	2	43.91	2.062	8	3.5
1	6	0	19.81	4.481	4	2.2	2	8	1	35.84	2.505	8	4.9	3	9	1	44.60	2.032	8	1.0
0	3	1	20.01	4.438	4	2.7	1	12	0	35.91	2.501	4	0.6	2	5	2	44.80	2.023	8	0.8
2	0	0	20.35	4.365	2	3.3	3	1	1	36.01	2.494	8	2.9	1	8	2	44.84	2.021	8	0.8
1	1	1	20.97	4.236	8	1.9	3	2	1	36.36	2.471	8	0.9	4	6	0	45.02	2.013	4	1.1
2	2	0	21.13	4.204	4	0.1	0	11	1	36.49	2.463	4	1.2	4	0	1	45.49	1.994	4	0.5
1	2	1	21.55	4.124	8	20.9	0	0	2	36.66	2.451	2	0.2	2	14	0	45.56	1.991	4	0.1
1	3	1	22.47	3.956	8	20.7	3	3	1	36.94	2.433	8	0.4	4	1	1	45.59	1.990	8	1.8
0	8	0	22.71	3.916	2	34.8	0	2	2	37.12	2.422	4	0.4	1	14	1	45.77	1.982	8	0.3
0	5	1	23.03	3.861	4	0.6	3	4	1	37.74	2.384	8	2.3	2	6	2	45.87	1.978	8	6.5
2	4	0	23.33	3.812	4	20.4	2	9	1	37.81	2.379	8	7.1	4	2	1	45.88	1.978	8	0.7
1	4	1	23.71	3.752	8	1.1	1	1	2	38.24	2.354	8	0.7	4	3	1	46.36	1.958	8	1.3
1	8	0	24.92	3.573	4	0.7	0	4	2	38.48	2.340	4	6.8	0	16	0	46.38	1.958	2	0.7
1	5	1	25.22	3.531	8	0.8	3	8	0	38.55	2.335	4	1.3	3	10	1	46.45	1.955	8	2.6
2	6	0	26.62	3.349	4	1.0	1	2	2	38.58	2.334	8	0.6	1	9	2	46.49	1.953	8	0.3
1	6	1	26.96	3.308	8	0.2	1	3	2	39.13	2.302	8	2.2	2	13	1	46.88	1.938	8	4.6
0	7	1	26.97	3.305	4	4.1	1	4	2	39.89	2.260	8	0.6	4	4	1	47.03	1.932	8	3.3
2	0	1	27.36	3.260	4	30.6	2	10	1	39.91	2.259	8	3.4	0	10	2	47.07	1.931	4	4.8
2	1	1	27.51	3.242	8	5.4	3	6	1	39.95	2.256	8	3.9	2	7	2	47.12	1.929	8	1.0
2	2	1	27.95	3.192	8	10.6	2	12	0	40.25	2.240	4	0.2	0	15	1	47.31	1.921	4	0.5
0	10	0	28.49	3.133	2	1.0	0	14	0	40.31	2.238	2	0.3	4	8	0	47.71	1.906	4	0.3
2	3	1	28.69	3.112	8	8.8	1	12	1	40.49	2.228	8	5.1	1	10	2	48.28	1.885	8	0.4
2	4	1	29.68	3.010	8	3.2	1	5	2	40.86	2.209	8	0.7	3	11	1	48.42	1.880	8	0.1
1	10	0	30.31	2.948	4	7.7	3	7	1	41.34	2.184	8	0.2	1	15	1	48.51	1.876	8	1.9
2	8	0	30.67	2.915	4	0.6	4	0	0	41.37	2.182	2	1.4	2	8	2	48.52	1.876	8	0.5
2	5	1	30.92	2.892	8	43.9	1	14	0	41.67	2.167	4	1.5	3	1	2	48.65	1.871	8	0.3
3	2	0	31.27	2.861	4	2.5	0	13	1	41.77	2.163	4	3.7	4	6	1	48.90	1.863	8	0.9
0	9	1	31.52	2.838	4	8.5	4	2	0	41.79	2.161	4	3.9	2	14	1	49.40	1.845	8	0.8
2	6	1	32.38	2.765	8	1.3	1	6	2	42.01	2.151	8	0.1							
3	4	0	32.84	2.728	4	0.2	2	0	2	42.28	2.137	4	2.0							

Chiavennite -CHI



CHEMICAL COMPOSITION: $|(C_7H_{14}NF)_{192}|\ [Ga_{768}P_{768}O_{2976}(OH)_{192}]$
$C_7H_{14}NF$ = quinuclidinium fluoride

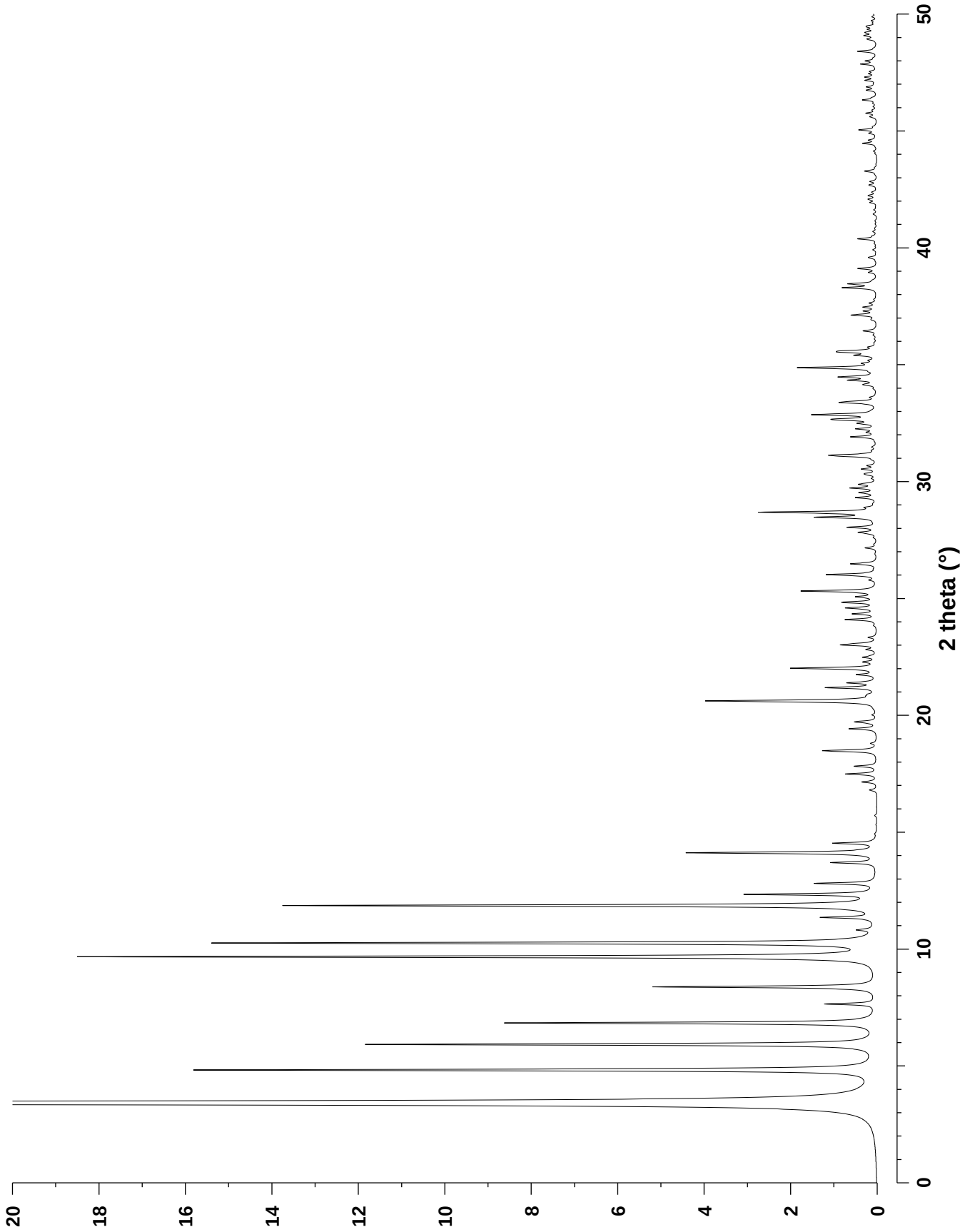
REFINED COMPOSITION: $|F_{192}|\ [Ga_{768}P_{768}O_{3168}]$

CRYSTAL DATA: $Fm\bar{3}c$ (No. 226)
$a = 51.7120$ Å $b = 51.7120$ Å $c = 51.7120$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.076$

REFERENCE: M. Estermann, L. B. McCusker, Ch. Baerlocher, A. Merrouche and H. Kessler, *Nature* **352** 320–322 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	3.42	25.856	6	100.0	10	10	2	24.59	3.621	24	0.7	16	10	4	33.42	2.681	48	0.4
2	2	0	4.83	18.283	12	15.7	12	8	0	24.83	3.586	24	0.8	18	6	4	33.60	2.667	48	0.1
2	2	2	5.92	14.928	8	11.8	14	4	0	25.07	3.552	24	0.3	18	8	0	34.15	2.625	24	0.2
4	0	0	6.84	12.928	6	8.6	12	8	2	25.07	3.552	48	0.2	16	10	6	34.33	2.612	48	0.1
4	2	0	7.65	11.563	24	1.2	12	6	6	25.31	3.519	24	1.7	14	14	0	34.33	2.612	12	0.3
4	2	2	8.38	10.556	24	5.2	12	8	4	25.78	3.455	48	0.1	18	8	2	34.33	2.612	48	0.2
4	4	0	9.67	9.141	12	18.4	14	4	4	26.02	3.425	24	0.8	15	11	7	34.47	2.602	48	0.6
6	0	0	10.26	8.619	6	15.3	10	8	8	26.02	3.425	24	0.3	15	13	3	34.83	2.576	48	0.2
6	2	0	10.82	8.176	24	0.4	14	6	2	26.48	3.366	48	0.4	16	12	2	34.87	2.573	48	0.1
6	2	2	11.35	7.796	24	1.2	10	10	6	26.48	3.366	24	0.2	14	12	8	34.87	2.573	48	1.6
4	4	4	11.86	7.464	8	13.7	12	10	2	27.16	3.284	48	0.2	14	14	4	35.05	2.560	24	0.2
6	4	0	12.34	7.171	24	3.0	14	8	0	27.82	3.207	24	0.3	16	12	4	35.40	2.535	48	0.4
6	4	2	12.81	6.910	48	1.4	10	10	8	28.04	3.183	24	0.5	19	7	3	35.53	2.526	48	0.6
8	0	0	13.70	6.464	6	1.0	14	8	2	28.04	3.183	48	0.2	16	10	8	35.58	2.523	48	0.6
8	2	0	14.12	6.271	24	2.9	16	4	0	28.47	3.136	24	0.4	18	10	0	35.75	2.511	24	0.1
6	4	4	14.12	6.271	24	1.5	12	8	8	28.47	3.136	24	0.9	14	12	10	36.44	2.465	48	0.2
8	2	2	14.53	6.094	24	0.6	16	4	2	28.68	3.113	48	0.2	16	14	2	37.12	2.422	48	0.3
6	6	0	14.53	6.094	12	0.4	14	8	4	28.68	3.113	48	2.5	16	10	10	37.12	2.422	24	0.2
8	4	4	16.80	5.278	24	0.2	12	10	6	28.89	3.090	48	0.2	18	10	6	37.29	2.411	48	0.3
8	6	0	17.15	5.171	24	0.3	12	12	0	29.31	3.047	12	0.4	20	8	0	37.46	2.401	24	0.2
8	6	2	17.49	5.071	48	0.7	16	6	0	29.52	3.026	24	0.3	14	12	12	38.29	2.351	24	0.2
6	6	6	17.82	4.976	8	0.4	14	8	6	29.72	3.006	48	0.2	22	0	0	38.29	2.351	6	0.5
10	4	0	18.48	4.801	24	1.3	14	10	0	29.72	3.006	24	0.3	18	12	4	38.29	2.351	48	0.1
10	4	2	18.80	4.721	48	0.1	17	3	1	29.88	2.991	48	0.2	22	2	0	38.45	2.341	24	0.6
8	8	0	19.42	4.571	12	0.6	15	9	1	30.28	2.951	48	0.1	22	4	2	39.11	2.303	48	0.1
8	8	2	19.72	4.501	24	0.4	16	6	4	30.33	2.947	48	0.2	20	10	2	39.11	2.303	48	0.2
12	0	0	20.61	4.309	6	0.2	14	10	4	30.53	2.928	48	0.3	14	14	12	40.38	2.234	24	0.3
8	8	4	20.61	4.309	24	3.7	15	9	3	30.68	2.914	48	0.1	24	0	0	41.93	2.155	6	0.1
10	6	4	21.18	4.194	48	1.2	17	5	3	31.08	2.877	48	0.5	20	14	4	43.28	2.090	48	0.1
11	5	3	21.39	4.154	48	0.5	12	12	6	31.13	2.873	24	0.2	18	16	8	44.46	2.038	48	0.2
9	7	5	21.39	4.154	48	0.1	16	8	2	31.13	2.873	48	0.6	18	18	0	44.60	2.031	12	0.1
12	4	0	21.74	4.088	24	0.4	18	4	0	31.91	2.804	24	0.4	16	16	12	44.89	2.019	24	0.1
8	8	6	22.01	4.038	24	0.7	14	12	0	31.91	2.804	24	0.2	20	16	2	45.04	2.013	48	0.2
10	8	0	22.01	4.038	24	1.3	12	10	10	32.10	2.788	24	0.1	20	14	8	45.04	2.013	48	0.2
10	8	2	22.28	3.990	48	0.3	15	11	1	32.25	2.776	48	0.4	26	2	0	45.75	1.983	24	0.1
11	7	1	22.48	3.955	48	0.3	12	12	8	32.48	2.756	24	0.4	26	4	2	46.32	1.960	48	0.2
12	4	4	22.81	3.898	24	0.2	15	9	7	32.63	2.745	48	0.1	16	16	14	46.74	1.943	24	0.1
11	7	3	23.01	3.865	48	0.4	15	11	3	32.63	2.745	48	0.4	26	6	0	46.88	1.938	24	0.1
13	3	1	23.01	3.865	48	0.3	16	8	6	32.67	2.741	48	0.1	20	16	8	47.16	1.927	48	0.2
12	6	0	23.07	3.854	24	0.2	18	4	4	32.67	2.741	24	0.4	18	16	12	47.30	1.922	48	0.2
10	8	4	23.07	3.854	48	0.1	18	6	0	32.86	2.725	24	0.5	20	14	12	47.85	1.901	48	0.2
12	6	2	23.33	3.812	48	0.2	16	10	2	32.86	2.725	48	1.0	22	14	8	47.99	1.896	48	0.1
14	0	0	24.09	3.694	6	0.6	13	11	9	33.37	2.685	48	0.1	22	16	4	48.40	1.881	48	0.3
10	10	0	24.34	3.657	12	0.4	19	3	1	33.37	2.685	48	0.4	22	14	10	49.21	1.852	48	0.2
14	2	0	24.34	3.657	24	0.1	15	11	5	33.37	2.685	48	0.2	28	0	0	49.34	1.847	6	0.2

Cloverite -CLO



CHEMICAL COMPOSITION: $[Si_{56}O_{112}]$

REFINED COMPOSITION: $[Si_{56}O_{112}]$

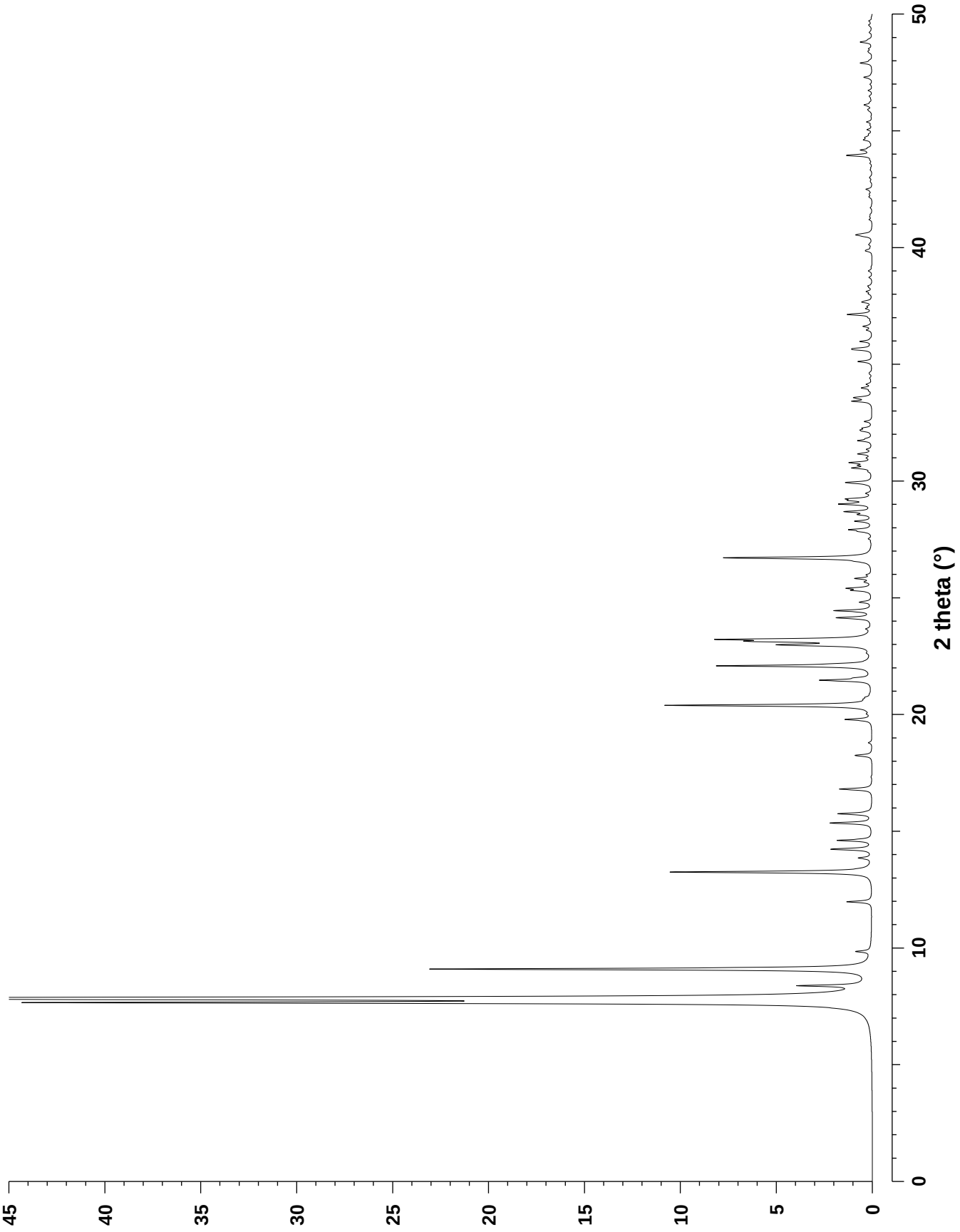
CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 22.6242$ Å $b = 13.3503$ Å $c = 12.3642$ Å
$\alpha = 90°$ $\beta = 68.913°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.136$, $R_F = 0.106$

REFERENCE: R. F. Lobo and M. E. Davis,
J. Am. Chem. Soc. **117** 3766–3779 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	7.66	11.536	2	40.5	-4	0	2	26.68	3.341	2	2.0	9	1	3	37.65	2.389	4	0.4
1	1	0	7.84	11.283	4	100.0	0	4	0	26.71	3.338	2	6.6	5	1	5	37.70	2.386	4	0.2
2	0	0	8.38	10.555	2	3.3	6	0	3	27.52	3.241	2	0.2	-1	5	2	38.01	2.367	4	0.2
2	0	1	9.10	9.722	2	23.4	0	4	1	27.83	3.206	4	0.5	-4	4	2	38.11	2.361	4	0.3
1	1	1	9.85	8.975	4	0.8	6	2	2	27.91	3.197	4	1.1	1	1	5	38.28	2.351	4	0.1
-1	1	1	11.98	7.387	4	1.3	2	4	1	28.27	3.157	4	0.9	-3	1	4	38.35	2.347	4	0.2
-2	0	1	13.25	6.681	2	8.0	7	1	1	28.56	3.125	4	0.6	-1	3	4	38.71	2.326	4	0.1
0	2	0	13.26	6.675	2	2.9	6	2	0	28.68	3.112	4	1.4	9	1	0	38.99	2.310	4	0.2
3	1	1	13.85	6.394	4	0.7	2	0	4	29.01	3.078	2	1.7	2	4	4	39.84	2.263	4	0.2
3	1	0	14.23	6.225	4	2.2	5	3	0	29.16	3.063	4	0.9	-6	4	1	39.89	2.260	4	0.2
2	0	2	14.61	6.062	2	1.8	5	3	2	29.23	3.056	4	1.1	7	3	4	40.12	2.248	4	0.1
0	2	1	15.34	5.778	4	1.0	4	0	4	29.47	3.031	2	0.3	1	5	3	40.47	2.229	4	0.2
0	0	2	15.36	5.768	2	1.4	-4	2	2	29.91	2.987	4	0.3	0	6	0	40.54	2.225	2	0.7
2	2	0	15.71	5.642	4	0.2	-2	4	1	29.93	2.986	4	1.2	6	2	5	40.59	2.223	4	0.2
4	0	1	15.75	5.625	2	1.7	7	1	0	30.39	2.941	4	0.1	-3	5	2	41.19	2.191	4	0.1
4	0	0	16.80	5.277	2	1.7	-2	2	3	30.55	2.926	4	0.9	10	2	2	42.17	2.143	4	0.1
-3	1	1	18.22	4.869	4	0.3	2	4	2	30.58	2.924	4	0.2	-8	0	2	42.49	2.127	2	0.3
4	0	2	18.25	4.861	2	0.7	6	2	3	30.67	2.915	4	0.5	4	0	6	43.94	2.061	2	1.3
-2	2	1	18.79	4.722	4	0.2	-3	3	2	30.78	2.905	4	1.1	8	2	5	43.96	2.060	4	0.1
2	2	2	19.78	4.488	4	1.4	-3	1	3	30.98	2.886	4	0.2	4	6	0	44.17	2.050	4	0.6
-2	0	2	20.02	4.435	2	0.1	4	4	1	31.16	2.870	4	0.7	7	5	2	44.27	2.046	4	0.2
0	2	2	20.35	4.364	4	0.4	5	1	4	31.35	2.853	4	0.3	11	1	2	44.59	2.032	4	0.1
1	3	0	20.39	4.354	4	10.8	4	4	0	31.72	2.821	4	0.7	9	1	5	44.60	2.032	4	0.2
4	2	1	20.65	4.302	4	0.2	8	0	2	31.81	2.813	2	0.2	-2	4	4	44.63	2.030	4	0.1
5	1	1	20.73	4.285	4	0.2	-5	3	1	32.13	2.785	4	0.4	3	1	6	44.68	2.028	4	0.1
4	2	0	21.46	4.140	4	2.7	-1	3	3	32.18	2.782	4	0.4	5	1	6	44.72	2.026	4	0.2
2	0	3	21.56	4.121	2	0.6	5	3	3	32.26	2.775	4	0.4	7	3	5	44.85	2.021	4	0.1
5	1	0	22.08	4.025	4	8.1	4	4	2	32.54	2.751	4	0.4	10	2	0	45.04	2.013	4	0.2
5	1	2	22.17	4.009	4	0.9	-4	0	3	33.41	2.682	2	1.0	7	5	0	45.37	1.999	4	0.3
4	2	2	22.63	3.929	4	0.1	-1	1	4	33.52	2.674	4	0.3	-1	3	5	45.85	1.979	4	0.1
1	1	3	22.95	3.874	4	2.0	8	0	3	33.57	2.669	2	0.8	-5	5	2	45.91	1.977	4	0.1
3	1	3	22.99	3.868	4	3.5	8	0	0	33.97	2.639	2	0.3	-3	1	5	46.10	1.969	4	0.3
0	0	3	23.13	3.845	2	5.0	-7	1	1	33.99	2.637	4	0.3	7	1	6	46.48	1.954	4	0.1
4	0	3	23.21	3.833	2	7.2	-4	4	1	34.14	2.626	4	0.3	10	0	5	46.72	1.944	2	0.2
3	3	0	23.66	3.761	4	0.2	-1	5	1	35.10	2.557	4	0.1	-9	1	2	47.29	1.922	4	0.4
-2	2	2	24.09	3.694	4	0.3	7	1	4	35.11	2.556	4	0.6	11	1	0	47.89	1.899	4	0.2
-3	1	2	24.14	3.686	4	1.7	0	4	3	35.62	2.521	4	0.8	1	7	0	47.89	1.899	4	0.4
6	0	2	24.44	3.642	2	2.0	4	4	3	35.67	2.517	4	0.7	-8	0	3	48.35	1.883	2	0.1
-4	2	1	24.81	3.588	4	0.6	7	3	0	35.97	2.496	4	0.1	-10	2	1	48.51	1.877	4	0.2
6	0	0	25.31	3.518	2	0.9	3	5	0	35.97	2.496	4	0.5	10	2	5	48.78	1.867	4	0.2
2	2	3	25.40	3.507	4	1.2	4	0	5	36.46	2.464	2	0.3	11	3	2	48.79	1.866	4	0.2
3	3	2	25.67	3.471	4	0.3	8	2	0	36.62	2.454	4	0.4	9	3	5	48.80	1.866	4	0.2
-5	1	1	25.82	3.450	4	0.9	6	4	0	37.13	2.421	4	1.3	-4	6	2	49.20	1.852	4	0.1
5	1	3	25.98	3.430	4	0.2	3	5	2	37.38	2.406	4	0.3	3	7	0	49.52	1.841	4	0.1
-1	3	2	26.55	3.358	4	0.4	-5	1	3	37.48	2.400	4	0.2	6	6	3	49.70	1.834	4	0.2

CIT-1

CON



CZP Chiral Sodium Zincophosphate, $P6_122$

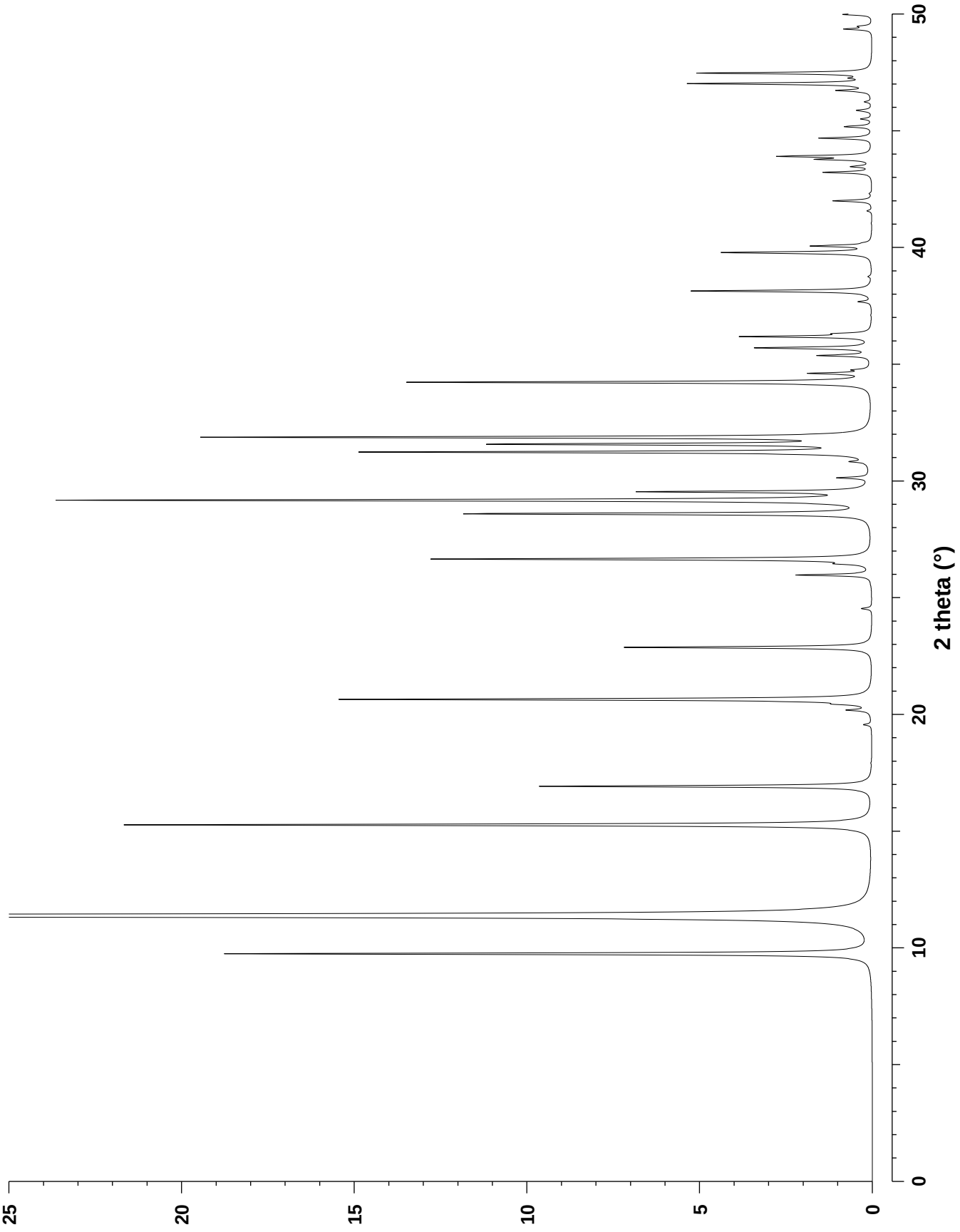
CHEMICAL COMPOSITION: $|Na_{12}(H_2O)_{12}|\ [Zn_{12}P_{12}O_{48}]$

REFINED COMPOSITION: $|Na_{6.06}O_{9.12}|\ [Zn_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P6_122$ (No. 178)
$a = 10.4797$ Å $b = 10.4797$ Å $c = 15.089$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 120.0°$
X-ray single crystal refinement, $R = 0.0599$, $R_w = 0.0529$

REFERENCE: W. T. A. Harrison, T. E. Gier, G. D. Stucky, R. W. Broach and R. A. Bedard, *Chemistry of Materials* **8** 145–151 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	9.75	9.076	6	18.7	2	1	3	31.57	2.834	24	10.6	3	1	4	43.21	2.094	24	1.4
1	0	1	11.38	7.777	12	100.0	3	0	2	31.87	2.808	12	19.2	3	2	0	43.46	2.082	12	0.6
1	0	2	15.27	5.802	12	21.7	2	2	0	34.22	2.620	6	13.4	4	0	3	43.77	2.068	12	1.4
1	1	0	16.92	5.240	6	9.6	3	0	3	34.60	2.592	12	1.7	3	2	1	43.90	2.063	24	2.6
2	0	0	19.56	4.538	6	0.2	2	2	1	34.75	2.581	12	0.4	2	1	6	44.68	2.028	24	1.5
1	0	3	20.18	4.399	12	0.6	2	1	4	35.37	2.538	24	1.5	3	2	2	45.17	2.007	24	0.8
2	0	1	20.44	4.346	12	0.6	3	1	0	35.67	2.517	12	0.7	1	1	7	45.50	1.993	12	0.3
1	1	2	20.64	4.304	12	15.4	0	0	6	35.70	2.515	2	2.8	2	2	5	45.87	1.978	12	0.4
2	0	2	22.87	3.889	12	7.2	3	1	1	36.18	2.483	24	3.7	4	1	1	46.23	1.964	24	0.2
1	1	3	24.53	3.629	12	0.3	2	2	2	36.30	2.475	12	0.8	2	0	7	46.65	1.947	12	0.1
2	1	0	25.97	3.430	12	2.2	3	1	2	37.67	2.388	24	0.4	4	0	4	46.72	1.944	12	0.9
2	0	3	26.45	3.369	12	0.6	3	0	4	38.13	2.360	12	5.2	3	0	6	46.98	1.934	12	0.3
2	1	1	26.65	3.345	24	12.7	4	0	0	39.73	2.269	6	0.5	3	1	5	47.01	1.933	24	5.1
2	1	2	28.59	3.123	24	11.7	1	1	6	39.76	2.267	12	0.9	3	2	3	47.25	1.924	24	0.4
1	1	4	29.17	3.061	12	23.5	2	1	5	39.78	2.266	24	3.4	4	1	2	47.46	1.916	24	5.0
3	0	0	29.53	3.025	6	6.5	3	1	3	40.06	2.251	24	1.7	1	0	8	49.35	1.847	12	0.8
3	0	1	30.13	2.966	12	0.9	4	0	1	40.19	2.244	12	0.1	4	1	3	49.46	1.843	24	0.3
2	0	4	30.82	2.901	12	0.5	4	0	2	41.56	2.173	12	0.1	2	1	7	49.97	1.825	24	0.9
1	0	5	31.23	2.864	12	14.6	2	2	4	41.99	2.152	12	1.1							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CZP Chiral Sodium Zincophosphate, $P6_522$

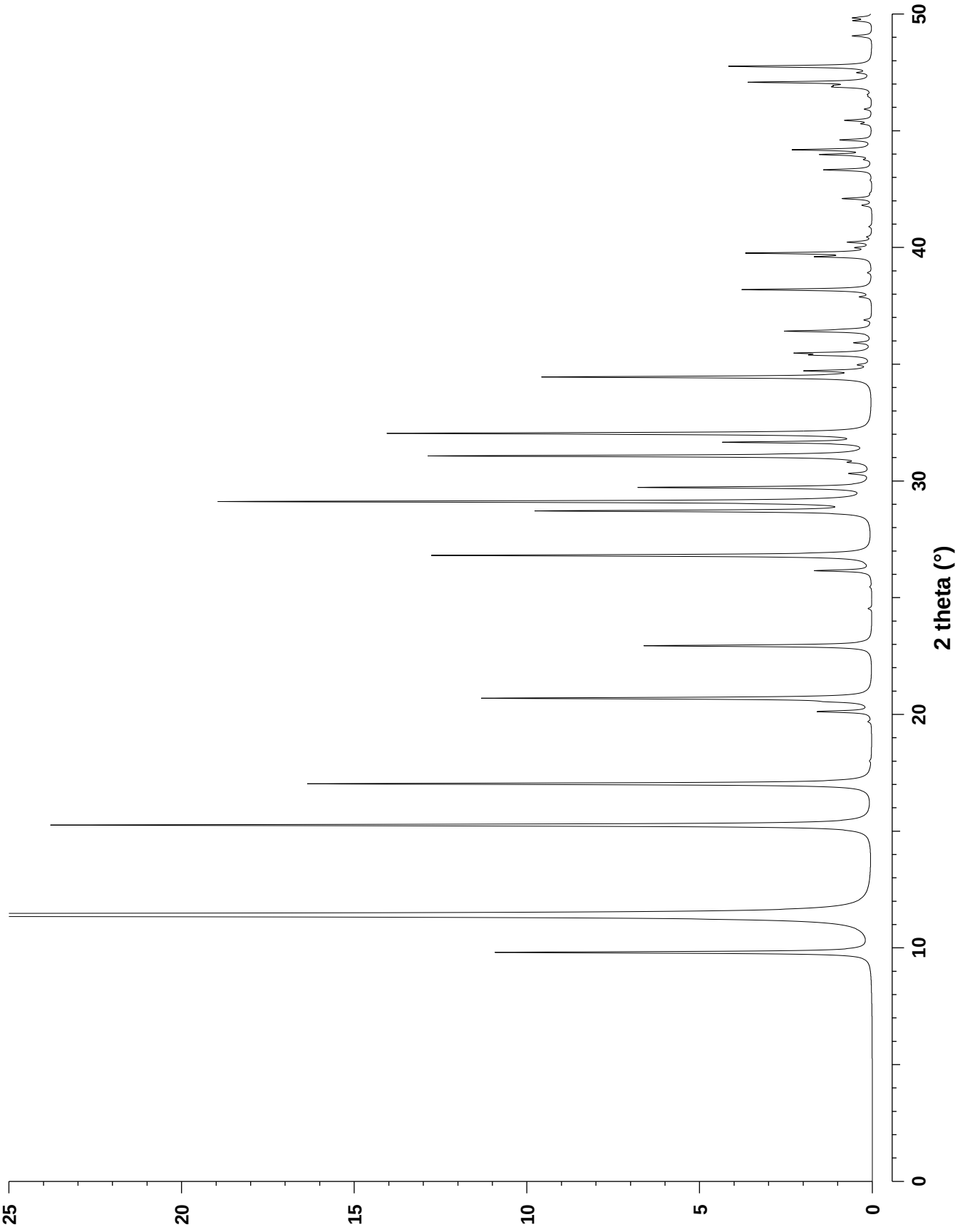
CHEMICAL COMPOSITION: $|Na_{12}(H_2O)_{12}|\ [Zn_{12}P_{12}O_{48}]$

REFINED COMPOSITION: $|Na_{2.04}O_{4.08}|\ [Zn_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P6_522$ (No. 179)
$a = 10.412$ Å $b = 10.412$ Å $c = 15.184$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 120.0°$
X-ray single crystal refinement, $R = 0.0690$, $R_w = 0.0810$

REFERENCE: W. T. A. Harrison, T. E. Gier, G. D. Stucky, R. W. Broach and R. A. Bedard, *Chemistry of Materials* **8** 145–151 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	9.81	9.017	6	10.9	3	0	2	32.03	2.795	12	14.0	4	0	2	41.80	2.161	12	0.3
1	0	1	11.41	7.753	12	100.0	2	2	0	34.45	2.603	6	9.5	2	2	4	42.09	2.147	12	0.9
1	0	2	15.26	5.808	12	23.8	3	0	3	34.71	2.584	12	1.7	3	1	4	43.32	2.088	24	1.4
1	1	0	17.03	5.206	6	16.4	2	2	1	34.97	2.566	12	0.3	3	2	0	43.76	2.069	12	0.2
1	0	3	20.12	4.414	12	1.5	2	1	4	35.39	2.536	24	1.4	4	0	3	43.97	2.059	12	1.4
2	0	1	20.55	4.322	12	0.6	0	0	6	35.47	2.531	2	2.0	3	2	1	44.18	2.050	24	2.3
1	1	2	20.69	4.294	12	11.3	3	1	0	35.91	2.501	12	0.5	2	1	6	44.60	2.032	24	0.9
2	0	2	22.94	3.877	12	6.6	3	1	1	36.41	2.468	24	2.4	1	1	7	45.29	2.002	12	0.3
1	1	3	24.53	3.629	12	0.1	2	2	2	36.49	2.462	12	0.5	3	2	2	45.44	1.996	24	0.8
2	1	0	26.15	3.408	12	1.6	1	0	6	36.89	2.437	12	0.2	2	2	5	45.92	1.976	12	0.2
2	1	1	26.81	3.325	24	12.8	3	1	2	37.88	2.375	24	0.3	4	0	4	46.87	1.938	12	0.8
2	1	2	28.71	3.109	24	9.6	3	0	4	38.19	2.356	12	3.8	3	0	6	46.93	1.936	12	0.6
1	1	4	29.11	3.067	12	18.8	2	2	3	38.91	2.315	12	0.1	3	1	5	47.07	1.931	24	3.5
3	0	0	29.72	3.006	6	6.7	1	1	6	39.60	2.276	12	1.4	3	2	3	47.48	1.915	24	0.3
3	0	1	30.31	2.948	12	0.6	2	1	5	39.75	2.267	24	3.6	4	1	2	47.75	1.905	24	4.1
2	0	4	30.79	2.904	12	0.4	4	0	0	39.99	2.254	6	0.4	1	0	8	49.05	1.857	12	0.6
1	0	5	31.07	2.878	12	12.8	3	1	3	40.22	2.242	24	0.7	4	1	3	49.71	1.834	24	0.5
2	1	3	31.65	2.827	24	4.1	4	0	1	40.45	2.230	12	0.1	2	1	7	49.83	1.830	24	0.5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DAC Dachiardite

CHEMICAL COMPOSITION: $|Na_{0.42}K_{0.92}Cs_{0.11}Ca_{1.54}Sr_{0.12}Ba_{0.01}(H_2O)_{12.56}|\ [Si_{18.96}Al_{4.86}Fe_{0.02}O_{48}]$
Elba, Italy

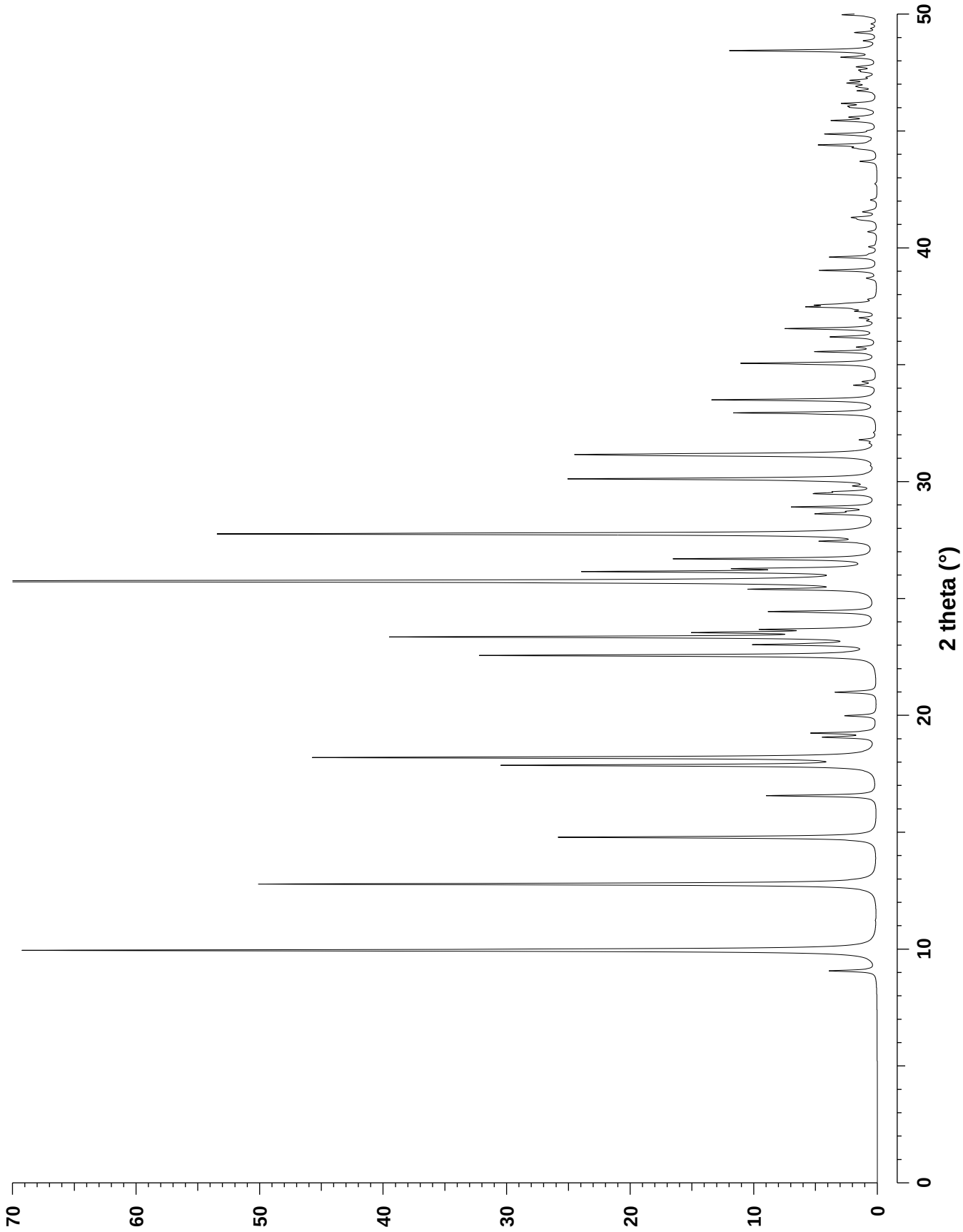
REFINED COMPOSITION: $|K_{0.62}Ca_{2.76}(H_2O)_{12}|\ [Si_{19.2}Al_{4.8}O_{48}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 18.676$ Å $b = 7.518$ Å $c = 10.246$ Å
$\alpha = 90°$ $\beta = 107.87°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: G. Vezzalini,
Z. Kristallogr. **166** 63–71 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	9.07	9.752	2	3.8	5	1	1	31.64	2.828	4	0.3	5	3	0	44.22	2.048	4	0.8
2	0	0	9.95	8.887	2	69.6	1	1	3	31.78	2.816	4	1.3	0	2	4	44.28	2.045	4	1.2
1	1	0	12.78	6.924	4	50.3	2	0	3	32.09	2.789	2	0.2	-2	0	5	44.39	2.041	2	4.6
-1	1	1	14.78	5.994	4	25.9	-4	2	2	32.93	2.720	4	11.6	8	0	1	44.51	2.035	2	0.2
1	1	1	16.56	5.352	4	9.0	2	2	2	33.49	2.676	4	13.4	-7	1	4	44.56	2.033	4	0.2
-2	0	2	17.86	4.965	2	29.9	-6	0	3	34.12	2.627	2	1.8	-4	0	5	44.64	2.030	2	0.1
0	0	2	18.19	4.876	2	45.5	4	2	1	34.27	2.616	4	1.0	5	1	3	44.82	2.022	4	0.8
-3	1	1	19.05	4.659	4	2.0	-2	0	4	35.05	2.560	2	11.0	-5	3	2	44.86	2.020	4	3.8
3	1	0	19.07	4.654	4	2.3	-2	2	3	35.55	2.525	4	4.9	-1	3	3	45.00	2.014	4	0.4
-4	0	1	19.24	4.613	2	5.1	-7	1	1	35.75	2.512	4	1.4	-3	3	3	45.39	1.998	4	0.4
4	0	0	19.98	4.444	2	2.6	-4	0	4	36.18	2.483	2	2.7	3	3	2	45.44	1.996	4	3.4
-1	1	2	20.99	4.232	4	3.4	1	3	0	36.20	2.481	4	1.2	-9	1	2	45.57	1.990	4	1.0
-4	0	2	22.56	3.941	2	32.1	-7	1	2	36.53	2.460	4	0.6	-9	1	1	45.60	1.989	4	1.3
-3	1	2	23.02	3.863	4	8.7	0	2	3	36.54	2.459	4	6.8	-3	1	5	45.91	1.977	4	0.2
3	1	1	23.08	3.854	4	1.7	0	0	4	36.87	2.438	2	0.6	3	1	4	46.00	1.973	4	1.5
2	0	2	23.35	3.810	2	38.7	-1	3	1	37.00	2.430	4	1.3	-8	0	4	46.06	1.971	2	1.6
1	1	2	23.54	3.780	4	12.6	-3	1	4	37.28	2.412	4	1.4	-8	2	2	46.17	1.966	4	2.6
0	2	0	23.67	3.759	2	7.8	3	1	3	37.37	2.406	4	0.8	7	1	2	46.71	1.945	4	1.5
4	0	1	24.43	3.644	2	8.6	-4	2	3	37.47	2.400	4	4.8	-1	1	5	46.86	1.939	4	0.8
0	2	1	25.39	3.507	4	9.0	5	1	2	37.55	2.395	4	3.8	5	3	1	46.91	1.937	4	1.1
2	2	0	25.73	3.462	4	100.0	-1	1	4	37.62	2.391	4	1.2	1	3	3	47.01	1.933	4	0.3
-2	0	3	26.14	3.409	2	22.2	1	3	1	37.79	2.381	4	0.5	-6	2	4	47.04	1.932	4	1.9
-2	2	1	26.27	3.393	4	9.2	-6	2	2	38.65	2.329	4	0.2	6	2	2	47.16	1.927	4	1.9
-5	1	1	26.69	3.340	4	16.1	6	2	0	38.70	2.327	4	0.7	-6	0	5	47.29	1.922	2	0.5
0	0	3	27.44	3.251	2	3.8	4	0	3	39.03	2.308	2	4.7	-5	1	5	47.34	1.920	4	0.1
5	1	0	27.76	3.214	4	53.5	-7	1	3	39.60	2.276	4	3.8	-9	1	3	47.52	1.914	4	0.7
-4	0	3	28.62	3.119	2	4.6	-5	1	4	39.73	2.269	4	0.3	8	2	0	47.54	1.913	4	0.4
-5	1	2	28.72	3.109	4	1.5	-6	0	4	40.04	2.252	2	0.6	9	1	0	47.60	1.910	4	1.1
-1	1	3	28.91	3.088	4	6.7	1	1	4	40.68	2.218	4	0.7	4	0	4	47.74	1.905	2	1.5
-3	1	3	29.48	3.030	4	4.5	7	1	1	41.18	2.192	4	0.7	-5	3	3	48.14	1.890	4	0.2
3	1	2	29.56	3.022	4	2.5	-3	3	2	41.22	2.190	4	0.8	2	2	4	48.15	1.890	4	2.5
-2	2	2	29.81	2.997	4	1.3	3	3	1	41.26	2.188	4	0.3	0	4	0	48.43	1.880	2	11.9
0	2	2	30.02	2.977	4	1.8	2	0	4	41.30	2.186	2	1.7	-10	0	2	48.85	1.864	2	1.0
-6	0	2	30.11	2.968	2	24.3	1	3	2	41.53	2.174	4	1.1	-10	0	1	49.20	1.852	2	1.8
6	0	0	30.17	2.962	2	1.5	-8	0	3	41.60	2.171	2	0.3	0	4	1	49.38	1.846	4	0.4
-4	2	1	30.68	2.914	4	0.2	6	2	1	42.04	2.149	4	0.5	2	4	0	49.57	1.839	4	0.4
4	0	2	31.11	2.874	2	10.7	-2	2	4	42.73	2.116	4	0.2	-2	4	1	49.88	1.828	4	0.2
4	2	0	31.16	2.870	4	20.4	-4	2	4	43.69	2.072	4	1.4	-7	3	1	49.96	1.826	4	2.8

Dachiardite DAC



DDR N_2, 1-aminoadamantane Deca-Dodecasil 3R

CHEMICAL COMPOSITION: $|(C_{10}H_{17}N)_6(N_2)_9|\ [Si_{120}O_{240}]$
$C_{10}H_{17}N$ = 1-aminoadamantane

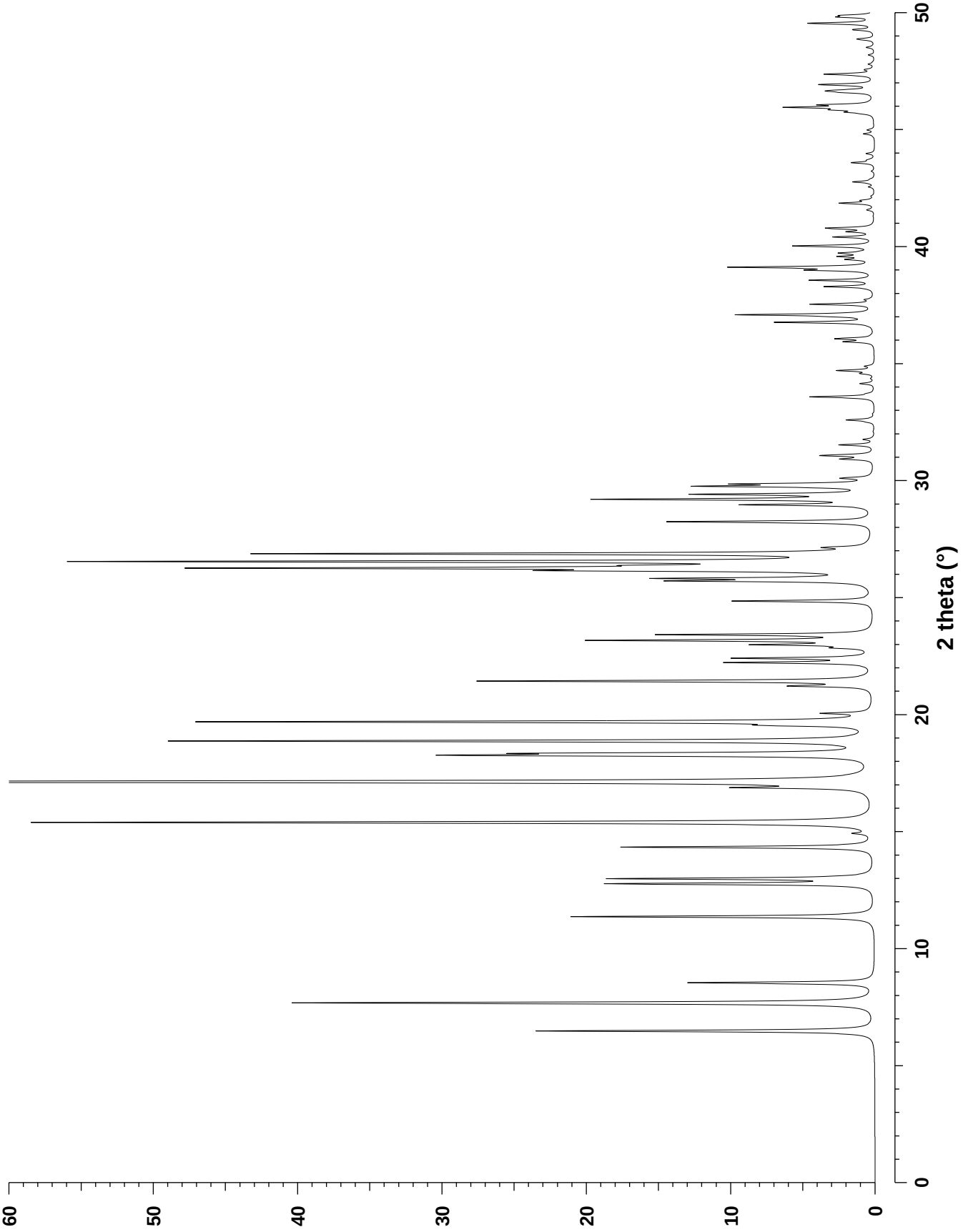
REFINED COMPOSITION: $|C_{69}N_6|\ [Si_{120}O_{240}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.860$ Å $b = 13.860$ Å $c = 40.891$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.066$

REFERENCE: H. Gies,
Z. Kristallogr. **175** 93–104 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	3	6.48	13.630	2	23.5	0	4	2	30.10	2.969	6	2.0	5	1	1	41.97	2.153	12	0.8
1	0	1	7.68	11.517	6	40.5	1	3	7	30.92	2.892	12	2.1	1	5	2	42.15	2.144	12	0.2
0	1	2	8.54	10.351	6	12.9	4	0	4	31.06	2.879	6	3.2	1	2	17	42.54	2.125	12	0.4
1	0	4	11.37	7.783	6	21.1	1	2	11	31.10	2.875	12	0.9	1	0	19	42.68	2.118	6	0.1
1	1	0	12.77	6.930	6	18.2	0	1	14	31.52	2.838	6	2.4	2	4	7	42.76	2.115	12	1.5
0	0	6	12.99	6.815	2	18.0	0	4	5	31.76	2.817	6	0.7	5	1	4	42.87	2.109	12	0.2
0	1	5	13.10	6.759	6	0.6	2	2	9	32.50	2.755	12	0.3	0	4	14	43.22	2.093	6	0.2
1	1	3	14.34	6.177	12	17.5	3	2	1	32.59	2.747	12	1.9	4	1	12	43.58	2.077	12	0.9
0	2	1	14.92	5.938	6	1.1	4	0	7	33.57	2.669	6	4.5	1	4	12	43.58	2.077	12	0.8
2	0	2	15.39	5.759	6	58.5	3	2	4	33.71	2.659	12	0.3	3	2	13	43.69	2.072	12	0.3
1	0	7	16.88	5.253	6	7.5	2	0	14	34.14	2.626	6	1.0	0	5	10	43.72	2.070	6	0.1
0	2	4	17.13	5.176	6	100.0	2	3	5	34.36	2.610	12	0.2	3	3	9	43.97	2.059	12	0.6
1	1	6	18.26	4.859	12	26.1	3	0	12	34.57	2.594	6	0.5	5	1	7	44.81	2.022	12	0.8
2	0	5	18.34	4.838	6	19.9	0	3	12	34.57	2.594	6	0.4	0	1	20	44.98	2.016	6	0.5
0	1	8	18.87	4.703	6	48.7	2	1	13	34.70	2.585	12	2.5	1	5	8	45.67	1.986	12	0.4
0	0	9	19.54	4.543	2	5.0	4	1	3	34.88	2.572	12	0.6	2	4	10	45.74	1.984	12	1.5
2	1	1	19.69	4.509	12	46.7	1	0	16	35.93	2.500	6	2.0	0	6	3	45.84	1.979	6	1.4
1	2	2	20.05	4.429	12	3.1	3	2	7	36.06	2.491	12	2.6	6	0	3	45.84	1.979	6	0.7
0	2	7	21.22	4.186	6	5.1	4	1	6	36.76	2.445	12	0.2	0	3	18	45.94	1.976	6	2.6
2	1	4	21.43	4.147	12	27.4	1	4	6	36.76	2.445	12	6.6	3	0	18	45.94	1.976	6	3.0
3	0	0	22.22	4.001	6	10.0	2	2	12	37.00	2.430	12	1.4	4	3	1	46.05	1.971	12	3.3
1	2	5	22.41	3.967	12	9.4	2	3	8	37.08	2.424	12	9.2	3	1	17	46.58	1.950	12	1.5
2	0	8	22.85	3.891	6	2.0	4	0	10	37.16	2.419	6	0.3	0	0	21	46.64	1.947	2	2.1
1	0	10	22.98	3.871	6	7.5	0	5	1	37.53	2.396	6	4.4	4	0	16	46.68	1.946	6	1.5
3	0	3	23.17	3.839	6	9.9	5	0	2	37.73	2.384	6	0.5	4	3	4	46.89	1.938	12	1.0
0	3	3	23.17	3.839	6	9.4	0	2	16	38.28	2.351	6	3.4	4	2	11	46.92	1.936	12	3.1
1	1	9	23.41	3.800	12	14.6	0	4	11	38.56	2.335	6	4.4	5	2	0	47.29	1.922	12	0.5
2	1	7	24.85	3.583	12	9.8	3	3	0	38.99	2.310	6	3.9	6	0	6	47.36	1.920	6	2.7
2	2	0	25.71	3.465	6	12.5	5	0	5	39.11	2.303	6	9.8	0	6	6	47.36	1.920	6	0.6
0	3	6	25.82	3.450	6	10.6	1	3	13	39.41	2.286	12	0.1	3	4	5	47.39	1.918	12	0.1
3	0	6	25.82	3.450	6	2.7	3	2	10	39.45	2.284	12	1.6	3	3	12	47.55	1.912	12	0.6
0	0	12	26.15	3.408	2	17.4	3	3	3	39.57	2.278	12	2.1	2	5	3	47.79	1.903	12	0.3
1	2	8	26.26	3.393	12	43.4	0	0	18	39.67	2.272	2	0.5	5	2	3	47.79	1.903	12	0.1
0	2	10	26.37	3.379	6	8.9	4	1	9	39.72	2.269	12	1.9	4	1	15	48.18	1.889	12	0.1
2	2	3	26.54	3.358	12	53.9	2	4	1	39.80	2.265	12	0.4	1	4	15	48.18	1.889	12	0.3
1	3	1	26.87	3.318	12	42.2	4	2	2	39.99	2.255	12	0.7	0	4	17	48.50	1.877	6	0.6
3	1	2	27.14	3.286	12	2.4	3	0	15	40.02	2.253	6	3.0	1	5	11	48.83	1.865	12	0.3
1	3	4	28.19	3.165	12	1.3	0	3	15	40.02	2.253	6	2.2	1	2	20	48.86	1.864	12	1.1
2	0	11	28.24	3.160	6	13.8	2	0	17	40.40	2.233	6	2.8	2	5	6	49.26	1.850	12	1.2
3	1	5	28.96	3.083	12	8.7	0	5	7	40.63	2.220	6	1.7	5	2	6	49.26	1.850	12	0.2
1	1	12	29.20	3.058	12	18.9	2	4	4	40.74	2.215	12	0.3	3	4	8	49.51	1.841	12	1.0
1	0	13	29.35	3.043	6	0.9	2	3	11	40.78	2.213	12	3.2	2	4	13	49.54	1.840	12	4.0
2	1	10	29.41	3.037	12	11.7	5	0	8	41.56	2.173	6	0.4	6	0	9	49.80	1.831	6	0.1
3	0	9	29.75	3.003	6	11.3	4	0	13	41.59	2.171	6	0.1	0	6	9	49.80	1.831	6	2.0
4	0	1	29.85	2.993	6	8.4	1	1	18	41.85	2.159	12	2.4	1	6	1	49.87	1.829	12	2.0

N_2, 1-aminoadamantane Deca-Dodecasil 3R DDR



CHEMICAL COMPOSITION: $|(C_{16}H_{38}N_2)_{7.92}(H_2O)_{40.26}|\ [Mg_{14.52}Al_{51.48}P_{66}O_{264}]$
$C_{16}H_{38}N_2^{2+}$ = decamethonium ion

REFINED COMPOSITION: $|C_{23}|\ [Si_{132}O_{264}]$

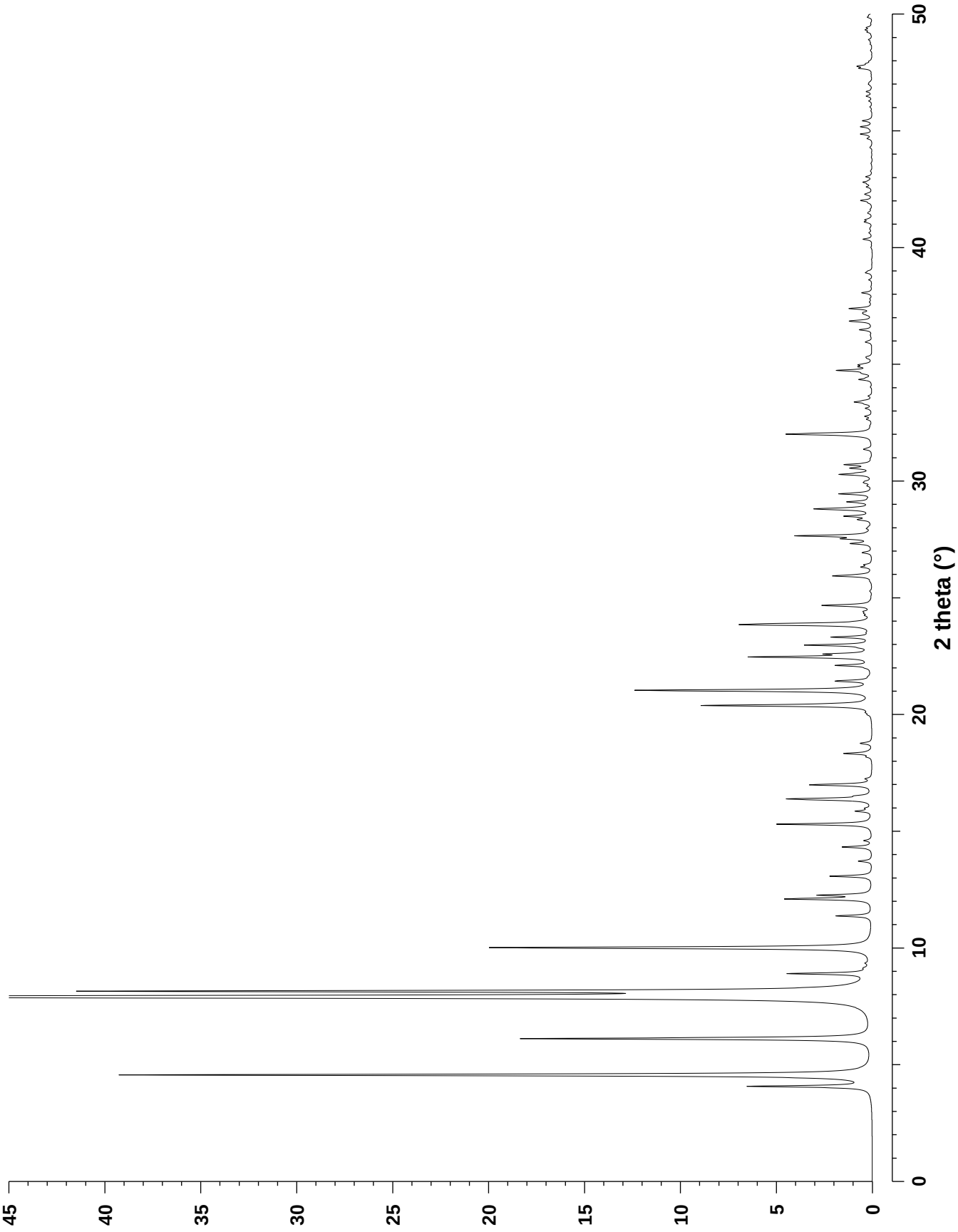
CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 22.351$ Å $b = 22.351$ Å $c = 21.693$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.122$

REFERENCE: P. A. Wright, R. H. Jones, S. Natarajan, R. G. Bell, J. Chen, M. B. Hursthouse and J. M. Thomas, *J. Chem. Soc., Chem. Comm.* 633–635 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	4.07	21.693	2	6.3	4	2	0	24.33	3.658	12	0.2	2	0	8	34.34	2.611	12	0.6
1	0	0	4.56	19.357	6	39.6	5	0	2	24.41	3.646	12	0.2	6	2	2	34.42	2.606	24	0.2
1	0	1	6.12	14.443	12	18.5	4	0	4	24.66	3.611	12	1.6	6	1	4	34.60	2.593	24	0.3
1	1	0	7.91	11.175	6	100.0	4	2	1	24.68	3.607	24	1.2	5	3	3	34.73	2.583	24	0.8
0	0	2	8.15	10.846	2	39.2	3	2	4	25.93	3.436	24	1.8	7	0	3	34.73	2.583	12	1.0
1	1	1	8.90	9.935	12	4.2	5	1	1	25.96	3.433	24	0.3	4	2	6	34.89	2.571	24	0.5
2	0	0	9.14	9.678	6	0.2	2	2	5	26.00	3.427	12	0.2	4	3	5	34.97	2.566	24	0.5
1	0	2	9.35	9.462	12	0.2	2	0	6	26.31	3.387	12	0.5	7	1	0	35.00	2.564	12	0.2
2	0	1	10.01	8.839	12	20.1	3	1	5	26.41	3.374	24	0.4	7	1	1	35.25	2.546	24	0.2
1	1	2	11.37	7.783	12	1.9	5	1	2	26.93	3.311	24	0.5	3	2	7	35.32	2.541	24	0.2
2	1	0	12.10	7.316	12	4.5	4	2	3	27.32	3.264	24	1.1	4	1	7	35.94	2.499	24	0.3
2	0	2	12.26	7.221	12	2.6	2	1	6	27.52	3.241	24	1.3	7	0	4	36.47	2.463	12	0.6
1	0	3	13.07	6.774	12	2.2	6	0	0	27.65	3.226	6	4.0	6	1	5	36.83	2.441	24	0.8
3	0	0	13.72	6.452	6	0.7	6	0	1	27.96	3.191	12	0.2	6	3	0	36.86	2.439	12	0.5
3	0	1	14.32	6.184	12	1.6	5	0	4	28.32	3.151	12	0.3	8	0	0	37.16	2.420	6	0.2
2	1	2	14.60	6.065	24	0.4	4	3	1	28.35	3.148	24	0.5	7	1	3	37.21	2.416	24	0.3
2	0	3	15.30	5.793	12	5.0	5	1	3	28.49	3.133	24	1.4	6	2	4	37.38	2.406	24	1.1
2	2	0	15.86	5.588	6	0.8	3	2	5	28.77	3.103	24	0.9	8	0	1	37.40	2.405	12	0.2
3	0	2	15.98	5.545	12	0.3	5	2	0	28.80	3.100	12	1.3	7	2	0	38.05	2.365	12	0.4
0	0	4	16.34	5.423	2	0.9	0	0	7	28.81	3.099	2	1.2	7	0	5	38.61	2.332	12	0.2
2	2	1	16.38	5.411	12	4.0	6	0	2	28.87	3.092	12	0.2	3	2	8	38.91	2.314	24	0.3
3	1	0	16.51	5.369	12	0.6	5	2	1	29.10	3.068	24	1.1	6	3	3	38.98	2.311	24	0.2
1	0	4	16.98	5.222	12	2.8	4	2	4	29.45	3.033	24	1.7	5	5	0	40.35	2.235	6	0.4
3	1	1	17.01	5.211	24	0.8	3	1	6	29.79	2.999	24	0.2	7	0	6	41.09	2.196	12	0.2
2	1	3	17.24	5.143	24	0.3	1	1	7	29.92	2.986	12	0.3	3	3	8	41.18	2.192	12	0.3
1	1	4	18.18	4.879	12	0.2	5	2	2	29.98	2.980	24	0.3	7	3	0	41.46	2.178	12	0.2
4	0	0	18.33	4.839	6	1.5	6	1	0	30.28	2.952	12	0.9	9	0	0	42.01	2.151	6	0.5
2	0	4	18.76	4.731	12	0.5	2	0	7	30.28	2.951	12	0.7	5	1	8	42.27	2.138	24	0.3
4	0	1	18.79	4.723	12	0.2	6	0	3	30.34	2.946	12	0.3	6	4	3	42.59	2.123	24	0.3
2	2	3	20.08	4.421	12	0.2	5	1	4	30.54	2.927	24	0.7	2	0	10	42.71	2.117	12	0.2
2	1	4	20.38	4.357	24	8.1	6	1	1	30.56	2.925	24	0.4	8	0	5	42.79	2.113	12	0.4
3	2	1	20.41	4.350	24	1.2	4	3	3	30.70	2.913	24	1.4	8	2	1	43.03	2.102	24	0.3
0	0	5	20.47	4.339	2	0.6	2	1	7	31.35	2.854	24	0.4	9	1	0	44.66	2.029	12	0.2
1	0	5	20.98	4.234	12	0.4	3	2	6	31.92	2.804	24	0.4	7	3	4	44.85	2.021	24	0.6
4	1	0	21.03	4.224	12	12.3	4	2	5	32.00	2.797	24	3.6	7	4	0	45.17	2.007	12	0.6
4	1	1	21.43	4.146	24	1.8	4	4	0	32.03	2.794	6	1.2	6	1	8	45.42	1.997	24	0.5
4	0	3	22.10	4.022	12	1.8	3	0	7	32.04	2.793	12	0.2	1	0	11	46.27	1.962	12	0.2
2	0	5	22.46	3.959	12	6.3	7	0	1	32.64	2.743	12	0.2	9	1	3	46.48	1.954	24	0.2
4	1	2	22.59	3.936	24	2.0	6	1	3	32.77	2.733	24	0.4	7	3	5	46.67	1.946	24	0.3
2	2	4	22.85	3.892	12	0.3	4	4	2	33.11	2.706	12	0.3	6	2	8	47.67	1.908	24	0.5
5	0	0	22.97	3.871	6	3.4	5	2	4	33.29	2.691	24	0.2	2	1	11	47.76	1.904	24	0.7
3	1	4	23.31	3.815	24	2.1	1	0	8	33.37	2.685	12	0.5	3	1	11	49.22	1.851	24	0.2
2	1	5	23.84	3.732	24	5.6	6	2	0	33.38	2.684	12	0.2	8	3	4	49.32	1.848	24	0.3
3	3	0	23.89	3.725	6	3.5	5	3	2	33.44	2.680	24	0.2	9	2	3	49.42	1.844	24	0.3
3	3	1	24.24	3.671	12	0.2	6	2	1	33.64	2.664	24	0.2	8	4	0	49.86	1.829	12	0.2

Decamethonium DAF-1

DFO



DFT Magnesium Phosphate UiO-20

CHEMICAL COMPOSITION: $|(NH_3(CH_2)_2NH_3)_{16}|$ $[Mg_{32}P_{32}O_{128}]$
$NH_2(CH_2)_2NH_2$ = ethylenediamine

REFINED COMPOSITION: $|C_{32}N_{32}|$ $[Mg_{32}P_{32}O_{128}]$

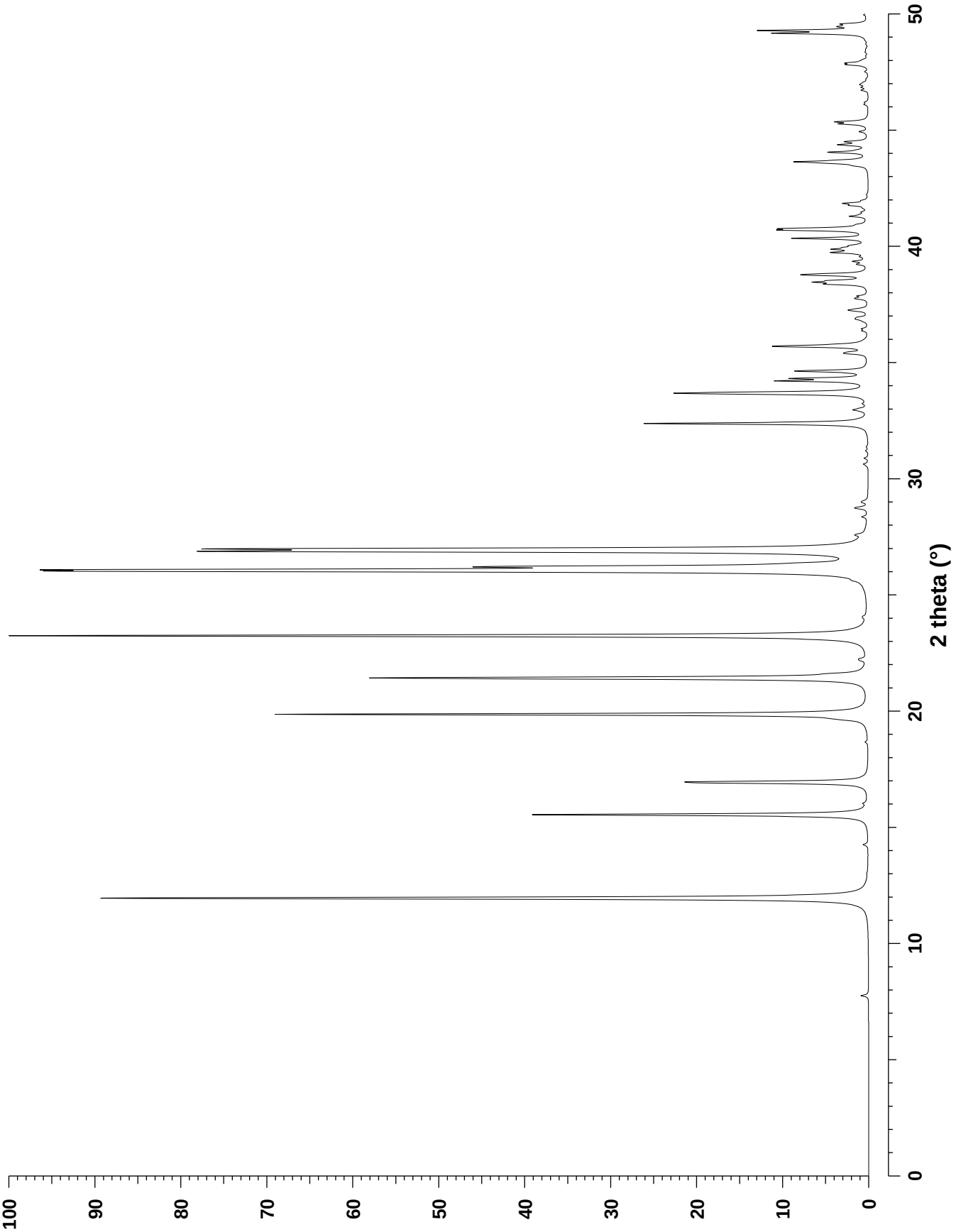
CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 20.9098$ Å $b = 17.8855$ Å $c = 14.7913$ Å
$\alpha = 90.0°$ $\beta = 134.842°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R = 0.1007, R_w = 0.0994$

REFERENCE: K. O. Kongshaug, H. Fjellvåg and K. P. Lillerud,
Chemistry of Materials **12** 1095–1099 (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
-1	1	1	7.76	11.398	4	1.2	-7	1	5	33.02	2.713	4	0.8	-8	4	4	39.95	2.256	4	1.0
2	0	0	11.94	7.413	2	73.7	2	4	2	33.64	2.664	4	8.0	-5	3	6	40.02	2.253	4	1.7
-2	0	2	11.97	7.396	2	71.1	-2	4	4	33.67	2.662	4	13.6	-7	3	6	40.06	2.251	4	0.8
2	2	0	15.53	5.707	4	30.3	-6	4	2	33.69	2.660	4	12.5	0	8	0	40.34	2.236	2	12.3
-2	2	2	15.55	5.699	4	28.5	-6	4	4	33.72	2.658	4	6.5	2	6	2	40.69	2.217	4	11.5
0	0	2	16.91	5.244	2	19.5	0	0	4	34.20	2.622	2	13.8	-6	6	2	40.74	2.215	4	0.6
-4	0	2	16.96	5.227	2	21.7	-8	0	4	34.31	2.614	2	11.1	-6	6	4	40.76	2.214	4	10.7
0	2	2	19.62	4.524	4	1.2	0	6	2	34.61	2.591	4	6.9	2	4	3	40.80	2.212	4	0.8
-4	2	2	19.67	4.513	4	1.4	-4	6	2	34.64	2.589	4	6.6	-8	4	5	40.93	2.205	4	0.9
0	4	0	19.86	4.471	2	97.4	3	5	1	35.38	2.537	4	2.1	0	8	1	41.29	2.187	4	1.4
2	2	1	21.39	4.155	4	17.9	-5	5	1	35.41	2.535	4	1.5	-2	8	1	41.29	2.186	4	1.3
-2	2	3	21.42	4.149	4	29.7	-5	5	4	35.45	2.532	4	1.5	3	5	2	41.36	2.183	4	0.6
-4	2	1	21.42	4.149	4	27.2	-1	7	1	35.66	2.518	4	0.5	-7	5	5	41.47	2.177	4	0.8
-4	2	3	21.45	4.142	4	21.1	0	2	4	35.68	2.516	4	2.6	6	4	0	41.76	2.163	4	2.4
0	4	1	21.60	4.113	4	1.7	2	6	1	35.68	2.516	4	6.5	-6	4	6	41.84	2.159	4	3.5
-2	4	1	21.62	4.111	4	1.2	-4	6	1	35.70	2.515	4	0.9	-9	3	5	41.97	2.153	4	0.5
-5	1	3	22.25	3.996	4	0.5	-2	6	3	35.70	2.515	4	0.9	4	6	1	43.46	2.082	4	0.5
2	4	0	23.23	3.829	4	75.2	-4	6	3	35.72	2.513	4	7.3	4	4	2	43.57	2.077	4	3.5
-2	4	2	23.25	3.826	4	74.9	-8	2	4	35.79	2.509	4	2.6	-4	4	6	43.63	2.074	4	5.3
4	2	0	26.02	3.424	4	100.0	6	0	0	36.36	2.471	2	0.8	-8	4	2	43.63	2.074	4	4.8
-4	2	4	26.08	3.417	4	97.4	-6	0	6	36.45	2.465	2	0.9	-8	4	6	43.70	2.071	4	2.8
0	4	2	26.19	3.402	4	30.5	-2	2	5	36.76	2.445	4	0.5	0	8	2	44.03	2.057	4	3.0
-4	4	2	26.23	3.398	4	32.6	4	4	1	36.86	2.438	4	0.8	-2	0	6	44.05	2.056	2	0.8
1	3	2	26.32	3.387	4	1.2	-4	4	5	36.92	2.435	4	0.7	-4	8	2	44.05	2.056	4	2.9
-1	3	3	26.33	3.385	4	1.7	-6	4	5	36.95	2.433	4	0.9	-10	0	4	44.14	2.052	2	0.8
-5	3	2	26.37	3.380	4	1.3	5	1	1	37.21	2.416	4	1.2	0	2	5	44.36	2.042	4	0.6
-5	3	3	26.38	3.378	4	2.1	-7	1	1	37.25	2.414	4	2.2	6	2	1	44.36	2.042	4	3.8
2	0	2	26.87	3.318	2	83.4	-5	1	6	37.30	2.411	4	1.1	-6	2	7	44.46	2.038	4	0.6
-2	0	4	26.91	3.313	2	21.1	1	7	1	37.73	2.384	4	0.7	-8	2	7	44.50	2.036	4	3.1
-6	0	2	26.94	3.309	2	20.6	6	2	0	37.77	2.382	4	1.1	-2	2	6	45.26	2.003	4	4.0
-6	0	4	26.98	3.305	2	82.8	-6	2	6	37.86	2.377	4	1.5	-10	2	4	45.35	2.000	4	4.8
2	4	1	27.56	3.237	4	0.7	4	0	2	38.37	2.346	2	5.6	0	6	4	46.10	1.969	4	0.6
-4	4	3	27.61	3.231	4	0.7	-4	0	6	38.45	2.341	2	3.3	-8	6	4	46.19	1.965	4	0.6
-1	5	2	28.35	3.148	4	0.5	-8	0	2	38.45	2.341	2	3.5	1	5	4	46.71	1.945	4	0.9
2	2	2	28.70	3.111	4	0.5	-8	0	6	38.52	2.337	2	4.6	-9	5	5	46.84	1.940	4	0.8
-2	2	4	28.73	3.107	4	1.1	4	6	0	38.76	2.323	4	7.4	6	6	0	47.81	1.902	4	2.7
-6	2	2	28.76	3.104	4	0.9	-4	6	4	38.80	2.321	4	6.1	-6	6	6	47.88	1.900	4	2.7
3	3	1	28.98	3.081	4	0.7	-1	1	5	39.23	2.297	4	1.1	-10	4	5	48.03	1.894	4	0.5
-3	5	3	30.88	2.895	4	0.6	-9	1	5	39.35	2.290	4	1.9	8	0	0	49.16	1.853	2	14.1
4	2	1	32.36	2.766	4	0.7	-7	5	4	39.55	2.279	4	0.8	-8	0	8	49.28	1.849	2	16.6
2	6	0	32.37	2.766	4	18.4	4	2	2	39.72	2.269	4	4.3	4	6	2	49.44	1.843	4	3.0
-2	6	2	32.38	2.765	4	18.7	0	6	3	39.74	2.268	4	1.2	-4	6	6	49.50	1.841	4	0.6
3	1	2	32.89	2.723	4	0.5	-6	6	3	39.79	2.265	4	1.2	-8	6	2	49.50	1.841	4	1.0
-3	1	5	32.95	2.719	4	1.0	-8	2	6	39.87	2.261	4	4.2	-8	6	6	49.56	1.839	4	3.5
-7	1	2	32.96	2.717	4	1.0	5	3	1	39.94	2.257	4	1.4	-7	1	8	49.95	1.826	4	0.5

Magnesium Phosphate UiO-20

DFT



DOH N_2, Piperidine Dodecasil 1H

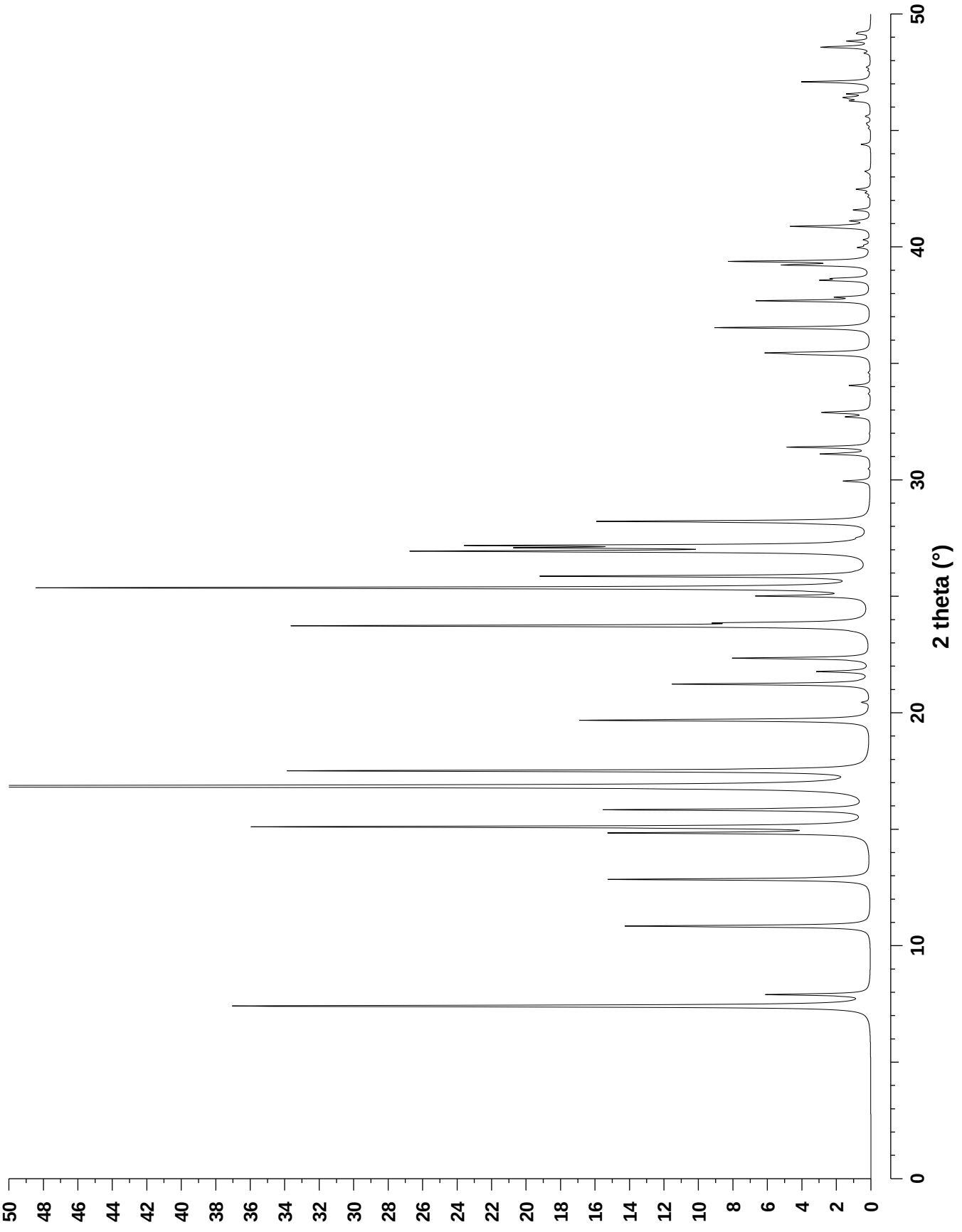
CHEMICAL COMPOSITION: $|(N_2)_3(N_2)_2C_5H_{10}NH|\ [Si_{34}O_{68}]$
$C_5H_{10}NH$ = piperidine

REFINED COMPOSITION: $|C_{15.4}|\ [Si_{34}O_{68}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 13.783$ Å $b = 13.783$ Å $c = 11.190$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.077$

REFERENCE: H. Gerke and H. Gies,
Z. Kristallogr. **166** 11–22 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.41	11.936	6	37.1	2	2	2	30.47	2.934	12	0.1	5	1	0	42.15	2.144	12	0.1
0	0	1	7.90	11.190	2	5.9	2	1	3	31.11	2.875	24	2.9	3	1	4	42.30	2.137	24	0.1
1	0	1	10.84	8.164	12	14.3	3	1	2	31.40	2.849	24	4.8	4	1	3	42.32	2.136	24	0.1
1	1	0	12.85	6.891	6	15.3	3	2	0	32.70	2.738	12	1.4	1	1	5	42.47	2.129	12	0.8
2	0	0	14.84	5.968	6	14.4	1	0	4	32.88	2.724	12	2.2	2	0	5	43.17	2.096	12	0.1
1	1	1	15.10	5.868	12	35.6	3	0	3	32.91	2.721	12	0.9	4	2	2	43.24	2.092	24	0.3
0	0	2	15.84	5.595	2	15.3	3	2	1	33.69	2.660	24	0.1	4	0	4	44.39	2.041	12	0.6
2	0	1	16.84	5.266	12	100.0	4	0	2	34.05	2.633	12	1.3	5	0	3	45.09	2.011	12	0.1
1	0	2	17.51	5.066	12	33.5	1	1	4	34.60	2.592	12	0.1	2	1	5	45.23	2.005	24	0.1
2	1	0	19.68	4.512	12	16.9	4	1	1	35.38	2.537	24	2.6	5	1	2	45.30	2.002	24	0.2
1	1	2	20.45	4.344	12	0.4	2	0	4	35.44	2.533	12	4.7	6	0	0	45.60	1.989	6	0.3
2	1	1	21.23	4.184	24	11.5	2	2	3	35.47	2.531	12	1.0	4	3	0	46.26	1.962	12	1.0
2	0	2	21.77	4.082	12	3.0	3	2	2	36.53	2.460	24	9.1	6	0	1	46.35	1.959	12	0.6
3	0	0	22.34	3.979	6	8.0	5	0	0	37.68	2.387	6	6.6	3	2	4	46.40	1.957	24	0.5
3	0	1	23.73	3.749	12	33.1	2	1	4	37.84	2.378	24	1.7	3	3	3	46.42	1.956	12	0.8
0	0	3	23.86	3.730	2	6.2	5	0	1	38.56	2.335	12	2.6	3	0	5	46.56	1.951	12	1.3
1	0	3	25.01	3.560	12	6.0	4	0	3	38.64	2.330	12	1.8	4	3	1	47.01	1.933	24	0.2
2	1	2	25.36	3.512	24	48.3	3	3	0	39.22	2.297	6	4.7	4	2	3	47.08	1.930	24	4.0
2	2	0	25.86	3.446	6	18.8	3	0	4	39.37	2.288	12	8.0	5	2	0	47.57	1.911	12	0.1
3	1	0	26.93	3.311	12	25.1	4	2	0	39.97	2.256	12	0.7	4	1	4	47.71	1.906	24	0.2
2	2	1	27.08	3.293	12	16.2	3	3	1	40.07	2.250	12	0.3	5	2	1	48.31	1.884	24	0.3
1	1	3	27.18	3.280	12	20.7	0	0	5	40.30	2.238	2	0.4	6	0	2	48.57	1.874	12	2.9
3	0	2	27.51	3.243	12	0.2	4	2	1	40.81	2.211	24	0.9	0	0	6	48.83	1.865	2	1.3
3	1	1	28.11	3.175	24	1.2	3	2	3	40.88	2.207	24	4.4	3	1	5	49.14	1.854	24	0.6
2	0	3	28.21	3.163	12	15.7	5	0	2	41.11	2.196	12	1.1	4	3	2	49.20	1.852	24	0.6
4	0	0	29.94	2.984	6	1.6	2	2	4	41.58	2.172	12	1.0							


0
10
20
30
40
50
2 theta (°)
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0

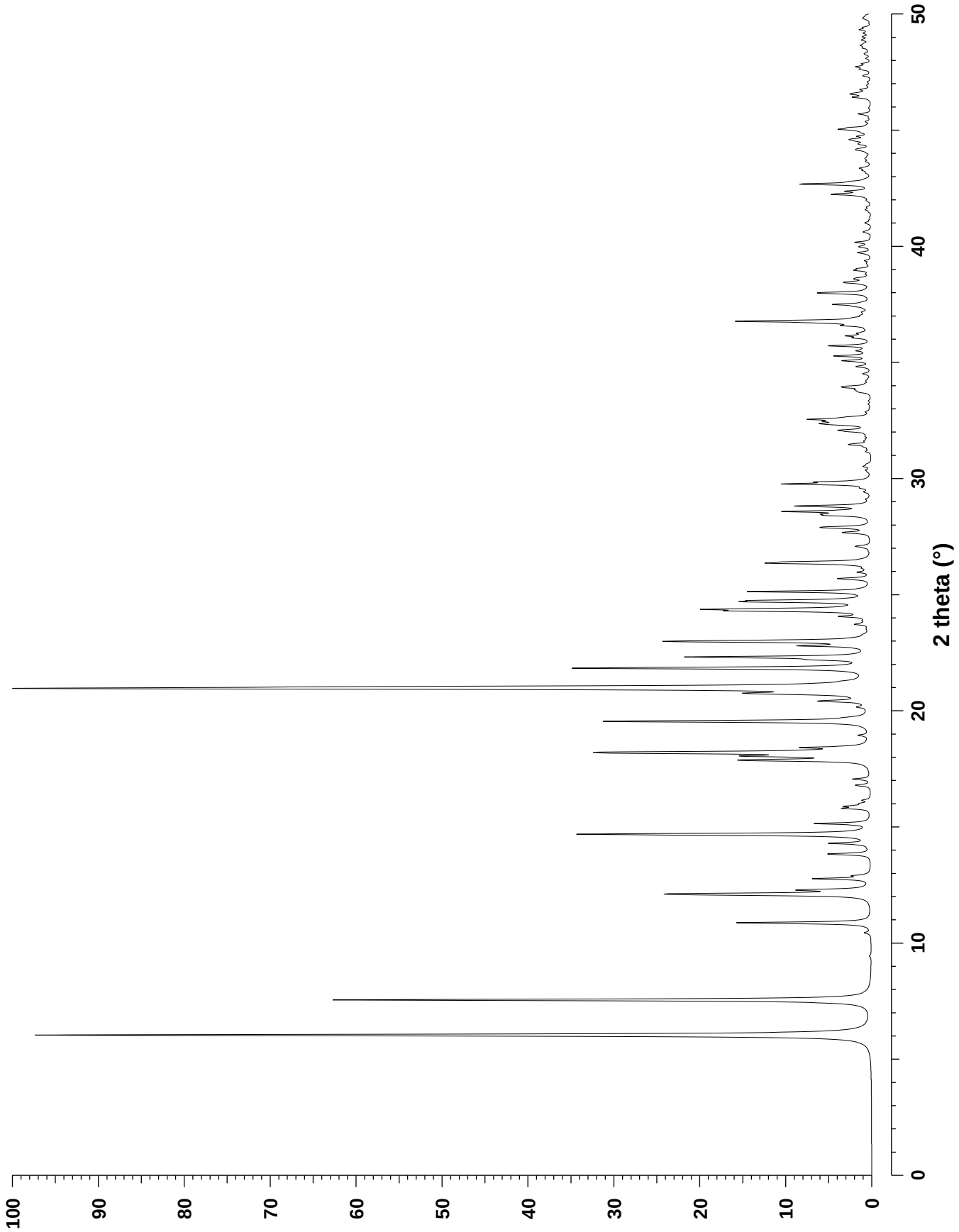
CHEMICAL COMPOSITION: $|((Cp^*)_2CoF_{0.075}OH_{0.25})_2|\ [Si_{64}O_{128}]$
$(Cp^*)_2CoOH$ = bis(pentamethylcyclopentadienyl)cobalt(III) hydroxide

REFINED COMPOSITION: $|Co_2C_{35}|\ [Si_{64}O_{128}]$

CRYSTAL DATA: *Pc* (No. 7) unique axis **b**, cell choice 1
$a = 14.9701$ Å $b = 8.4761$ Å $c = 30.0278$ Å
$\alpha = 90°$ $\beta = 102.65°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_F = 0.041$, $R_{wp} = 0.134$

REFERENCE: T. Wessels, Ch. Baerlocher, L. B. McCusker and E. J. Creyghton, *J. Am. Chem. Soc.* **121** 6242–6247 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	6.03	14.649	2	62.1	1	2	0	21.84	4.070	4	19.6	-3	1	10	33.76	2.655	4	1.1
1	0	0	6.05	14.607	2	65.5	-2	1	6	22.19	4.006	4	3.6	-5	1	6	33.82	2.651	4	1.3
-1	0	2	7.55	11.704	2	77.3	-3	1	4	22.22	4.001	4	2.4	1	2	8	33.91	2.643	4	2.5
0	1	1	10.87	8.142	4	19.3	-1	2	2	22.31	3.985	4	25.4	4	2	2	33.96	2.640	4	2.8
0	1	2	12.06	7.337	4	3.0	-3	0	6	22.79	3.901	2	8.9	-4	0	10	34.81	2.577	2	1.6
1	1	0	12.07	7.331	4	2.4	1	1	6	22.97	3.872	4	16.8	1	3	4	35.06	2.559	4	3.2
0	0	4	12.08	7.325	2	10.1	3	1	2	23.00	3.866	4	14.0	-2	3	4	35.27	2.544	4	4.9
-1	1	1	12.12	7.303	4	12.5	1	2	2	23.03	3.861	4	5.4	5	0	4	35.49	2.530	2	1.7
2	0	0	12.12	7.303	2	9.2	-1	0	8	23.72	3.751	2	1.4	3	2	6	35.71	2.514	4	6.0
-1	0	4	12.27	7.211	2	5.9	2	0	6	24.04	3.702	2	1.1	-6	0	2	36.05	2.491	2	2.0
-2	0	2	12.30	7.196	2	4.3	3	0	4	24.06	3.699	2	2.9	-2	0	12	36.14	2.485	2	3.1
1	1	1	12.77	6.935	4	8.1	0	0	8	24.30	3.662	2	15.4	-6	0	4	36.25	2.478	2	1.2
-1	1	2	12.90	6.865	4	2.1	4	0	0	24.37	3.652	2	20.0	-1	3	6	36.58	2.456	4	2.6
0	1	3	13.83	6.401	4	6.1	-2	0	8	24.69	3.605	2	14.2	-1	2	10	36.68	2.450	4	1.9
-1	1	3	14.29	6.199	4	5.6	-4	0	4	24.75	3.598	2	12.6	0	3	6	36.75	2.446	4	10.9
1	0	4	14.67	6.039	2	22.3	-3	1	6	25.13	3.544	4	17.4	-5	2	2	36.76	2.445	4	1.8
2	0	2	14.69	6.030	2	22.5	1	2	4	25.68	3.469	4	2.3	3	3	0	36.78	2.444	4	8.2
-2	0	4	15.14	5.852	2	7.9	2	2	2	25.69	3.467	4	2.4	-3	0	12	37.41	2.404	2	1.2
-2	1	1	15.80	5.609	4	3.7	1	0	8	26.35	3.382	2	12.2	-3	3	4	37.49	2.399	4	2.7
1	1	3	15.89	5.576	4	3.2	4	0	2	26.41	3.374	2	8.9	-6	0	6	37.50	2.399	2	2.0
2	1	1	16.79	5.279	4	2.2	-3	0	8	27.07	3.294	2	1.7	1	3	6	37.96	2.370	4	1.8
-2	1	3	17.06	5.198	4	2.5	-1	2	6	27.66	3.225	4	2.2	3	3	2	37.99	2.369	4	6.3
-1	0	6	17.85	4.970	2	10.6	-3	2	2	27.69	3.221	4	2.0	4	0	8	38.43	2.342	2	2.7
-3	0	2	17.89	4.957	2	11.4	0	2	6	27.87	3.201	4	4.1	6	1	0	38.47	2.340	4	1.0
1	1	4	18.04	4.918	4	5.9	3	2	0	27.91	3.197	4	4.3	-3	2	10	38.58	2.333	4	1.6
2	1	2	18.05	4.914	4	8.3	1	1	8	28.41	3.141	4	4.1	-5	2	6	38.63	2.331	4	1.3
0	0	6	18.17	4.883	2	24.5	4	1	2	28.47	3.135	4	4.3	1	2	10	38.96	2.312	4	1.3
3	0	0	18.22	4.869	2	27.6	3	0	6	28.58	3.123	2	11.7	-6	0	8	39.72	2.269	2	1.7
-1	1	5	18.31	4.844	4	2.1	-2	2	6	28.80	3.100	4	5.0	3	3	4	40.16	2.245	4	2.0
-2	1	4	18.42	4.816	4	7.2	-3	2	4	28.82	3.098	4	5.8	-2	0	14	42.23	2.140	2	4.6
2	0	4	18.94	4.684	2	1.5	-1	0	10	29.76	3.002	2	11.8	-7	0	4	42.36	2.134	2	2.9
-2	0	6	19.53	4.545	2	23.5	-5	0	2	29.85	2.993	2	5.9	0	4	0	42.67	2.119	2	9.8
-3	0	4	19.56	4.539	2	20.0	2	1	8	31.45	2.844	4	2.3	-6	0	10	42.78	2.114	2	1.5
2	1	3	19.71	4.504	4	1.4	4	1	4	31.49	2.841	4	1.4	-5	1	12	44.13	2.052	4	1.1
-2	1	5	20.16	4.404	4	1.3	-3	0	10	32.02	2.795	2	1.9	-2	3	10	44.38	2.041	4	1.0
1	0	6	20.40	4.353	2	3.5	-5	0	6	32.07	2.791	2	3.5	-4	3	8	44.58	2.033	4	1.3
1	1	5	20.42	4.350	4	1.8	0	2	8	32.31	2.771	4	1.8	7	1	0	44.73	2.026	4	1.6
3	0	2	20.44	4.344	2	2.3	0	1	10	32.33	2.769	4	1.5	3	0	12	45.03	2.013	2	3.7
-1	1	6	20.72	4.287	4	6.8	4	2	0	32.36	2.766	4	1.8	6	0	6	45.10	2.010	2	2.3
-3	1	2	20.76	4.279	4	9.3	-4	1	8	32.37	2.766	4	2.8	-5	3	6	45.69	1.985	4	1.7
0	2	0	20.96	4.238	2	100.0	5	1	0	32.42	2.762	4	1.1	1	1	14	46.41	1.956	4	1.9
0	1	6	21.00	4.231	4	32.0	1	0	10	32.46	2.759	2	3.9	7	1	2	46.53	1.952	4	1.6
3	1	0	21.04	4.222	4	32.2	5	0	2	32.54	2.752	2	7.2	-2	2	14	47.61	1.910	4	1.0
0	2	2	21.83	4.071	4	22.4	-2	2	8	32.61	2.746	4	1.3	-7	2	4	47.72	1.906	4	1.6
3	1	1	21.83	4.071	4	1.2	-4	2	4	32.65	2.743	4	1.6	-6	1	12	47.85	1.901	4	1.2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Bellbergite

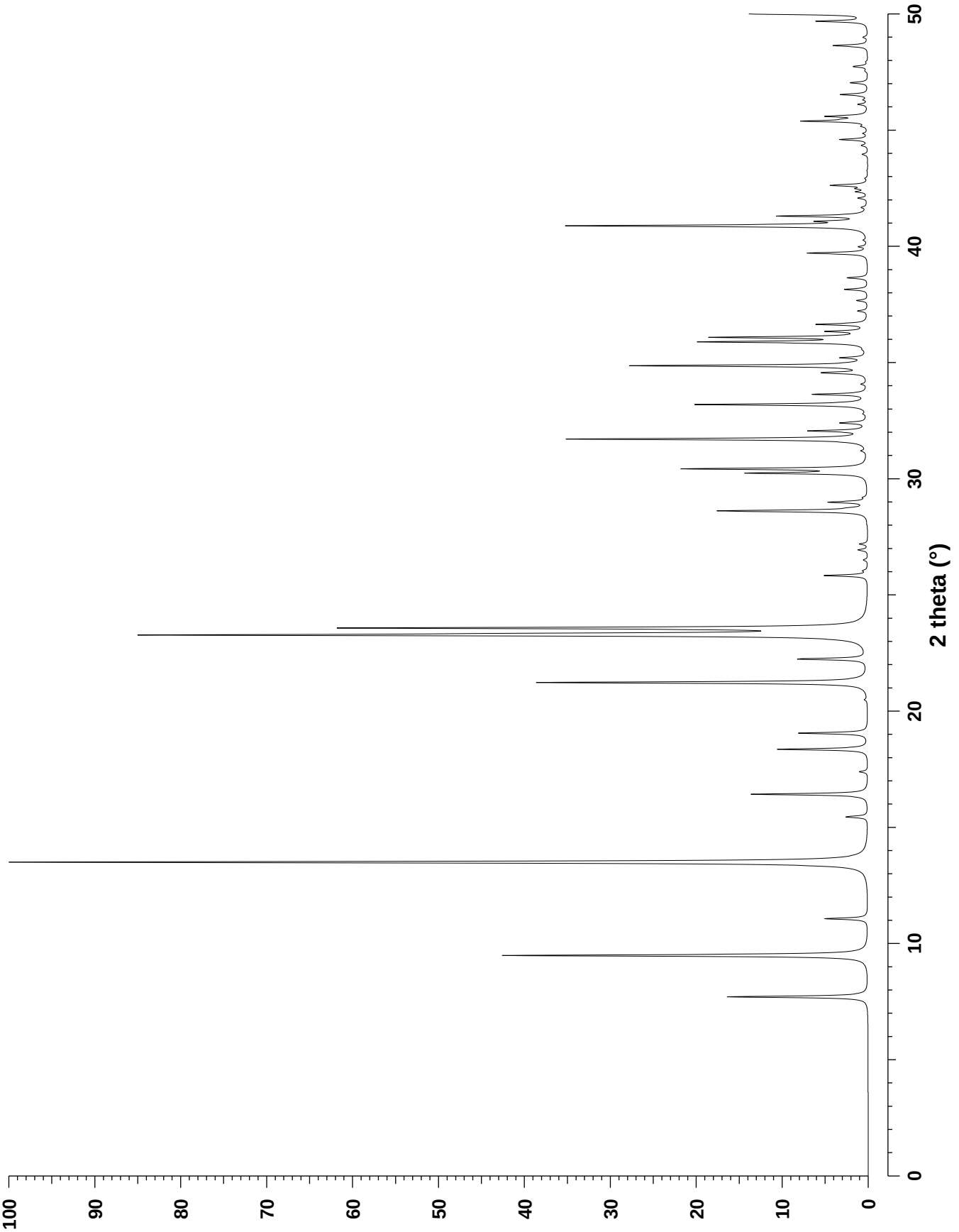
CHEMICAL COMPOSITION: $|Ba_{0.26}Na_{0.72}K_{1.33}Ca_{5.32}Sr_{2.36}(H_2O)_{30}|\ [Si_{18.36}Al_{17.55}O_{72}]$
Bellberg Volcano, Eifel, Germany

REFINED COMPOSITION: $|K_2Ca_6Sr_2(H_2O)_{30}|\ [Si_{18.45}Al_{17.55}O_{72}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.244$ Å $b = 13.244$ Å $c = 15.988$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.122$

REFERENCE: B. Rüdinger, E. Tillmanns and G. Hentschel,
Mineralogy and Petrology **48** 147–152 (1993).

h	k	l	2θ	d	M	I_{rel}
1	0	0	7.71	11.470	6	16.4
1	0	1	9.49	9.320	12	42.6
0	0	2	11.07	7.994	2	5.0
1	1	0	13.37	6.622	6	0.6
1	0	2	13.50	6.558	12	100.0
2	0	0	15.45	5.735	6	2.5
2	0	1	16.42	5.398	12	13.6
1	1	2	17.39	5.100	12	1.0
1	0	3	18.36	4.833	12	10.5
2	0	2	19.05	4.660	12	8.1
2	1	0	20.49	4.335	12	0.3
2	1	1	21.23	4.184	24	38.6
0	0	4	22.24	3.997	2	8.0
3	0	0	23.27	3.823	6	78.1
2	1	2	23.34	3.811	24	23.9
1	0	4	23.57	3.774	12	59.8
3	0	2	25.83	3.449	12	5.1
1	1	4	26.04	3.422	12	0.4
2	1	3	26.50	3.363	24	0.5
2	2	0	26.93	3.311	6	1.1
2	0	4	27.19	3.279	12	1.0
3	1	1	28.61	3.120	24	17.5
3	0	3	28.74	3.107	12	1.0
1	0	5	28.99	3.080	12	4.5
2	2	2	29.19	3.059	12	0.4
3	1	2	30.24	2.956	24	13.4
2	1	4	30.42	2.939	24	21.1
4	0	0	31.19	2.867	6	0.6
4	0	1	31.70	2.822	12	35.0
2	0	5	32.05	2.793	12	6.5
3	0	4	32.40	2.763	12	3.1
3	1	3	32.79	2.731	24	0.3
4	0	2	33.19	2.699	12	20.1
0	0	6	33.63	2.665	2	6.3
3	2	0	34.07	2.631	12	0.6
3	2	1	34.54	2.596	24	1.4
1	0	6	34.56	2.596	12	3.8
2	1	5	34.86	2.573	24	27.6
2	2	4	35.20	2.550	12	2.8
4	0	3	35.55	2.525	12	0.2
4	1	0	35.88	2.503	12	19.1
3	1	4	36.08	2.489	24	17.7
4	1	1	36.33	2.473	24	3.8
1	1	6	36.34	2.472	12	0.6
3	0	5	36.64	2.453	12	5.9
2	0	6	37.21	2.417	12	1.2
4	1	2	37.66	2.389	24	1.3
3	2	3	38.14	2.359	24	2.7
4	0	4	38.64	2.330	12	2.4
2	1	6	39.70	2.270	24	7.0
3	1	5	39.98	2.255	24	0.9
1	0	7	40.26	2.240	12	0.4
3	3	0	40.88	2.207	6	34.8
5	0	2	40.93	2.205	12	0.3
3	2	4	41.07	2.198	24	4.5
3	0	6	41.30	2.186	12	10.2
4	2	0	41.67	2.168	12	0.6
4	2	1	42.07	2.148	24	1.1
4	0	5	42.34	2.135	12	1.3
3	3	2	42.48	2.128	12	1.1
2	0	7	42.61	2.122	12	0.1
4	1	4	42.62	2.121	24	4.2
5	0	3	42.92	2.107	12	0.3
5	1	0	43.95	2.060	12	0.7
5	1	1	44.33	2.043	24	0.3
3	1	6	44.34	2.043	24	0.4
3	2	5	44.59	2.032	24	3.3
2	1	7	44.85	2.021	24	0.5
4	2	3	45.16	2.008	24	0.5
0	0	8	45.38	1.998	2	7.4
5	1	2	45.47	1.995	24	1.5
5	0	4	45.59	1.990	12	4.7
1	0	8	46.10	1.969	12	1.1
3	0	7	46.30	1.961	12	0.5
4	0	6	46.52	1.952	12	3.2
3	3	4	47.03	1.932	12	2.1
1	1	8	47.52	1.913	12	0.2
6	0	0	47.57	1.912	6	0.2
4	2	4	47.73	1.905	24	1.7
6	0	1	47.93	1.898	12	0.2
4	3	1	48.62	1.873	24	1.5
3	2	6	48.63	1.872	24	2.6
6	0	2	48.99	1.859	12	0.5
5	2	0	49.64	1.837	12	0.4
4	3	2	49.68	1.835	24	5.7
5	1	4	49.80	1.831	24	0.2
5	2	1	49.99	1.825	24	0.6
4	1	6	49.99	1.824	24	13.2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EAB (Na, Tetramethylammonium)-E

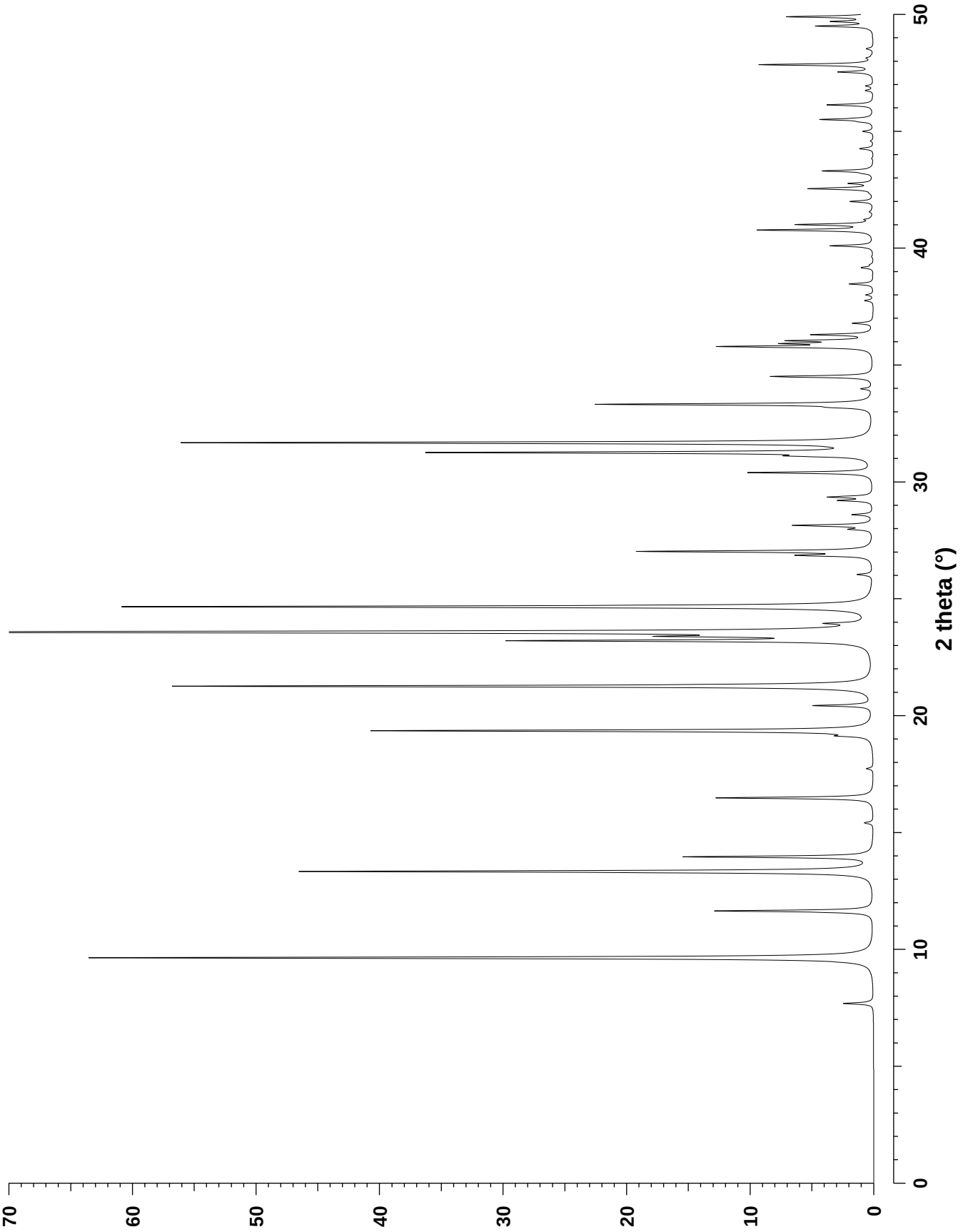
CHEMICAL COMPOSITION: $|Na_{8.1}((CH_3)_4N)_{2.2}(H_2O)_{25}|\ [Si_{26.6}Al_{9.4}O_{72}]$
$(CH_3)_4N$ = tetramethylammonium

REFINED COMPOSITION: $|(H_2O)_{39.5}|\ [Si_{26.6}Al_{9.4}O_{72}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.28$ Å $b = 13.28$ Å $c = 15.21$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R = 0.19$

REFERENCE: W. M. Meier and M. Groner,
J. Solid State Chem. **37** 204–218 (1981).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.69	11.501	6	2.5	2	1	4	31.25	2.862	24	35.8	3	3	2	42.54	2.125	12	5.3
1	0	1	9.64	9.174	12	64.2	4	0	1	31.67	2.825	12	56.3	3	0	6	42.76	2.115	12	1.9
0	0	2	11.64	7.605	2	13.0	3	1	3	33.18	2.700	24	0.1	5	0	3	43.19	2.095	12	0.2
1	1	0	13.33	6.640	6	46.9	3	0	4	33.18	2.700	12	1.6	4	1	4	43.19	2.095	24	0.3
1	0	2	13.96	6.344	12	15.4	4	0	2	33.31	2.689	12	21.8	4	2	2	43.29	2.090	24	1.0
2	0	0	15.41	5.750	6	0.7	2	0	5	33.32	2.689	12	0.9	4	0	5	43.30	2.090	12	3.2
2	0	1	16.48	5.379	12	12.9	3	2	0	33.98	2.638	12	0.9	5	1	0	43.83	2.066	12	0.1
1	1	2	17.73	5.002	12	0.6	3	2	1	34.50	2.600	24	8.4	5	1	1	44.25	2.047	24	1.1
1	0	3	19.13	4.639	12	1.9	4	1	0	35.78	2.510	12	12.2	2	0	7	44.58	2.033	12	0.2
2	0	2	19.35	4.587	12	41.0	4	0	3	35.91	2.501	12	2.6	2	2	6	44.99	2.015	12	0.9
2	1	0	20.43	4.347	12	4.8	2	2	4	35.91	2.501	12	3.5	4	2	3	45.40	1.998	24	0.7
2	1	1	21.26	4.180	24	57.3	3	2	2	36.03	2.493	24	3.2	5	1	2	45.50	1.993	24	4.3
3	0	0	23.20	3.834	6	28.4	2	1	5	36.04	2.492	24	3.3	5	0	4	46.12	1.968	12	3.8
2	0	3	23.39	3.803	12	6.4	1	0	6	36.29	2.476	12	4.8	2	1	7	46.74	1.944	24	0.6
0	0	4	23.39	3.802	2	5.6	3	1	4	36.78	2.444	24	1.7	4	1	5	46.93	1.936	24	0.6
2	1	2	23.57	3.774	24	100.0	4	1	2	37.75	2.383	24	0.7	5	1	3	47.53	1.913	24	0.3
3	0	1	23.94	3.717	12	2.7	1	1	6	37.99	2.368	12	0.6	3	3	4	47.53	1.913	12	2.4
1	0	4	24.66	3.610	12	61.3	3	2	3	38.46	2.341	24	2.0	6	0	1	47.83	1.902	12	0.3
3	0	2	26.03	3.423	12	1.2	5	0	0	39.16	2.300	6	1.0	0	0	8	47.84	1.901	2	9.1
2	2	0	26.85	3.320	6	5.4	4	0	4	39.28	2.293	12	0.2	4	3	0	48.12	1.891	12	0.3
2	1	3	27.02	3.300	24	15.5	5	0	1	39.63	2.274	12	0.1	3	0	7	48.13	1.890	12	0.1
1	1	4	27.02	3.300	12	3.5	4	1	3	40.09	2.249	24	3.5	4	3	1	48.52	1.876	24	0.5
3	1	0	27.97	3.190	12	1.7	3	3	0	40.77	2.213	6	9.4	5	2	0	49.49	1.842	12	4.6
2	0	4	28.13	3.172	12	6.5	5	0	2	40.99	2.202	12	0.5	4	3	2	49.69	1.835	24	1.0
3	1	1	28.59	3.122	24	1.7	3	1	5	41.00	2.201	24	5.7	5	0	5	49.69	1.835	12	2.1
3	0	3	29.20	3.058	12	2.7	2	1	6	41.22	2.190	24	0.5	5	2	1	49.88	1.828	24	1.1
2	2	2	29.35	3.043	12	3.6	4	2	0	41.55	2.173	12	0.3	3	2	6	49.89	1.828	24	4.2
1	0	5	30.39	2.941	12	10.2	4	2	1	41.99	2.152	24	1.9	1	1	8	49.89	1.828	12	1.8
4	0	0	31.10	2.875	6	4.7	1	0	7	42.33	2.135	12	0.1							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CHEMICAL COMPOSITION: $|Ba_2(H_2O)_7|\ [Si_6Al_4O_{20}]$
Bathurst, New Brunswick, Canada

REFINED COMPOSITION: $|Ba_{1.95}(H_2O)_7|\ [Si_6Al_4O_{20}]$

CRYSTAL DATA: $P2_12_12$ (No. 18)
$a = 9.537$ Å $b = 9.651$ Å $c = 6.509$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{wp} = 0.070$, $R_{F^2} = 0.055$

REFERENCE: Å. Kvick and J. V. Smith,
J. Chem. Phys. **79** 2356–2362 (1983).

h	k	l	2θ	d	M	I_{rel}
1	1	0	13.05	6.784	4	1.4
0	0	1	13.60	6.509	2	90.4
0	1	1	16.43	5.396	4	34.9
1	0	1	16.49	5.376	4	46.3
0	2	0	18.39	4.826	2	53.7
2	0	0	18.61	4.768	2	43.7
1	1	1	18.89	4.697	8	86.1
1	2	0	20.63	4.306	4	9.0
2	1	0	20.78	4.275	4	4.0
0	2	1	22.94	3.876	4	5.6
2	0	1	23.12	3.847	4	1.6
1	2	1	24.79	3.591	8	100.0
2	1	1	24.92	3.573	8	86.7
2	2	0	26.27	3.392	4	20.6
0	0	2	27.40	3.254	2	11.1
0	1	2	28.95	3.084	4	15.0
1	0	2	28.99	3.080	4	13.3
1	3	0	29.30	3.048	4	29.3
3	1	0	29.58	3.019	4	30.2
2	2	1	29.70	3.008	8	20.8
1	1	2	30.46	2.934	8	35.5
0	3	1	31.01	2.884	4	1.2
3	0	1	31.31	2.857	4	1.5
1	3	1	32.43	2.761	8	84.4
3	1	1	32.69	2.739	8	91.2
0	2	2	33.20	2.698	4	0.4
2	0	2	33.33	2.688	4	0.6
2	3	0	33.60	2.667	4	5.2
3	2	0	33.76	2.655	4	5.9
1	2	2	34.55	2.596	8	41.2
2	1	2	34.64	2.590	8	49.6
2	3	1	36.41	2.468	8	6.0
3	2	1	36.55	2.458	8	7.8
0	4	0	37.27	2.413	2	1.5
4	0	0	37.73	2.384	2	1.4
2	2	2	38.33	2.348	8	2.9
0	3	2	39.38	2.288	4	35.2
3	0	2	39.63	2.274	4	29.6
0	4	1	39.85	2.262	4	3.1
3	3	0	39.87	2.261	4	34.2
4	0	1	40.28	2.239	4	2.5
1	3	2	40.55	2.225	8	1.7
3	1	2	40.76	2.213	8	1.9
1	4	1	41.00	2.201	8	20.9
4	1	1	41.40	2.181	8	18.0
0	0	3	41.62	2.170	2	4.7
2	4	0	41.96	2.153	4	12.6
4	2	0	42.28	2.138	4	13.8
3	3	1	42.31	2.136	8	12.3
0	1	3	42.71	2.117	4	3.0
1	0	3	42.74	2.116	4	2.8
1	1	3	43.81	2.067	8	16.3
2	3	2	43.89	2.063	8	8.0
3	2	2	44.02	2.057	8	7.6
2	4	1	44.32	2.044	8	6.9
4	2	1	44.62	2.031	8	6.9
0	2	3	45.86	1.979	4	3.7
2	0	3	45.95	1.975	4	5.3
1	2	3	46.89	1.938	8	8.4
2	1	3	46.96	1.935	8	8.4
4	0	2	47.26	1.923	4	0.2
3	4	0	47.30	1.922	4	1.4
4	3	0	47.46	1.916	4	2.1
1	4	2	47.89	1.899	8	7.4
1	5	0	48.09	1.892	4	2.0
4	1	2	48.25	1.886	8	8.5
5	1	0	48.66	1.871	4	1.9
3	3	2	49.06	1.857	8	2.0
0	5	1	49.24	1.851	4	5.7
3	4	1	49.45	1.843	8	10.4
4	3	1	49.61	1.838	8	11.3
5	0	1	49.82	1.830	4	5.8
2	2	3	49.89	1.828	8	18.1

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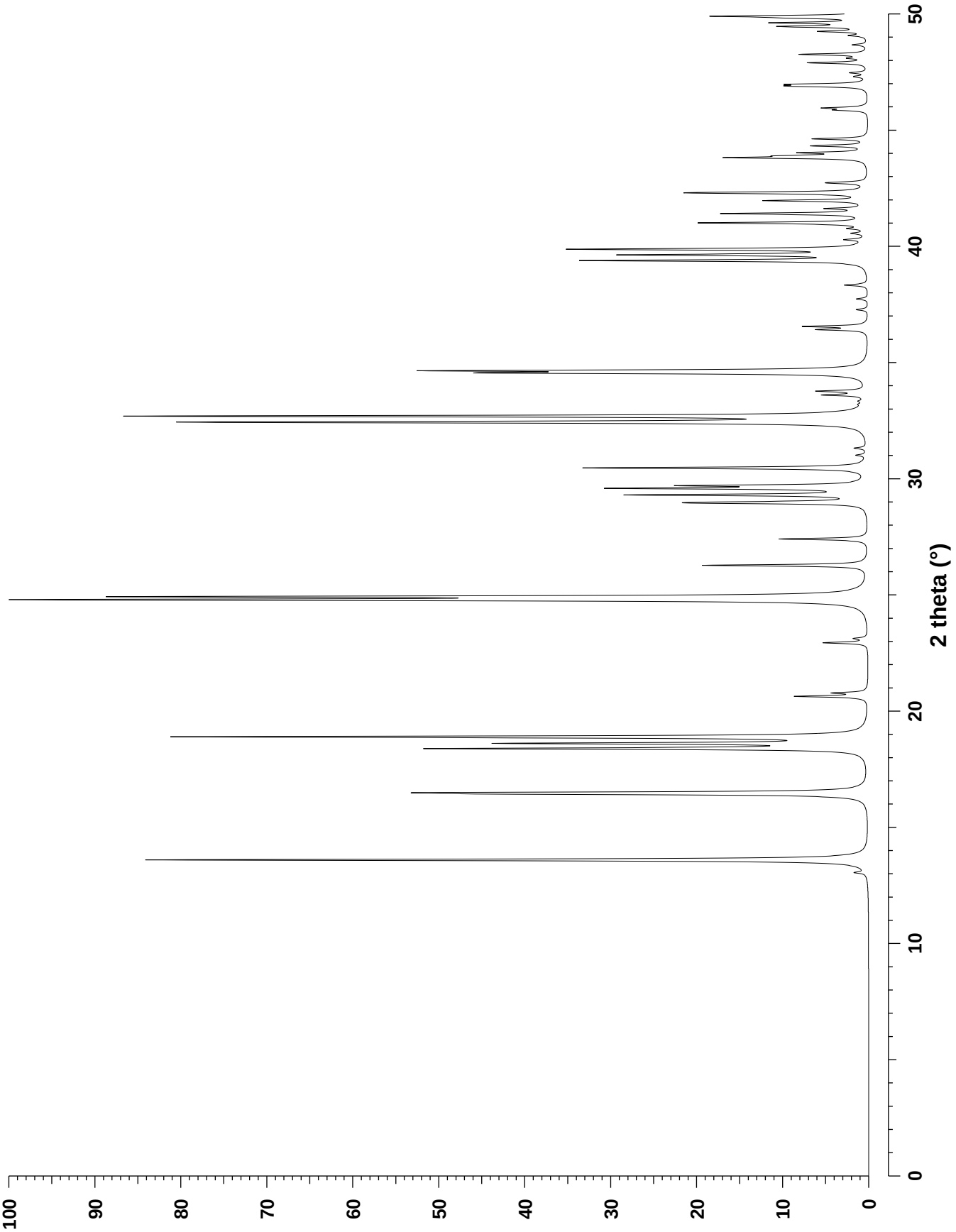


EMT

EMC-2, Calcined

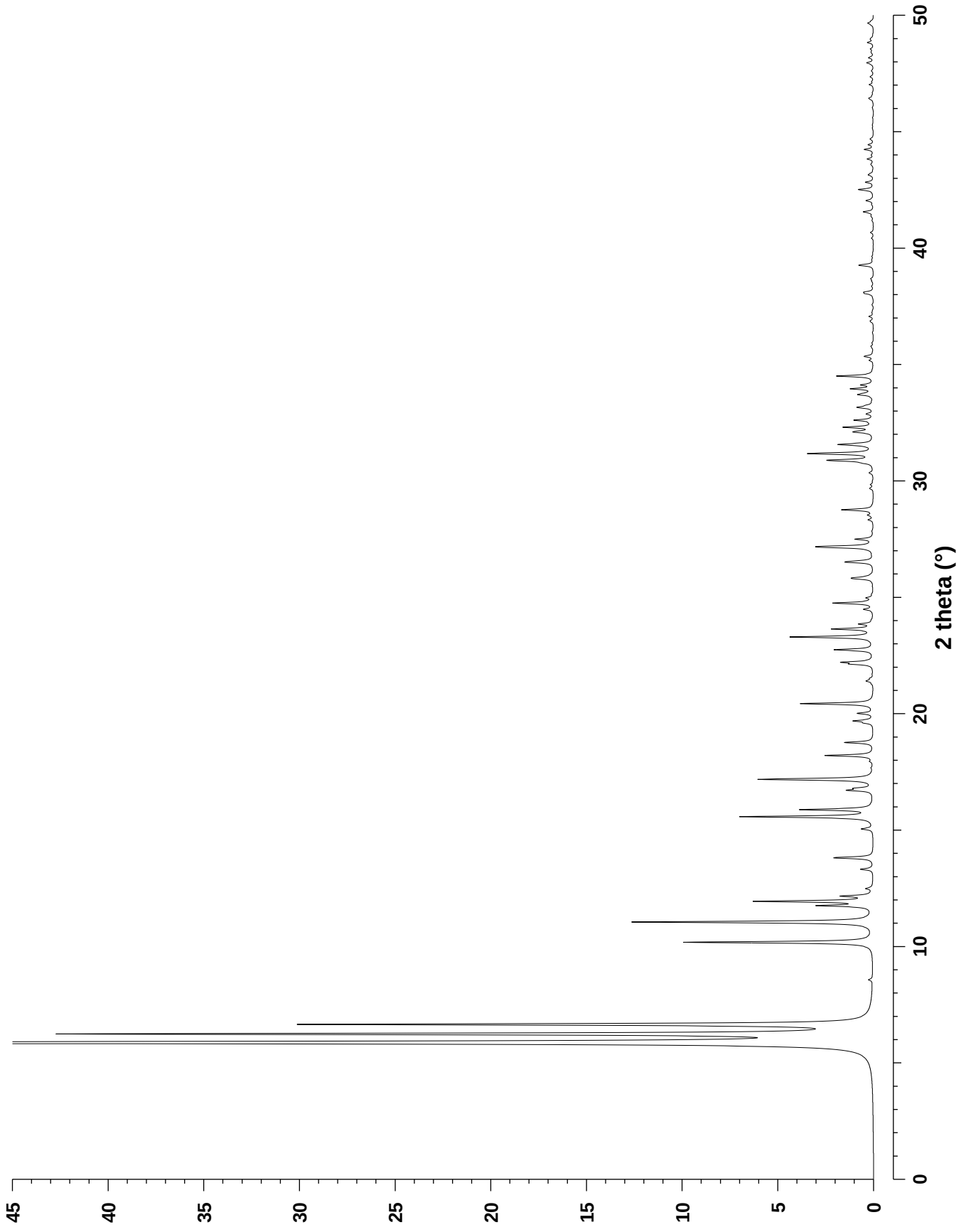
CHEMICAL COMPOSITION: $|Na_{8.3}(H_2O)_6|\ [Si_{76}Al_{20}O_{192}]$

REFINED COMPOSITION: $|Na_{8.3}(H_2O)_6|\ [Si_{76.03}Al_{19.97}O_{192}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 17.3864$ Å $b = 17.3864$ Å $c = 28.3459$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.181$, $R_{wp} = 0.206$, $R_F = 0.074$

REFERENCE: Ch. Baerlocher, L. B. McCusker and R. Chiappetta, *Microporous Materials* **2** 269–280 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.87	15.057	6	100.0	4	0	2	24.47	3.638	12	0.4	5	1	2	33.74	2.656	24	0.2
0	0	2	6.24	14.173	2	41.5	2	1	6	24.49	3.635	24	0.1	4	2	4	33.95	2.641	24	1.2
1	0	1	6.65	13.297	12	29.6	3	1	4	24.75	3.598	24	2.1	3	2	7	34.12	2.628	24	0.6
1	0	2	8.57	10.320	12	0.2	2	0	7	24.97	3.566	12	0.3	5	1	3	34.50	2.600	24	1.9
1	1	0	10.18	8.693	6	9.9	3	2	0	25.79	3.454	12	0.7	4	1	7	35.17	2.551	24	0.2
1	0	3	11.05	8.003	12	12.7	1	0	8	25.83	3.449	12	0.7	1	0	11	35.34	2.540	12	0.4
2	0	0	11.75	7.529	6	2.7	3	0	6	25.90	3.440	12	0.2	6	0	0	35.78	2.510	6	0.1
1	1	2	11.94	7.410	12	6.1	3	1	5	26.51	3.362	24	1.4	6	0	3	37.06	2.425	12	0.2
2	0	1	12.16	7.276	12	1.5	3	2	2	26.56	3.356	24	0.3	6	0	4	38.04	2.366	12	0.4
0	0	4	12.49	7.086	2	0.3	4	1	0	27.14	3.286	12	1.7	0	0	12	38.10	2.362	2	0.4
2	0	2	13.32	6.649	12	0.7	1	1	8	27.18	3.281	12	2.1	6	0	5	39.26	2.295	12	0.7
1	0	4	13.81	6.412	12	2.1	3	2	3	27.49	3.244	24	0.9	4	2	8	40.66	2.219	24	0.1
2	0	3	15.05	5.888	12	0.6	3	0	7	28.32	3.152	12	0.3	4	4	0	41.55	2.173	6	0.5
2	1	0	15.57	5.691	12	7.0	3	1	6	28.53	3.129	24	0.2	5	1	8	42.03	2.150	24	0.3
2	1	1	15.88	5.580	24	3.8	3	2	4	28.75	3.105	24	1.6	6	1	5	42.47	2.128	24	0.1
1	0	5	16.71	5.306	12	1.2	5	0	0	29.66	3.011	6	0.1	7	0	2	42.51	2.127	12	0.1
2	1	2	16.79	5.281	24	0.8	5	0	1	29.84	2.995	12	0.1	4	0	11	42.51	2.126	12	0.6
2	0	4	17.18	5.160	12	6.1	5	0	2	30.34	2.946	12	0.2	4	3	7	42.82	2.112	24	0.4
3	0	1	17.95	4.942	12	0.1	2	0	9	30.77	2.906	12	0.3	5	3	3	43.13	2.097	24	0.1
2	1	3	18.20	4.875	24	2.5	3	3	0	30.86	2.898	6	1.3	2	0	13	43.19	2.094	12	0.1
3	0	2	18.76	4.731	12	1.4	3	0	8	30.89	2.895	12	1.4	6	2	2	43.82	2.066	24	0.3
0	0	6	18.78	4.724	2	0.2	5	0	3	31.17	2.869	12	3.4	6	0	8	44.23	2.048	12	0.5
2	0	5	19.60	4.529	12	0.4	3	3	2	31.51	2.839	12	0.2	6	2	3	44.43	2.039	24	0.3
1	0	6	19.69	4.508	12	1.0	0	0	10	31.56	2.835	2	1.6	2	0	14	46.44	1.955	12	0.2
2	1	4	20.01	4.437	24	0.7	4	2	1	31.60	2.831	24	0.2	3	1	13	47.01	1.933	24	0.2
3	0	3	20.03	4.432	12	0.1	4	2	2	32.08	2.790	24	0.5	7	1	4	47.35	1.920	24	0.2
2	2	0	20.43	4.347	6	3.8	3	2	6	32.10	2.788	24	0.3	6	3	0	47.95	1.897	12	0.3
1	1	6	21.41	4.151	12	0.3	1	0	10	32.13	2.786	12	0.3	5	4	3	48.17	1.889	24	0.2
3	1	1	21.51	4.131	24	0.2	5	0	4	32.30	2.772	12	1.5	1	0	15	48.55	1.875	12	0.1
2	1	5	22.13	4.016	24	1.0	2	2	8	32.60	2.746	12	1.0	5	1	11	48.82	1.866	24	0.3
2	0	6	22.21	4.002	12	1.5	4	2	3	32.87	2.725	24	0.3	5	4	4	48.96	1.860	24	0.1
1	0	7	22.74	3.910	12	2.0	5	1	0	33.13	2.704	12	0.3	5	2	10	49.64	1.837	24	0.1
3	1	3	23.29	3.820	24	4.4	3	1	8	33.16	2.702	24	0.6	7	2	1	49.66	1.836	24	0.1
4	0	0	23.63	3.764	6	2.1	1	1	10	33.24	2.695	12	0.2							
4	0	1	23.85	3.732	12	0.7	5	0	5	33.70	2.659	12	0.7							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EMT EMC-2, Partially Dehydrated

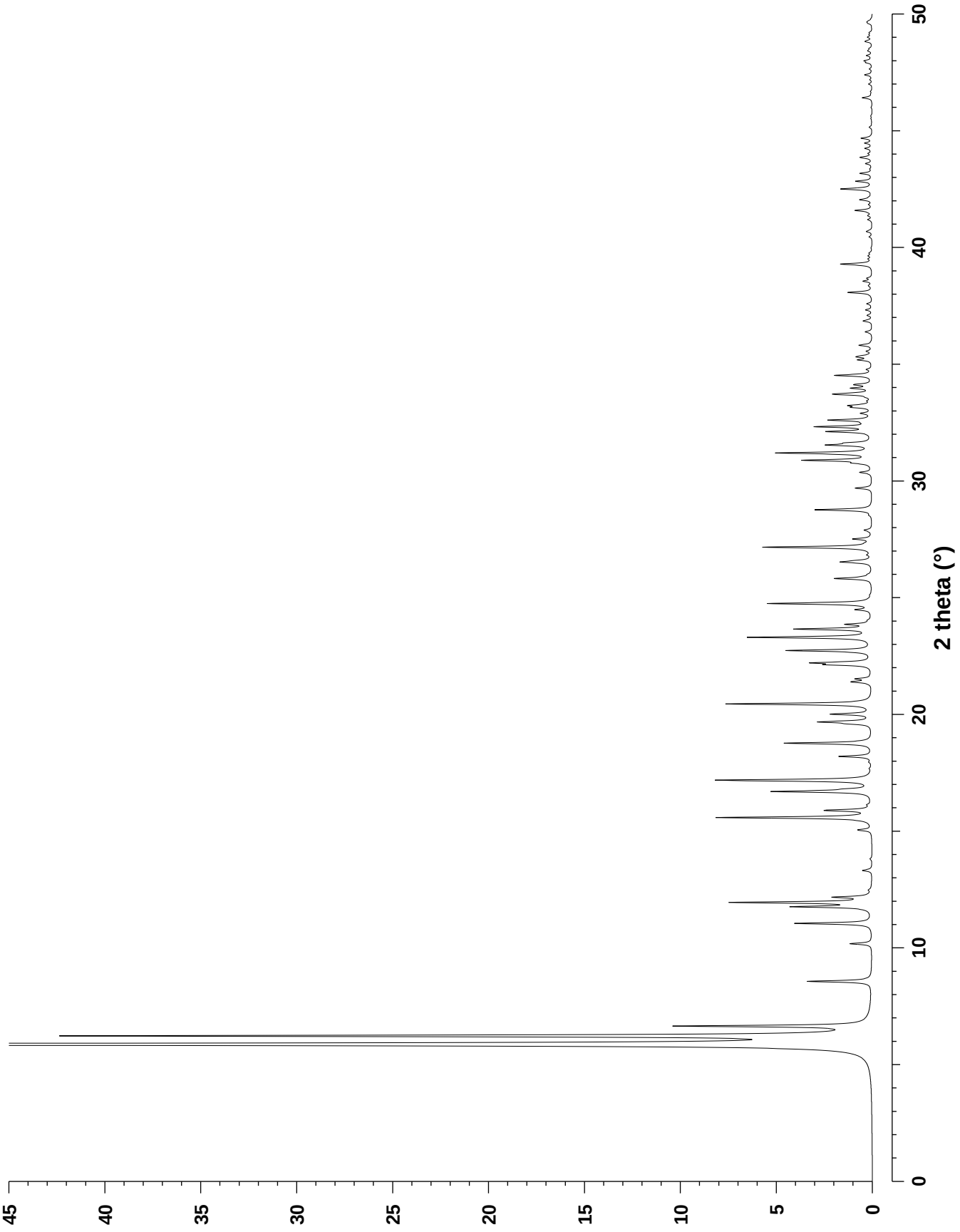
CHEMICAL COMPOSITION: $|Na_{20}(C_{12}H_{24}O_6)_4(H_2O)_{22.6}|\ [Si_{76}Al_{20}O_{192}]$
$C_{12}H_{24}O_6$ = 1,4,7,10,13,16-hexaoxacyclooctadecane (18-crown-6 ether)

REFINED COMPOSITION: $|Na_{20}C_{60}O_{24}(H_2O)_{22.6}|\ [Si_{76.03}Al_{19.97}O_{192}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 17.3741$ Å $b = 17.3741$ Å $c = 28.3646$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.037$, $R_{wp} = 0.186$, $R_F = 0.068$

REFERENCE: Ch. Baerlocher, L. B. McCusker and R. Chiappetta,
Microporous Materials **2** 269–280 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.87	15.046	6	100.0	4	1	0	27.16	3.283	12	3.3	4	2	7	38.68	2.328	24	0.2
0	0	2	6.23	14.182	2	41.3	1	1	8	27.16	3.283	12	2.4	6	1	0	39.26	2.295	12	0.1
1	0	1	6.65	13.292	12	9.8	3	2	3	27.51	3.243	24	0.9	5	0	8	39.27	2.294	12	0.2
1	0	2	8.57	10.320	12	3.4	4	1	2	27.89	3.199	24	0.4	6	0	5	39.28	2.294	12	1.3
1	1	0	10.18	8.687	6	1.1	3	2	4	28.76	3.104	24	3.0	3	0	11	39.29	2.293	12	0.2
1	0	3	11.05	8.006	12	4.0	2	1	8	29.69	3.009	24	0.8	4	1	9	39.64	2.274	24	0.2
2	0	0	11.76	7.523	6	4.0	5	0	2	30.36	2.944	12	0.5	4	3	5	39.75	2.267	24	0.1
1	1	2	11.95	7.408	12	7.3	2	0	9	30.76	2.907	12	0.7	6	1	3	40.45	2.230	24	0.2
2	0	1	12.17	7.272	12	1.8	3	3	0	30.88	2.896	6	1.4	4	2	8	40.67	2.218	24	0.2
0	0	4	12.48	7.091	2	0.1	3	0	8	30.88	2.895	12	2.1	5	2	5	40.68	2.218	24	0.1
2	0	2	13.32	6.646	12	0.5	5	0	3	31.19	2.868	12	5.0	3	2	10	41.19	2.192	24	0.2
2	0	3	15.05	5.887	12	0.7	3	3	2	31.53	2.837	12	0.5	6	1	4	41.36	2.183	24	0.2
2	1	0	15.58	5.687	12	8.1	0	0	10	31.54	2.836	2	1.6	4	4	0	41.58	2.172	6	0.9
2	1	1	15.89	5.576	24	2.4	4	2	1	31.62	2.829	24	1.0	1	0	13	41.83	2.159	12	0.1
1	1	4	16.13	5.493	12	0.2	4	2	2	32.10	2.788	24	0.6	5	1	8	42.04	2.149	24	0.5
1	0	5	16.70	5.308	12	5.1	3	2	6	32.11	2.788	24	0.6	6	1	5	42.50	2.127	24	0.4
2	1	2	16.80	5.278	24	0.8	1	0	10	32.11	2.787	12	1.1	4	0	11	42.50	2.127	12	1.2
2	0	4	17.18	5.160	12	8.2	5	0	4	32.32	2.770	12	2.9	7	0	2	42.54	2.125	12	0.2
2	1	3	18.20	4.873	24	1.7	2	1	9	32.48	2.757	24	0.2	4	3	7	42.83	2.111	24	0.8
3	0	2	18.77	4.728	12	4.5	2	2	8	32.60	2.747	12	2.2	5	3	3	43.16	2.096	24	0.2
0	0	6	18.77	4.727	2	0.1	4	2	3	32.89	2.723	24	0.5	7	0	3	43.16	2.096	12	0.1
2	0	5	19.60	4.530	12	0.9	5	1	0	33.15	2.702	12	0.6	2	0	13	43.17	2.096	12	0.3
1	0	6	19.68	4.510	12	2.6	3	1	8	33.15	2.702	24	0.3	4	4	4	43.58	2.077	12	0.2
2	1	4	20.01	4.437	24	1.9	1	1	10	33.23	2.696	12	1.1	2	2	12	43.59	2.076	12	0.1
3	0	3	20.04	4.431	12	0.2	3	3	4	33.42	2.681	12	0.2	3	2	11	43.82	2.066	24	0.1
2	2	0	20.45	4.344	6	7.6	3	0	9	33.58	2.669	12	0.2	6	2	2	43.86	2.064	24	0.5
2	2	2	21.39	4.153	12	0.8	5	0	5	33.71	2.658	12	1.9	6	0	8	44.24	2.047	12	0.4
1	1	6	21.40	4.152	12	0.2	5	1	2	33.76	2.655	24	0.4	6	2	3	44.46	2.038	24	0.3
3	1	1	21.52	4.129	24	0.8	4	2	4	33.97	2.639	24	1.0	4	3	8	44.67	2.029	24	0.3
2	1	5	22.13	4.016	24	2.0	3	2	7	34.12	2.628	24	0.9	4	1	11	44.68	2.028	24	0.3
2	0	6	22.21	4.003	12	2.9	5	1	3	34.52	2.598	24	2.0	5	1	10	46.41	1.957	24	0.1
1	0	7	22.73	3.913	12	4.5	4	0	8	34.77	2.580	12	0.3	2	0	14	46.41	1.956	12	0.3
3	1	3	23.30	3.818	24	6.5	4	1	7	35.18	2.551	24	0.7	3	1	13	46.99	1.934	24	0.2
4	0	0	23.65	3.762	6	3.8	1	0	11	35.31	2.542	12	0.6	7	1	4	47.38	1.919	24	0.3
3	0	5	23.68	3.758	12	0.3	2	1	10	35.36	2.538	24	0.3	4	1	12	47.39	1.918	24	0.1
4	0	1	23.86	3.729	12	1.3	5	1	4	35.55	2.525	24	0.3	7	0	7	47.91	1.899	12	0.2
4	0	2	24.48	3.636	12	0.7	6	0	0	35.81	2.508	6	0.7	6	3	0	47.99	1.896	12	0.4
3	1	4	24.75	3.597	24	5.5	6	0	2	36.38	2.469	12	0.3	5	4	3	48.21	1.888	24	0.2
3	2	0	25.81	3.452	12	0.6	5	1	5	36.84	2.440	24	0.3	7	1	5	48.41	1.880	24	0.1
1	0	8	25.82	3.451	12	1.3	6	0	3	37.09	2.424	12	0.2	1	0	15	48.52	1.876	12	0.1
3	0	6	25.90	3.440	12	0.2	5	2	0	37.32	2.409	12	0.3	5	1	11	48.81	1.866	24	0.3
3	2	1	26.00	3.427	24	0.1	4	3	3	37.58	2.393	24	0.3	4	3	10	48.85	1.864	24	0.2
3	1	5	26.52	3.362	24	1.5	6	0	4	38.06	2.364	12	0.5	5	0	12	49.00	1.859	12	0.1
3	2	2	26.58	3.354	24	0.6	0	0	12	38.07	2.364	2	0.8	4	4	8	49.20	1.852	12	0.1
4	0	4	26.83	3.323	12	0.2	1	0	12	38.55	2.335	12	0.4	7	0	8	49.59	1.838	12	0.2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EPI Epistilbite

CHEMICAL COMPOSITION: $|Na_{1.06}K_{0.1}Ca_{2.59}(H_2O)_{15.74}|\ [Si_{17.71}Al_{6.29}O_{48}]$
Teigarhorn, Iceland

REFINED COMPOSITION: $|Na_{1.04}Ca_{2.56}(H_2O)_{15.75}|\ [Si_{17.76}Al_{6.24}O_{48}]$

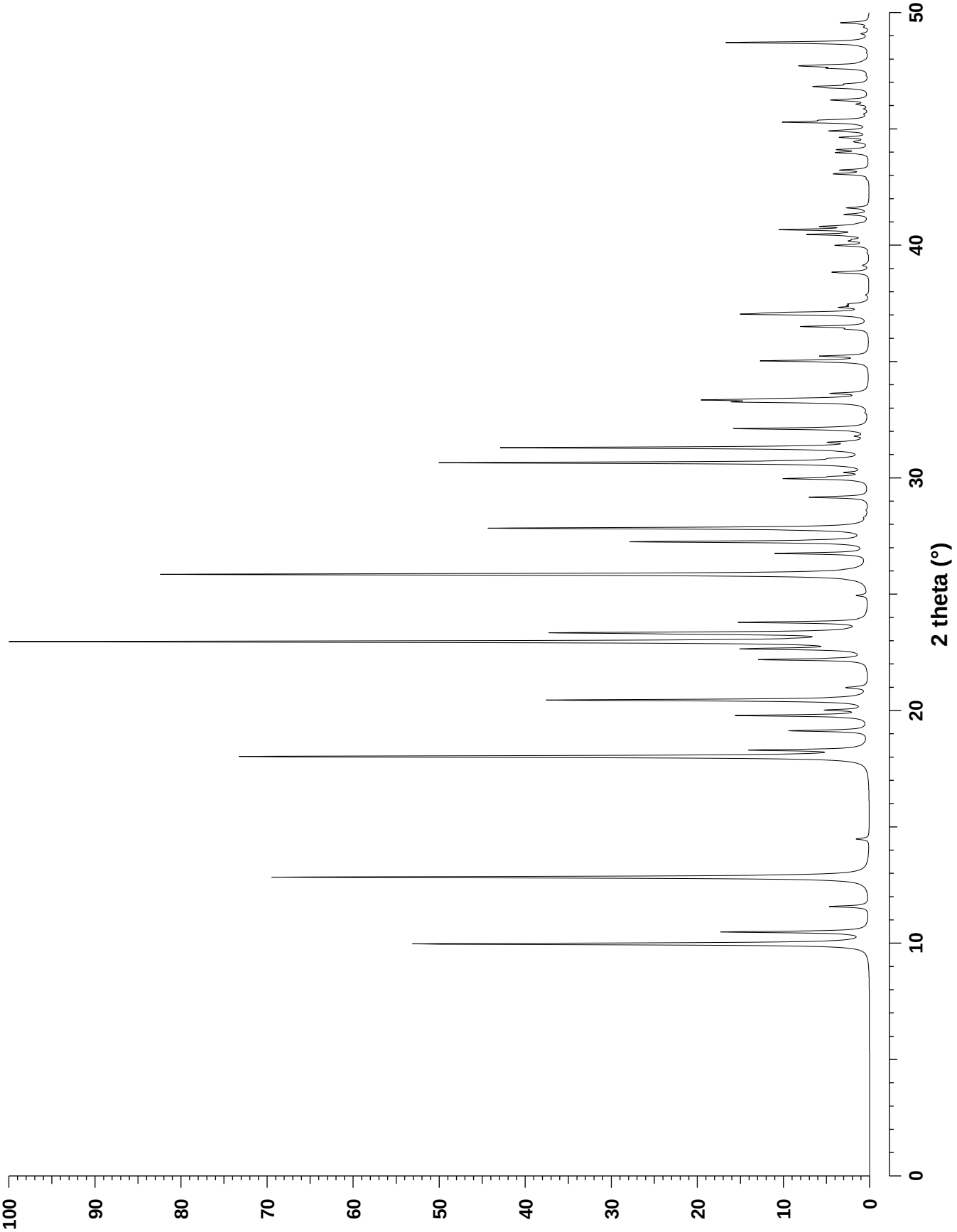
CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.08$ Å $b = 17.74$ Å $c = 10.25$ Å
$\alpha = 90°$ $\beta = 124.54°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.16$

REFERENCE: A. J. Perrotta,
Mineral. Mag. **36** 480–490 (1967).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	9.97	8.870	2	53.4	0	6	1	32.07	2.791	4	0.7	2	2	2	41.60	2.171	4	2.6
0	0	1	10.48	8.443	2	17.1	-3	1	3	32.11	2.788	4	15.2	0	0	4	42.84	2.111	2	0.2
-1	1	1	11.58	7.642	4	4.6	1	5	1	32.19	2.781	4	0.6	1	3	3	43.06	2.101	4	4.0
1	1	0	12.84	6.892	4	70.0	2	2	1	32.80	2.730	4	0.2	-4	0	1	43.22	2.093	2	3.2
0	2	1	14.48	6.116	4	1.5	-3	3	2	33.26	2.693	4	12.6	2	6	1	43.97	2.059	4	0.7
-1	1	2	18.02	4.924	4	73.6	1	3	2	33.34	2.687	4	15.2	-4	2	4	43.97	2.059	4	3.0
-1	3	1	18.30	4.848	4	12.7	0	2	3	33.40	2.683	4	6.3	0	2	4	44.10	2.053	4	3.5
1	3	0	19.13	4.639	4	9.3	-2	4	3	33.63	2.665	4	4.0	3	5	0	44.41	2.040	4	0.6
-2	0	1	19.78	4.489	2	15.4	-2	0	4	35.02	2.562	2	12.6	0	6	3	44.44	2.039	4	0.8
0	4	0	20.02	4.435	2	4.5	-3	3	3	35.23	2.547	4	5.4	-4	2	1	44.47	2.037	4	0.6
1	1	1	20.45	4.342	4	37.7	3	1	0	36.39	2.469	4	1.9	-2	0	5	44.63	2.030	2	3.3
-2	0	2	20.98	4.234	2	2.4	-2	2	4	36.50	2.462	4	7.8	-3	1	5	44.90	2.019	4	4.2
0	0	2	21.04	4.222	2	0.3	-1	7	1	37.03	2.428	4	0.6	-1	7	3	44.95	2.016	4	1.0
-2	2	1	22.19	4.006	4	12.6	-1	5	3	37.03	2.428	4	11.8	-3	5	4	45.27	2.003	4	1.4
0	4	1	22.65	3.926	4	13.3	-2	6	2	37.09	2.424	4	8.0	-4	4	2	45.28	2.003	4	8.0
-1	3	2	22.96	3.873	4	100.0	0	6	2	37.12	2.422	4	0.5	-1	5	4	45.34	2.000	4	0.7
-2	2	2	23.28	3.821	4	11.0	2	4	1	37.32	2.409	4	2.8	2	4	2	45.37	1.999	4	3.8
0	2	2	23.34	3.812	4	32.9	-3	1	4	37.41	2.404	4	1.5	-2	8	1	45.63	1.988	4	0.4
2	0	0	23.79	3.740	2	14.8	1	7	0	37.47	2.400	4	0.3	-2	2	5	45.85	1.979	4	0.5
1	3	1	24.94	3.570	4	1.3	-1	1	4	37.48	2.400	4	1.5	3	3	1	46.05	1.971	4	1.3
2	2	0	25.85	3.446	4	83.0	0	4	3	37.86	2.376	4	0.3	-2	8	2	46.21	1.964	4	1.4
-2	0	3	26.75	3.333	2	10.7	2	6	0	38.83	2.319	4	4.4	0	8	2	46.24	1.963	4	3.5
-1	5	1	27.25	3.272	4	16.9	-3	5	2	39.13	2.302	4	0.7	-3	7	2	46.76	1.943	4	3.4
-1	1	3	27.26	3.272	4	11.5	3	3	0	39.21	2.297	4	0.2	1	7	2	46.82	1.940	4	5.3
1	5	0	27.83	3.206	4	44.5	-1	7	2	39.67	2.272	4	0.2	-2	6	4	46.92	1.936	4	2.0
-2	4	1	28.29	3.155	4	0.3	-4	0	3	39.99	2.254	2	3.9	-3	3	5	47.30	1.922	4	0.1
-2	2	3	28.61	3.120	4	0.2	-3	3	4	40.17	2.245	4	1.6	-4	4	4	47.60	1.910	4	3.7
-2	4	2	29.16	3.062	4	6.6	-4	0	2	40.17	2.245	2	0.2	2	8	0	47.68	1.907	4	3.3
0	4	2	29.20	3.058	4	0.7	-1	3	4	40.24	2.241	4	1.2	1	9	0	47.71	1.906	4	2.1
-3	1	2	29.96	2.982	4	9.4	-3	5	1	40.38	2.233	4	0.7	0	4	4	47.72	1.906	4	3.8
1	1	2	30.05	2.974	4	2.9	1	1	3	40.46	2.230	4	6.7	-3	7	1	47.85	1.901	4	0.5
0	6	0	30.23	2.957	2	2.1	-2	4	4	40.66	2.219	4	9.7	-4	0	5	47.93	1.898	2	0.3
-1	5	2	30.65	2.917	4	50.1	0	8	0	40.69	2.217	2	0.3	-3	7	3	48.26	1.886	4	0.1
-1	3	3	30.83	2.901	4	2.1	-2	6	3	40.80	2.212	4	4.5	4	0	0	48.70	1.870	2	16.8
2	0	1	31.17	2.870	2	0.7	-3	5	3	40.85	2.209	4	1.0	-4	2	5	49.08	1.856	4	0.8
2	4	0	31.29	2.859	4	42.8	1	7	1	40.92	2.206	4	0.6	-2	4	5	49.37	1.846	4	0.4
-3	1	1	31.53	2.837	4	3.6	-4	2	3	41.32	2.185	4	2.9	-1	9	2	49.55	1.840	4	3.4
0	0	3	31.79	2.814	2	1.1	-4	2	2	41.50	2.176	4	0.2							

Epistilbite

EPI



ERI Erionite

CHEMICAL COMPOSITION: $|K_{2.02}Na_{1.94}Ca_{1.25}Mg_{0.63}(H_2O)_{10.4}|\ [Si_{26.16}Al_{9.31}Fe_{0.53}O_{72}]$
Wenatchee, Washington, U.S.A.

REFINED COMPOSITION: $|K_2Na_{1.86}Ca_{1.3}Mg_{0.7}(H_2O)_{6.12}|\ [Si_{27}Al_9O_{72}]$

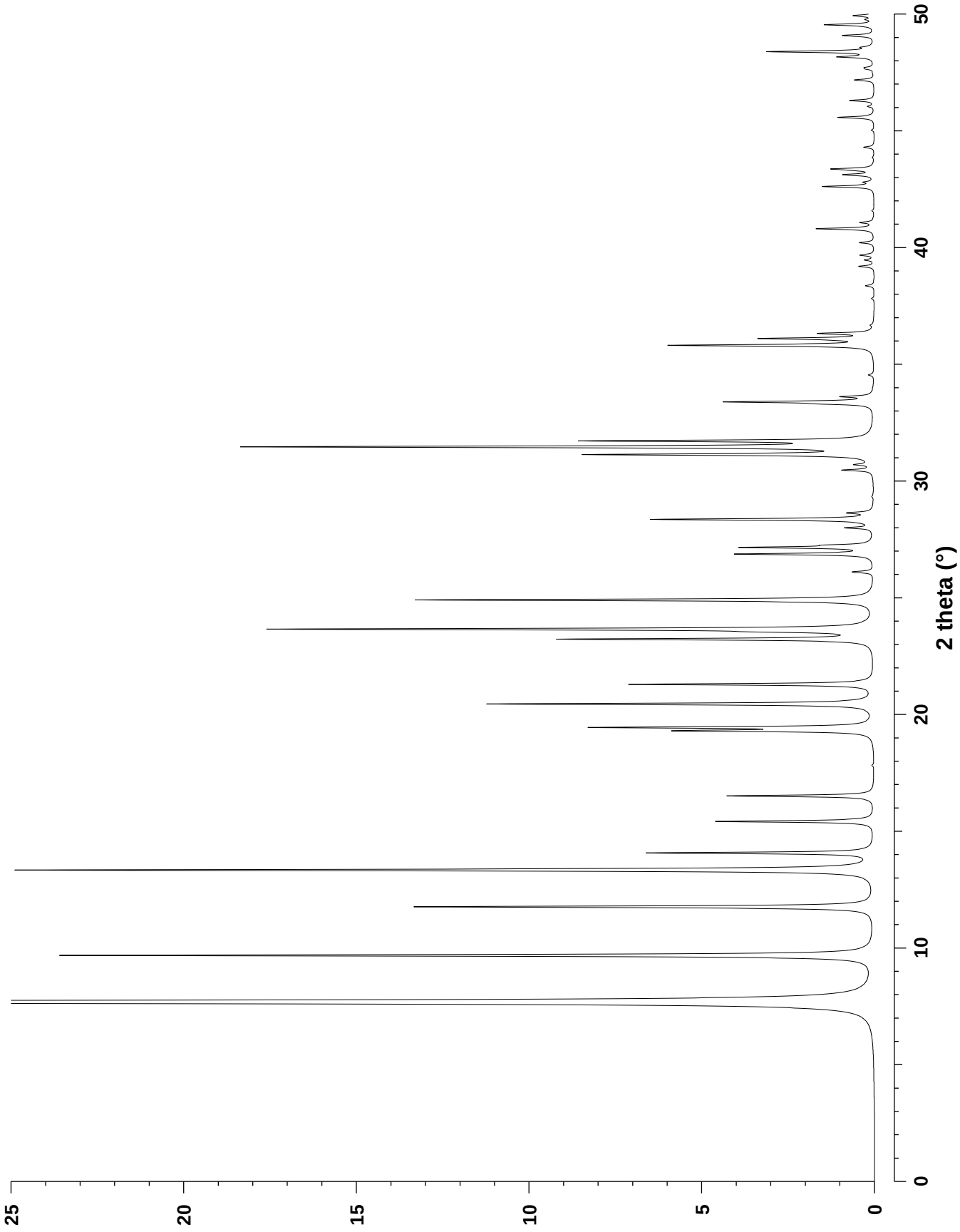
CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.27$ Å $b = 13.27$ Å $c = 15.05$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.15$

REFERENCE: J. A. Gard and J. M. Tait,
in *Proceedings of the Third International Conference on Molecular Sieves; Recent Progress Reports, Zurich*,
Ed. by J. B. Uytterhoeven (Leuven University Press) 94–99 (1973).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.69	11.492	6	100.0	3	1	2	30.46	2.935	24	0.9	5	0	2	41.06	2.198	12	0.4
1	0	1	9.68	9.134	12	23.6	1	0	5	30.70	2.912	12	0.5	3	3	2	42.61	2.122	12	1.5
0	0	2	11.76	7.525	2	13.3	4	0	0	31.13	2.873	6	8.2	1	0	7	42.79	2.113	12	0.2
1	1	0	13.34	6.635	6	24.9	2	1	4	31.46	2.844	24	18.0	3	0	6	43.11	2.098	12	0.9
1	0	2	14.07	6.295	12	6.5	4	0	1	31.71	2.822	12	8.1	5	0	3	43.30	2.090	12	0.3
2	0	0	15.42	5.746	6	4.6	3	1	3	33.30	2.690	24	0.8	4	2	2	43.36	2.087	24	1.1
2	0	1	16.51	5.368	12	4.3	4	0	2	33.38	2.684	12	4.2	5	1	1	44.29	2.045	24	0.3
1	0	3	19.30	4.598	12	5.3	2	0	5	33.61	2.666	12	0.9	5	1	2	45.57	1.991	24	1.1
2	0	2	19.44	4.567	12	7.9	3	2	1	34.54	2.597	24	0.2	3	1	6	46.04	1.971	24	0.2
2	1	0	20.45	4.344	12	11.2	0	0	6	35.80	2.508	2	0.9	5	0	4	46.29	1.961	12	0.7
2	1	1	21.29	4.173	24	7.1	4	1	0	35.81	2.508	12	5.1	2	1	7	47.17	1.927	24	0.2
3	0	0	23.22	3.831	6	9.0	4	0	3	36.02	2.493	12	0.3	4	1	5	47.17	1.927	24	0.4
2	0	3	23.54	3.779	12	1.4	2	2	4	36.09	2.488	12	0.8	5	1	3	47.64	1.909	24	0.2
0	0	4	23.65	3.762	2	2.2	3	2	2	36.10	2.488	24	2.4	3	3	4	47.70	1.907	12	0.2
2	1	2	23.65	3.762	24	15.1	2	1	5	36.31	2.474	24	1.3	4	0	6	48.16	1.890	12	0.9
1	0	4	24.90	3.576	12	13.3	4	1	1	36.32	2.474	24	0.2	4	3	0	48.16	1.889	12	0.1
3	0	2	26.10	3.414	12	0.6	1	1	6	38.36	2.346	12	0.3	0	0	8	48.38	1.881	2	2.9
2	2	0	26.87	3.317	6	4.0	2	0	6	39.19	2.299	12	0.1	4	2	4	48.39	1.881	24	0.2
2	1	3	27.15	3.284	24	3.7	5	0	0	39.19	2.298	6	0.3	4	3	1	48.57	1.875	24	0.3
1	1	4	27.25	3.273	12	1.0	4	0	4	39.46	2.283	12	0.3	1	0	8	49.07	1.857	12	0.9
3	1	0	27.99	3.187	12	0.8	5	0	1	39.67	2.272	12	0.4	5	2	0	49.53	1.840	12	1.4
2	0	4	28.35	3.148	12	6.5	4	1	3	40.20	2.243	24	0.4	4	3	2	49.76	1.832	24	0.2
3	1	1	28.63	3.118	24	0.7	3	3	0	40.80	2.212	6	1.7	5	0	5	49.92	1.827	12	0.6

Erionite

ERI



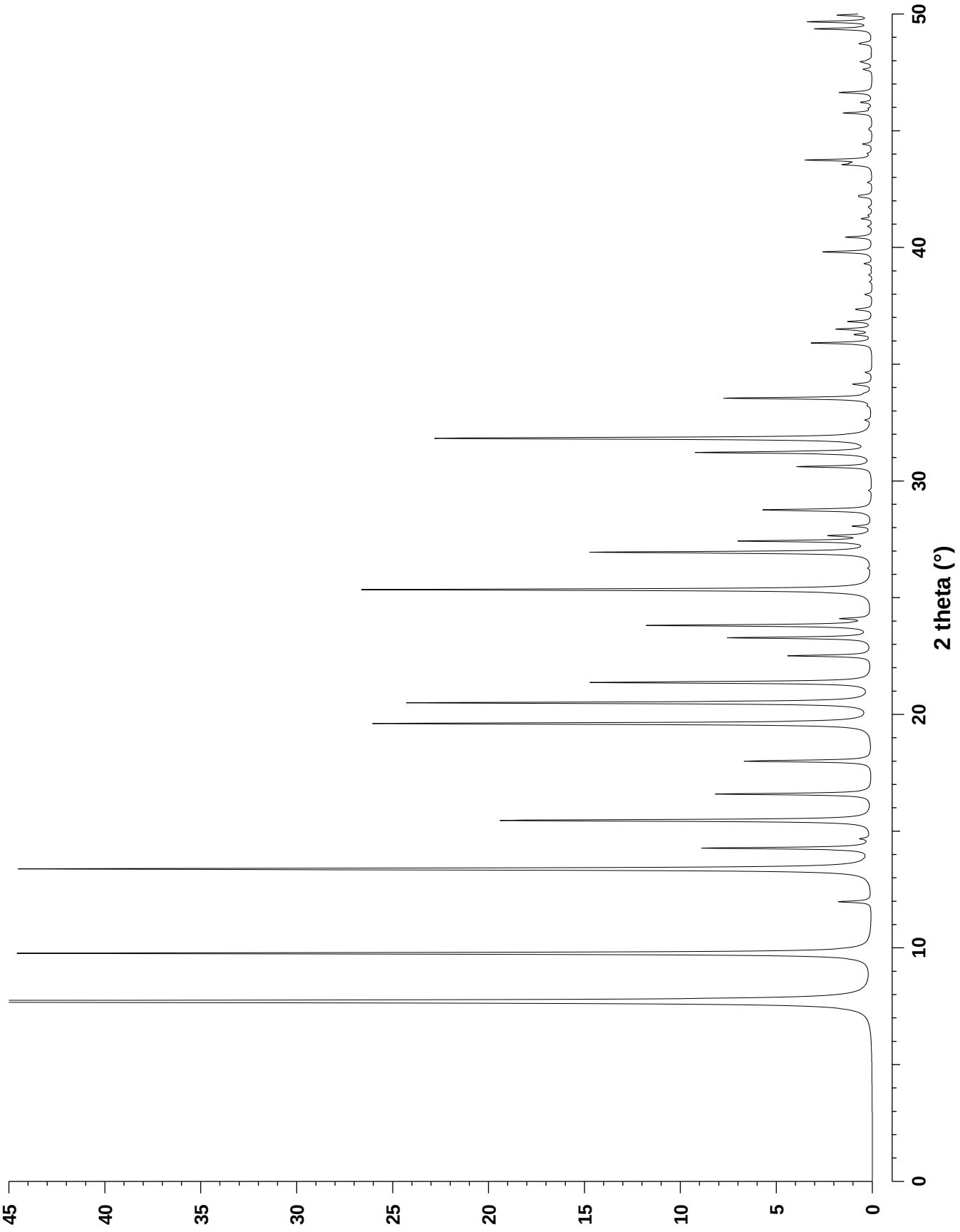
CHEMICAL COMPOSITION: $|(C_5H_{10}NH)_4(H_2O)_4|\ [Al_{18}P_{18}O_{72}]$
$C_5H_{10}NH$ = piperidine

REFINED COMPOSITION: $|C_{24}O_{4.14}|\ [Al_{18}P_{18}O_{72}]$

CRYSTAL DATA: $P6_3/m$ (No. 176)
$a = 13.2371$ Å $b = 13.2371$ Å $c = 14.7708$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.081$

REFERENCE: J. J. Pluth, J. V. Smith and J. M. Bennett,
Acta Cryst. **C42** 283–286 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.71	11.464	6	100.0	1	0	5	31.27	2.861	12	1.1	2	4	1	42.16	2.143	12	0.2
1	0	1	9.77	9.056	12	44.5	4	0	1	31.81	2.813	12	14.1	3	2	4	42.18	2.142	12	0.2
0	0	2	11.98	7.385	2	1.7	1	2	4	31.84	2.810	12	4.8	1	2	6	42.22	2.140	12	0.3
1	1	0	13.38	6.619	6	44.5	2	1	4	31.84	2.810	12	7.0	2	1	6	42.22	2.140	12	0.2
1	0	2	14.27	6.209	12	8.8	2	2	3	32.60	2.747	12	0.3	3	3	2	42.78	2.114	12	0.2
1	1	1	14.67	6.040	12	0.5	1	1	5	33.21	2.698	12	0.1	4	2	2	43.53	2.079	12	0.4
2	0	0	15.46	5.732	6	19.4	4	0	2	33.54	2.672	12	6.6	5	0	3	43.54	2.078	12	0.9
2	0	1	16.59	5.344	12	8.1	3	1	3	33.55	2.671	12	1.1	1	0	7	43.61	2.075	12	0.6
1	1	2	18.00	4.929	12	6.6	3	0	4	33.75	2.655	12	0.2	3	0	6	43.74	2.070	12	3.4
2	0	2	19.60	4.528	12	12.4	3	2	0	34.09	2.630	6	0.1	4	0	5	44.02	2.057	12	0.2
1	0	3	19.62	4.524	12	15.2	2	0	5	34.14	2.626	12	0.9	1	5	1	44.42	2.039	12	0.4
1	2	0	20.50	4.333	6	14.6	3	2	1	34.64	2.589	12	0.3	3	3	3	45.03	2.013	12	0.1
2	1	0	20.50	4.333	6	9.6	4	1	0	35.90	2.502	6	2.2	1	1	7	45.10	2.010	12	0.1
2	1	1	21.37	4.158	12	4.8	1	4	0	35.90	2.502	6	0.9	5	1	2	45.75	1.983	12	1.0
1	2	1	21.37	4.158	12	9.8	2	3	2	36.26	2.478	12	0.5	1	5	2	45.75	1.983	12	0.5
1	1	3	22.51	3.950	12	4.3	3	2	2	36.26	2.478	12	0.2	2	2	6	45.95	1.975	12	0.1
3	0	0	23.28	3.821	6	7.5	4	0	3	36.27	2.477	12	0.2	2	3	5	46.21	1.964	12	0.6
2	1	2	23.81	3.737	12	6.5	1	4	1	36.43	2.466	12	0.2	5	0	4	46.63	1.948	12	1.7
1	2	2	23.81	3.737	12	3.7	0	0	6	36.50	2.462	2	1.8	6	0	0	47.59	1.911	6	0.1
2	0	3	23.82	3.735	12	1.6	1	2	5	36.82	2.441	12	1.2	4	1	5	47.63	1.909	12	0.3
0	0	4	24.10	3.693	2	1.4	1	3	4	37.32	2.409	12	0.1	1	4	5	47.63	1.909	12	0.1
1	0	4	25.34	3.515	12	26.6	3	1	4	37.32	2.409	12	0.3	5	1	3	47.89	1.900	12	0.2
3	0	2	26.26	3.394	12	0.1	1	0	6	37.36	2.407	12	0.6	2	1	7	47.95	1.897	12	0.2
2	2	0	26.94	3.309	6	14.7	4	1	2	37.98	2.369	12	0.4	1	2	7	47.95	1.897	12	0.3
2	1	3	27.42	3.253	12	6.8	3	0	5	38.52	2.337	12	0.1	3	3	4	48.04	1.894	12	0.1
2	2	1	27.62	3.229	12	0.4	2	3	3	38.82	2.320	12	0.1	3	4	1	48.71	1.869	12	0.2
1	1	4	27.66	3.225	12	1.9	5	0	0	39.30	2.293	6	0.4	4	3	1	48.71	1.869	12	0.3
3	1	0	28.06	3.179	6	0.4	5	0	1	39.79	2.266	12	1.0	4	0	6	48.76	1.867	12	0.3
1	3	0	28.06	3.179	6	0.6	4	0	4	39.81	2.264	12	1.7	0	0	8	49.36	1.846	2	2.9
3	1	1	28.72	3.108	12	1.6	1	4	3	40.44	2.230	12	0.6	2	5	0	49.66	1.836	6	0.9
2	0	4	28.76	3.104	12	4.9	4	1	3	40.44	2.230	12	0.8	5	2	0	49.66	1.836	6	2.4
2	2	2	29.58	3.020	12	0.1	3	3	0	40.90	2.206	6	0.2	3	4	2	49.94	1.826	12	1.1
1	3	2	30.61	2.920	12	1.2	5	0	2	41.23	2.190	12	0.6	4	3	2	49.94	1.826	12	0.6
3	1	2	30.61	2.920	12	2.6	3	3	1	41.38	2.182	12	0.2							
4	0	0	31.21	2.866	6	8.8	3	1	5	41.74	2.164	12	0.1							


0
10
20
30
40
50
2 theta (°)
45
40
35
30
25
20
15
10
5
0

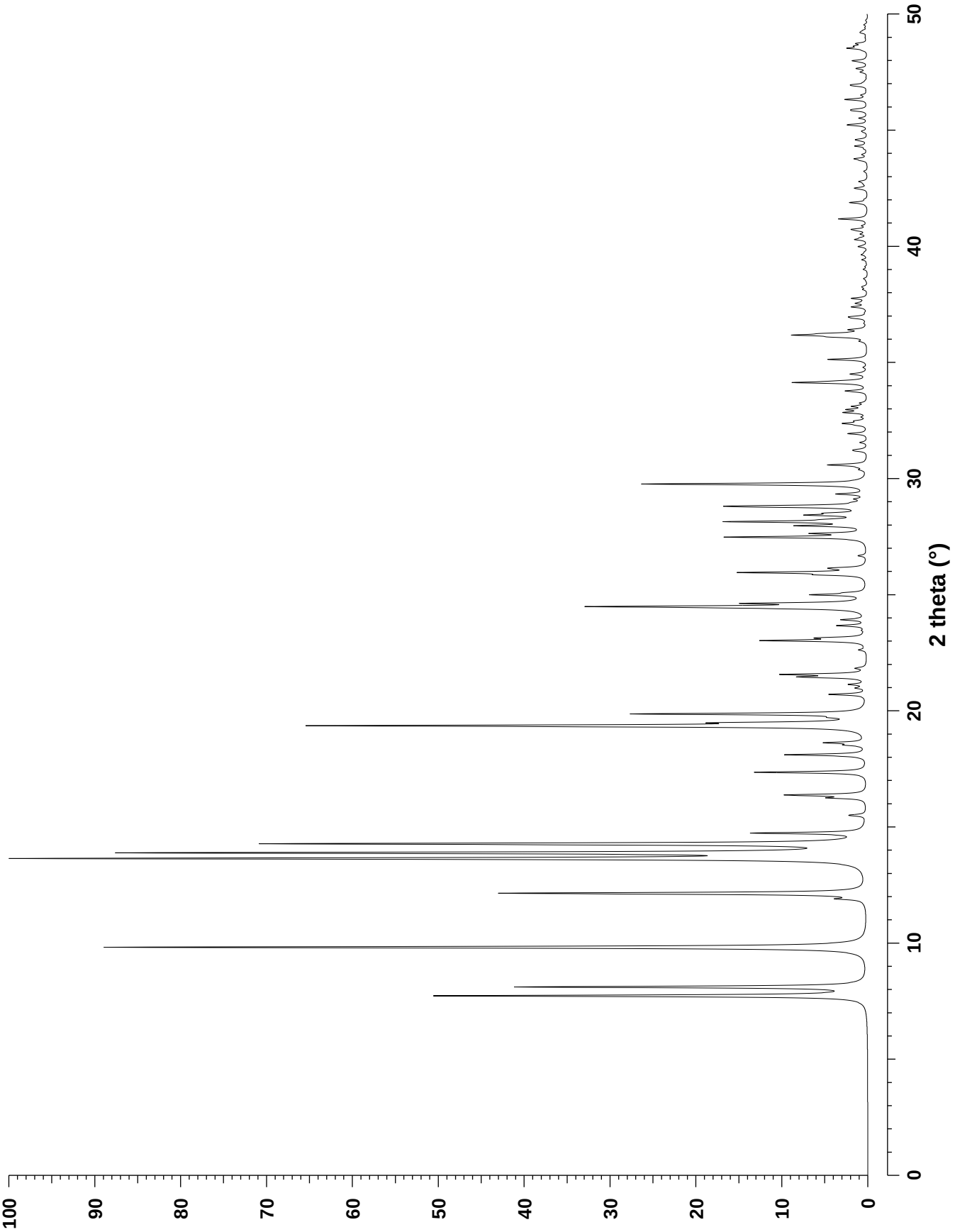
CHEMICAL COMPOSITION: $[Al_{1.4}Si_{46.6}O_{96}]$

REFINED COMPOSITION: $[Si_{48}O_{96}]$

CRYSTAL DATA: *Pnma* (No. 62)
$a = 9.7998$ Å $b = 12.4116$ Å $c = 22.8606$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.056$, $R_{wp} = 0.0611$

REFERENCE: R. Millini, G. Perego, L. Carluccio, G. Bellussi, D. E. Cox, B. J. Campbell and A. K. Cheetham, in *Proc. of the 12th International Zeolite Conference*, Ed. by M. M. J. Treacy, B. K. Marcus, J. B. Higgins and M. E. Bisher (Materials Research Society: Warrendale) vol. **I** 541–548 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	7.73	11.430	2	51.5	2	3	0	28.23	3.161	4	1.8	4	0	2	37.54	2.396	4	1.2
0	1	1	8.11	10.908	4	41.6	0	1	7	28.26	3.158	4	0.4	2	4	4	37.75	2.383	8	1.9
1	0	1	9.82	9.007	4	91.2	3	0	2	28.42	3.141	4	6.2	0	5	3	38.13	2.360	4	0.5
1	0	2	11.90	7.440	4	2.7	2	3	1	28.50	3.131	8	2.8	4	1	2	38.26	2.352	8	0.5
1	1	1	12.14	7.290	8	43.9	3	1	1	28.52	3.129	8	0.9	4	0	3	38.60	2.332	4	0.4
0	1	3	13.64	6.494	4	100.0	0	4	0	28.77	3.103	2	8.1	3	0	7	39.00	2.310	4	0.5
1	1	2	13.88	6.381	8	86.5	1	0	7	28.81	3.098	4	12.4	0	0	10	39.41	2.286	2	0.5
0	2	0	14.27	6.206	2	71.3	1	2	6	28.97	3.082	8	0.7	2	4	5	39.63	2.274	8	0.6
1	0	3	14.73	6.016	4	13.2	0	3	5	29.11	3.068	4	1.0	2	0	9	39.98	2.255	4	1.0
0	0	4	15.50	5.715	2	2.0	3	1	2	29.33	3.045	8	3.4	3	4	1	40.28	2.239	8	1.3
0	2	2	16.25	5.454	4	4.0	2	0	6	29.70	3.008	4	1.0	4	2	2	40.36	2.235	8	0.6
1	1	3	16.37	5.413	8	9.5	1	1	7	29.72	3.006	8	0.6	1	0	10	40.52	2.226	4	0.7
1	2	1	17.35	5.110	8	13.4	3	0	3	29.76	3.002	4	26.3	2	1	9	40.66	2.219	8	0.7
2	0	0	18.10	4.900	2	9.8	2	2	5	30.37	2.943	8	0.7	4	1	4	40.72	2.216	8	1.6
2	0	1	18.52	4.791	4	2.1	1	4	1	30.47	2.934	8	0.6	3	4	2	40.88	2.207	8	0.5
1	2	2	18.62	4.766	8	4.7	2	1	6	30.58	2.923	8	4.4	1	4	7	41.17	2.192	8	3.5
1	1	4	19.35	4.587	8	65.8	3	2	1	31.19	2.868	8	1.1	3	4	3	41.87	2.158	8	2.1
2	1	0	19.48	4.558	4	13.2	1	4	2	31.23	2.864	8	1.0	4	1	5	42.49	2.128	8	0.6
2	0	2	19.71	4.504	4	1.8	3	0	4	31.55	2.836	4	0.8	3	3	6	42.50	2.127	8	0.6
2	1	1	19.86	4.470	8	27.7	3	2	2	31.93	2.802	8	2.3	1	3	9	42.78	2.114	8	0.9
0	1	5	20.70	4.290	4	4.4	1	2	7	32.29	2.772	8	0.8	2	0	10	43.69	2.072	4	0.6
2	1	2	20.98	4.233	8	1.1	2	3	4	32.36	2.766	8	1.6	0	6	0	43.76	2.069	2	1.5
0	2	4	21.13	4.204	4	2.0	3	1	4	32.38	2.765	8	1.3	4	0	6	43.94	2.061	4	0.6
1	0	5	21.45	4.143	4	7.3	1	4	3	32.47	2.758	8	1.2	2	4	7	44.31	2.044	8	1.4
2	0	3	21.56	4.121	4	9.6	1	0	8	32.64	2.743	4	0.5	1	0	11	44.57	2.033	4	0.6
0	3	1	21.83	4.071	4	1.2	0	4	4	32.84	2.727	4	2.7	3	2	8	44.59	2.032	8	0.5
1	1	5	22.62	3.930	8	0.9	2	0	7	32.96	2.718	4	2.2	3	3	7	44.95	2.017	8	0.5
1	2	4	23.02	3.863	8	12.3	2	2	6	33.10	2.707	8	1.6	3	0	9	45.22	2.005	4	2.3
2	2	0	23.13	3.846	4	4.9	1	3	6	33.25	2.695	8	0.8	2	5	5	45.51	1.993	8	1.0
1	3	1	23.66	3.760	8	3.5	2	1	7	33.76	2.655	8	2.5	2	3	9	45.83	1.980	8	1.3
2	0	4	23.92	3.720	4	2.9	1	4	4	34.13	2.627	8	8.6	4	3	4	45.88	1.978	8	1.3
2	2	2	24.42	3.645	8	8.1	2	4	0	34.20	2.621	4	1.5	1	3	10	46.31	1.960	8	2.5
0	3	3	24.48	3.636	4	30.3	2	3	5	34.49	2.600	8	1.5	5	0	1	46.50	1.953	4	0.7
1	3	2	24.62	3.616	8	12.6	3	1	5	34.51	2.599	8	0.5	1	5	7	46.90	1.937	8	0.9
2	1	4	24.99	3.563	8	6.3	3	2	4	34.78	2.579	8	0.4	4	1	7	46.94	1.936	8	1.5
1	0	6	25.08	3.551	4	1.7	2	4	2	35.12	2.555	8	4.7	4	3	5	47.49	1.914	8	0.7
1	2	5	25.85	3.446	8	4.3	3	3	2	35.90	2.502	8	0.7	5	1	2	47.64	1.909	8	0.8
2	2	3	25.95	3.433	8	14.7	0	1	9	36.09	2.488	4	3.0	1	6	4	47.66	1.908	8	0.5
1	1	6	26.10	3.414	8	1.7	1	4	5	36.17	2.484	8	7.5	5	0	3	47.92	1.898	4	0.5
1	3	3	26.14	3.409	8	3.0	2	4	3	36.24	2.479	8	3.5	4	4	2	47.98	1.896	8	1.7
2	0	5	26.67	3.343	4	1.0	2	0	8	36.40	2.468	4	1.7	5	1	3	48.52	1.876	8	2.2
0	2	6	27.47	3.247	4	16.7	4	0	1	36.90	2.436	4	1.3	3	0	10	48.61	1.873	4	1.2
2	1	5	27.63	3.228	8	5.8	2	3	6	36.95	2.433	8	0.8	4	2	7	48.72	1.869	8	1.1
2	2	4	27.96	3.191	8	7.7	3	1	6	36.96	2.432	8	1.0	2	3	10	49.18	1.852	8	0.6
1	3	4	28.14	3.171	8	16.2	0	4	6	37.38	2.406	4	1.7	1	6	5	49.23	1.851	8	0.4


100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
2 theta (°)

EUO EU-1, Calcined, Rehydrated

CHEMICAL COMPOSITION: $|(H_2O)_{36.16}|\ [Si_{112}O_{224}]$

REFINED COMPOSITION: $|O_{36.16}|\ [Si_{112}O_{224}]$

CRYSTAL DATA: *Cmme* (No. 67)
$a = 13.695$ Å $b = 22.326$ Å $c = 20.178$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld limited refinement. No R-factor reported.

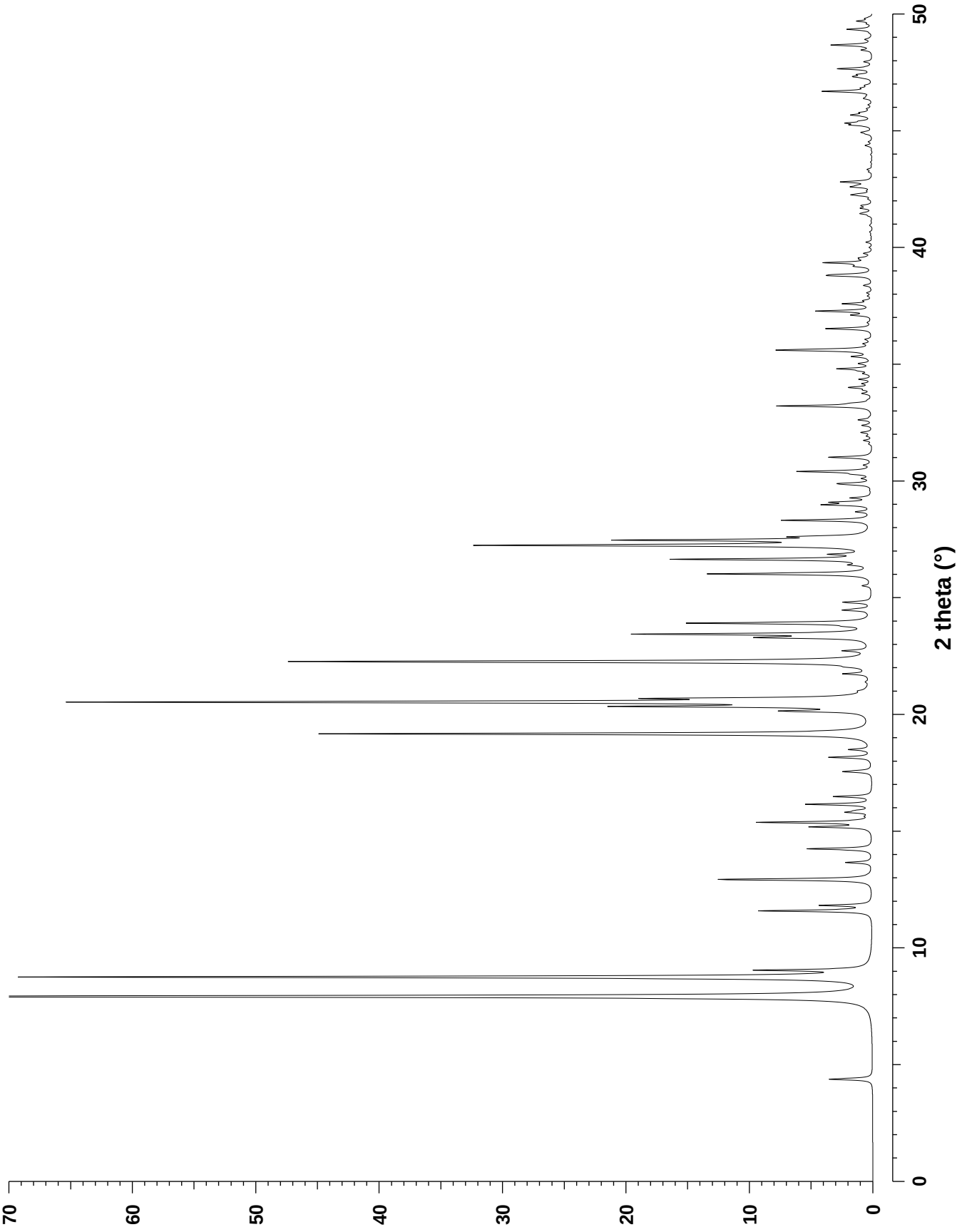
REFERENCE: N. A. Briscoe, D. W. Johnson, M. D. Shannon, G. T. Kokotailo and L. B. McCusker, *Zeolites* **8** 74–76 (1988).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	4.38	20.178	2	3.5	4	2	0	27.24	3.273	4	28.3	5	3	2	36.06	2.491	8	0.5
0	2	0	7.92	11.163	2	100.0	0	4	5	27.27	3.270	4	2.2	0	2	8	36.52	2.460	4	3.7
1	1	1	8.75	10.105	8	64.0	2	6	0	27.28	3.269	4	3.5	1	9	1	37.10	2.423	8	1.0
0	0	2	8.76	10.089	2	5.3	0	6	3	27.39	3.256	4	0.9	3	1	7	37.10	2.423	8	0.5
0	2	1	9.05	9.768	4	8.4	1	5	4	27.46	3.248	8	19.1	2	8	3	37.27	2.412	8	4.5
1	1	2	11.59	7.633	8	9.1	4	0	2	27.51	3.242	4	0.6	5	1	4	37.58	2.393	8	2.3
0	2	2	11.82	7.485	4	4.1	1	1	6	27.60	3.232	8	4.1	1	5	7	37.72	2.385	8	0.6
2	0	0	12.93	6.847	2	12.5	2	6	1	27.64	3.227	8	1.7	4	2	6	38.37	2.346	8	0.7
2	0	1	13.66	6.484	4	2.1	3	5	1	28.31	3.153	8	7.3	3	7	4	38.79	2.321	8	2.7
1	3	1	14.24	6.220	8	5.3	4	2	2	28.67	3.113	8	1.1	5	5	1	38.83	2.319	8	1.9
2	2	0	15.18	5.837	4	4.8	3	3	4	28.98	3.081	8	3.7	0	4	8	39.19	2.298	4	1.0
0	2	3	15.38	5.761	4	9.2	1	7	1	29.08	3.070	8	2.9	0	8	5	39.25	2.295	4	0.5
2	2	1	15.81	5.607	8	1.9	4	0	3	29.27	3.051	4	1.6	5	3	4	39.34	2.290	8	3.8
0	4	0	15.88	5.582	2	0.9	0	6	4	29.84	2.994	4	0.8	1	7	6	39.49	2.282	8	0.5
1	3	2	16.15	5.487	8	5.4	1	3	6	29.88	2.991	8	2.4	0	6	7	39.55	2.279	4	0.8
0	4	1	16.48	5.379	4	3.1	1	7	2	30.10	2.969	8	0.7	6	0	1	39.74	2.268	4	0.6
2	2	2	17.55	5.052	8	2.1	2	4	5	30.29	2.951	8	1.0	0	0	9	40.22	2.242	2	0.5
0	0	4	17.58	5.044	2	0.4	4	2	3	30.37	2.943	8	0.5	2	4	8	41.44	2.179	8	0.8
0	4	2	18.16	4.884	4	3.5	2	6	3	30.40	2.940	8	5.7	3	9	1	41.68	2.167	8	0.7
2	0	3	18.49	4.798	4	1.7	2	2	6	30.68	2.914	8	0.6	6	0	3	41.79	2.161	4	0.7
1	1	4	19.17	4.631	8	44.9	3	5	3	31.01	2.884	8	2.4	3	5	7	42.24	2.139	8	1.5
2	2	3	20.14	4.408	8	6.2	0	0	7	31.02	2.883	2	1.1	4	6	5	42.29	2.137	8	0.6
3	1	1	20.34	4.366	8	18.3	1	7	3	31.73	2.820	8	0.7	2	10	0	42.59	2.123	4	1.4
2	4	0	20.53	4.326	4	63.6	0	2	7	32.07	2.791	4	0.5	5	5	4	42.67	2.119	8	0.5
0	4	3	20.68	4.295	4	14.4	0	8	0	32.07	2.791	2	0.4	1	7	7	42.80	2.113	8	0.5
2	4	1	21.00	4.230	8	0.4	0	8	1	32.38	2.764	4	0.8	6	4	0	42.80	2.113	4	1.8
3	1	2	21.74	4.089	8	2.0	4	2	4	32.61	2.746	8	1.0	5	3	6	44.36	2.042	8	0.5
0	0	5	22.03	4.036	2	0.8	3	5	4	33.21	2.697	8	7.7	0	0	10	44.92	2.018	2	0.8
1	3	4	22.26	3.994	8	47.2	0	8	2	33.31	2.690	4	0.4	3	1	9	45.24	2.004	8	1.3
2	4	2	22.36	3.976	8	0.6	3	1	6	33.33	2.688	8	0.6	3	9	4	45.32	2.001	8	1.8
1	5	2	22.72	3.913	8	2.0	2	0	7	33.74	2.657	4	0.7	2	6	8	45.41	1.997	8	0.7
3	3	1	23.28	3.821	8	6.5	1	7	4	33.89	2.645	8	0.5	6	0	5	45.66	1.987	4	1.3
2	2	4	23.31	3.817	8	1.5	1	3	7	33.99	2.638	8	0.8	1	5	9	45.77	1.983	8	0.8
1	1	5	23.32	3.814	8	1.5	1	5	6	34.01	2.636	8	1.1	1	7	8	46.37	1.958	8	0.5
0	2	5	23.44	3.795	4	18.7	5	1	2	34.16	2.625	8	0.7	6	6	0	46.68	1.946	4	4.0
0	4	4	23.77	3.742	4	1.0	4	0	5	34.35	2.611	4	1.0	7	1	1	46.83	1.940	8	0.6
0	6	0	23.91	3.721	2	14.8	3	7	1	34.59	2.593	8	0.6	5	7	4	47.31	1.921	8	1.2
2	4	3	24.46	3.639	8	2.1	2	8	0	34.71	2.584	4	0.4	3	9	5	47.40	1.918	8	0.7
3	3	2	24.52	3.631	8	0.7	0	8	3	34.80	2.578	4	2.7	4	4	8	47.65	1.908	8	2.7
1	5	3	24.80	3.590	8	2.3	2	8	1	35.00	2.563	8	0.4	4	6	7	47.95	1.897	8	0.5
0	6	2	25.51	3.491	4	0.7	0	4	7	35.03	2.561	4	0.7	2	10	5	48.45	1.879	8	0.8
4	0	0	26.02	3.424	2	13.3	2	6	5	35.33	2.540	8	1.2	0	8	8	48.66	1.871	4	2.9
4	0	1	26.40	3.376	4	1.3	0	0	8	35.59	2.522	2	6.0	3	11	1	49.34	1.847	8	1.9
3	1	4	26.64	3.347	8	16.1	5	1	3	35.62	2.521	8	0.9	3	5	9	49.69	1.835	8	1.2
2	2	5	26.86	3.319	8	2.7	4	6	0	35.63	2.519	4	2.1	5	9	1	49.80	1.831	8	0.5

The space group symbol *Cmme* now replaces the older form, *Cmma*.

EU-1, Calcined, Rehydrated

EUO



FAU Faujasite

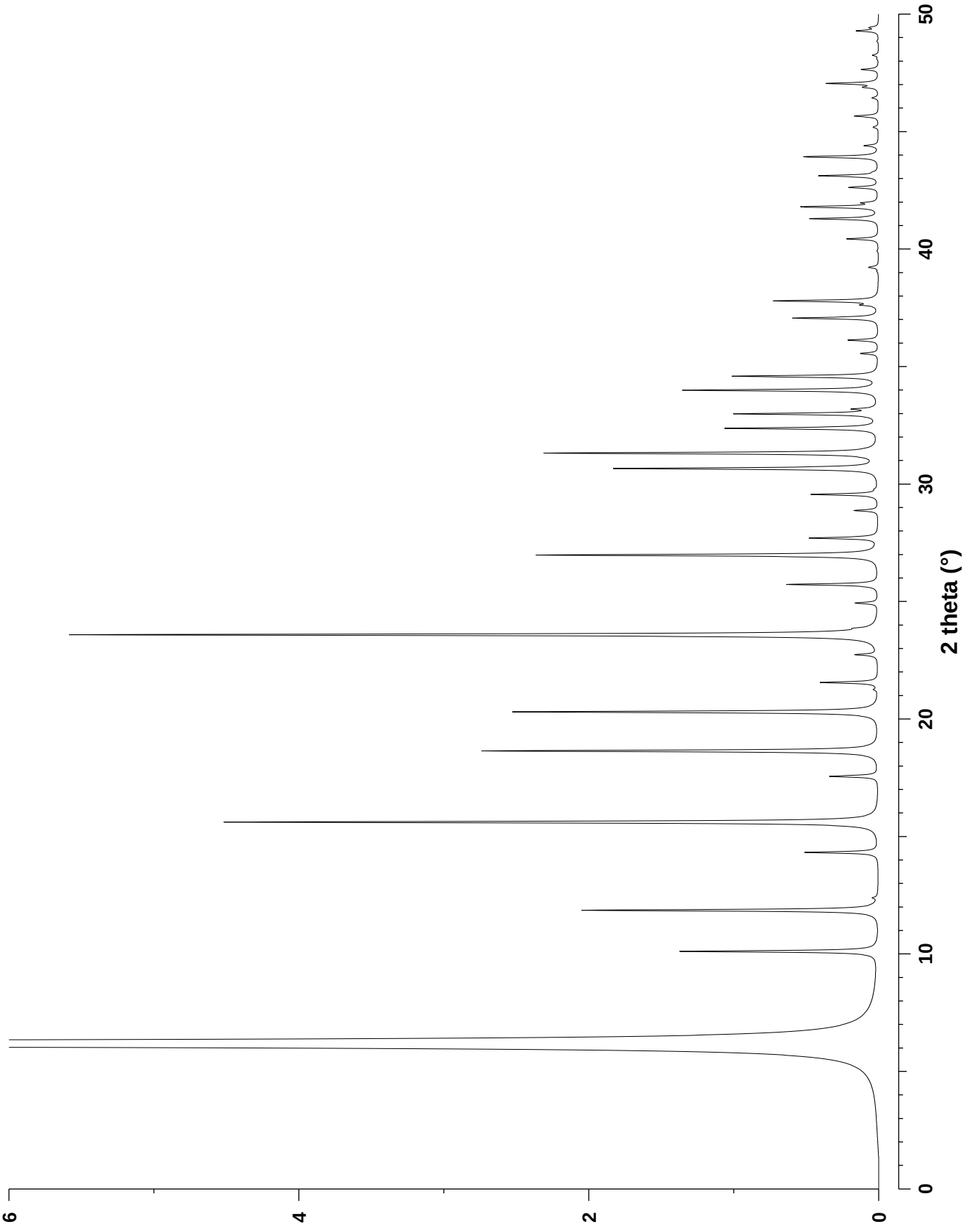
CHEMICAL COMPOSITION: $|Na_{28.8}Ca_{14.4}(H_2O)_{263}|\ [Si_{134.4}Al_{57.6}O_{384}]$
Kaiserstuhl, Germany

REFINED COMPOSITION: $|Na_{16}Ca_{16}(H_2O)_{42.7}|\ [Si_{134.4}Al_{57.6}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}m$ (No. 227) origin at centre ($\overline{3}m$)
$a = 24.74$ Å $b = 24.74$ Å $c = 24.74$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.13$

REFERENCE: W. H. Baur,
American Mineralogist **49** 697–704 (1964).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	6.19	14.284	8	100.0	7	3	1	27.70	3.221	48	0.5	8	6	2	37.06	2.426	48	0.3
2	2	0	10.11	8.747	12	1.4	8	0	0	28.87	3.092	6	0.2	10	2	0	37.06	2.426	24	0.3
3	1	1	11.86	7.459	24	2.0	7	3	3	29.55	3.022	24	0.5	6	6	6	37.79	2.381	8	0.6
4	0	0	14.32	6.185	6	0.5	8	2	2	30.66	2.916	24	1.1	7	7	5	40.43	2.231	24	0.2
3	3	1	15.61	5.676	24	4.5	6	6	0	30.66	2.916	12	0.7	8	8	0	41.29	2.187	12	0.5
4	2	2	17.56	5.050	24	0.3	5	5	5	31.31	2.857	8	2.0	11	3	1	41.79	2.162	48	0.2
5	1	1	18.64	4.761	24	2.7	7	5	1	31.31	2.857	48	0.3	9	7	1	41.79	2.162	48	0.3
4	4	0	20.30	4.373	12	2.5	8	4	0	32.37	2.766	24	1.1	10	6	0	42.62	2.121	24	0.2
4	4	2	21.55	4.123	24	0.4	9	1	1	32.98	2.716	24	0.5	11	3	3	43.11	2.098	24	0.2
6	2	0	22.73	3.912	24	0.2	7	5	3	32.98	2.716	48	0.5	9	7	3	43.11	2.098	48	0.2
5	3	3	23.58	3.773	24	5.6	8	4	2	33.19	2.699	48	0.1	8	8	4	43.92	2.062	24	0.5
4	4	4	24.93	3.571	8	0.2	6	6	4	33.99	2.637	24	1.3	12	4	2	47.04	1.932	48	0.3
7	1	1	25.72	3.464	24	0.1	9	3	1	34.58	2.593	48	1.0	10	8	2	47.64	1.909	48	0.1
5	5	1	25.72	3.464	24	0.5	8	4	4	35.55	2.525	24	0.1	13	3	1	49.28	1.849	48	0.1
6	4	2	26.97	3.306	48	2.4	7	5	5	36.12	2.486	24	0.1							


0
10
20
30
40
50
2 theta (°)
0
2
4
6

FAU

Na-X, Dehydrated

CHEMICAL COMPOSITION: $|Na_{88}|\ [Si_{104}Al_{88}O_{384}]$

REFINED COMPOSITION: $|Na_{92.9}|\ [Si_{103.68}Al_{88.32}O_{384}]$

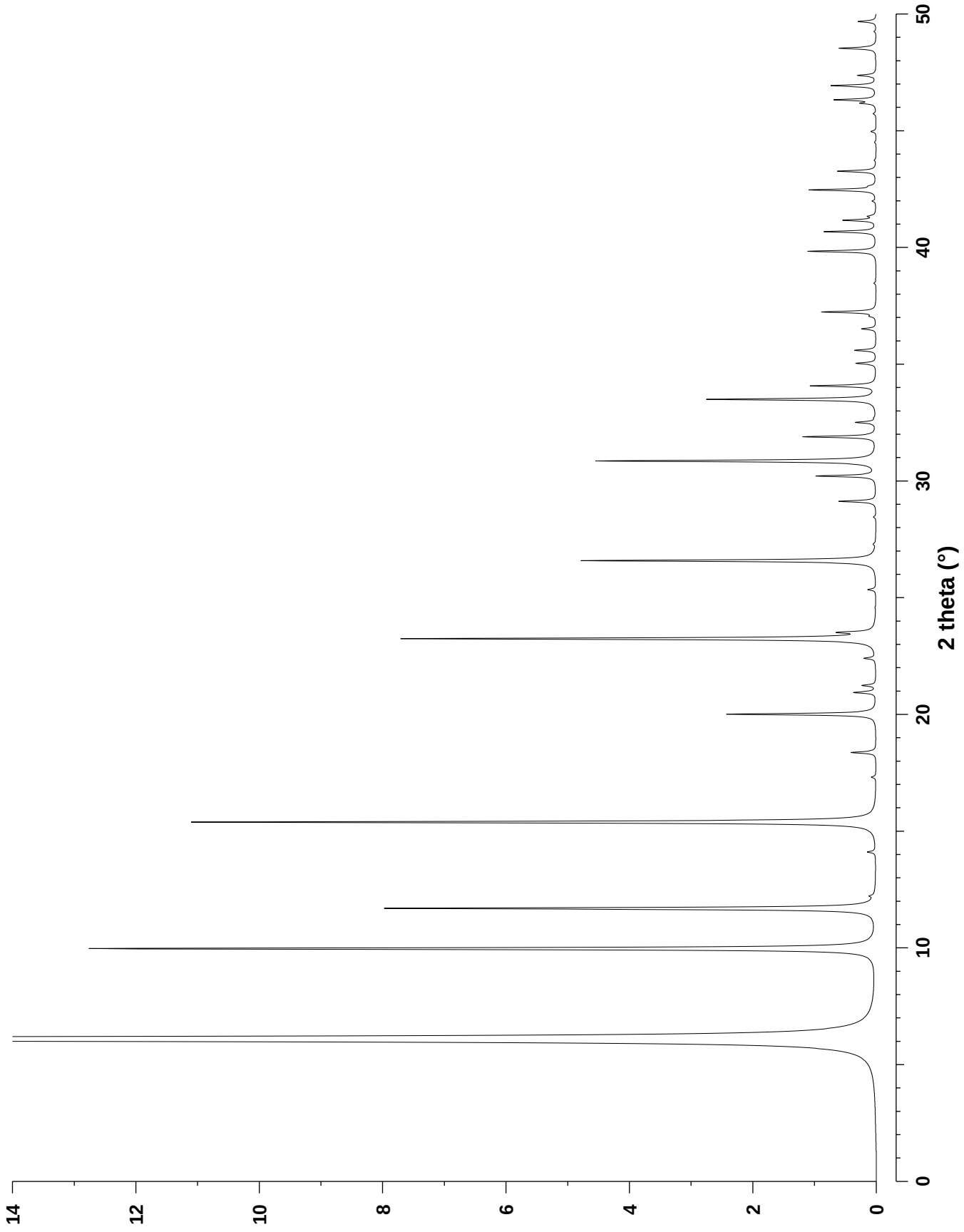
CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 25.099$ Å $b = 25.099$ Å $c = 25.099$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.046$

REFERENCE: D. H. Olson,
Zeolites **15** 439–443 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	6.10	14.491	8	100.0	5	5	5	30.85	2.898	8	4.5	11	1	3	41.16	2.193	24	0.1
2	2	0	9.97	8.874	12	12.7	8	0	4	31.89	2.806	12	0.5	9	1	7	41.16	2.193	24	0.1
3	1	1	11.69	7.568	24	8.0	8	4	0	31.89	2.806	12	0.7	10	4	4	41.33	2.185	24	0.1
4	0	0	14.11	6.275	6	0.1	7	5	3	32.50	2.755	24	0.2	11	3	3	42.46	2.129	24	1.0
3	3	1	15.39	5.758	24	11.1	7	3	5	32.50	2.755	24	0.1	12	0	0	43.26	2.092	6	0.3
5	1	1	18.37	4.830	24	0.4	6	6	4	33.49	2.676	24	2.7	8	8	4	43.26	2.092	24	0.3
4	4	0	20.01	4.437	12	2.4	9	1	3	34.07	2.631	24	0.5	9	9	1	46.17	1.966	24	0.2
5	3	1	20.94	4.243	24	0.4	9	3	1	34.07	2.631	24	0.5	12	4	2	46.32	1.960	24	0.2
4	4	2	21.24	4.183	24	0.2	8	4	4	35.03	2.562	24	0.3	8	8	6	46.32	1.960	24	0.2
6	2	0	22.40	3.969	12	0.2	7	5	5	35.59	2.523	24	0.3	12	2	4	46.32	1.960	24	0.2
5	3	3	23.24	3.828	24	7.7	8	2	6	36.51	2.461	24	0.1	10	2	8	46.92	1.936	24	0.3
6	2	2	23.51	3.784	24	0.5	10	2	2	37.23	2.415	24	0.3	10	8	2	46.92	1.936	24	0.4
6	4	2	26.58	3.354	24	2.8	6	6	6	37.23	2.415	8	0.6	9	9	3	47.36	1.919	24	0.2
6	2	4	26.58	3.354	24	2.0	11	1	1	39.83	2.263	24	0.8	11	3	7	48.53	1.876	24	0.2
7	3	3	29.12	3.066	24	0.6	7	7	5	39.83	2.263	24	0.3	9	7	7	48.53	1.876	24	0.2
8	2	2	30.21	2.958	24	0.5	8	8	0	40.67	2.218	12	0.8	11	7	3	48.53	1.876	24	0.2
6	6	0	30.21	2.958	12	0.4	11	3	1	41.16	2.193	24	0.2	9	9	5	49.67	1.835	24	0.2

Na-X, Dehydrated

FAU



FAU Na-X, Hydrated

CHEMICAL COMPOSITION: $|Na_{88}(H_2O)_{220}|\ [Si_{104}Al_{88}O_{384}]$

REFINED COMPOSITION: $|Na_{40.32}(H_2O)_{171.84}|\ [Si_{103.68}Al_{88.32}O_{384}]$

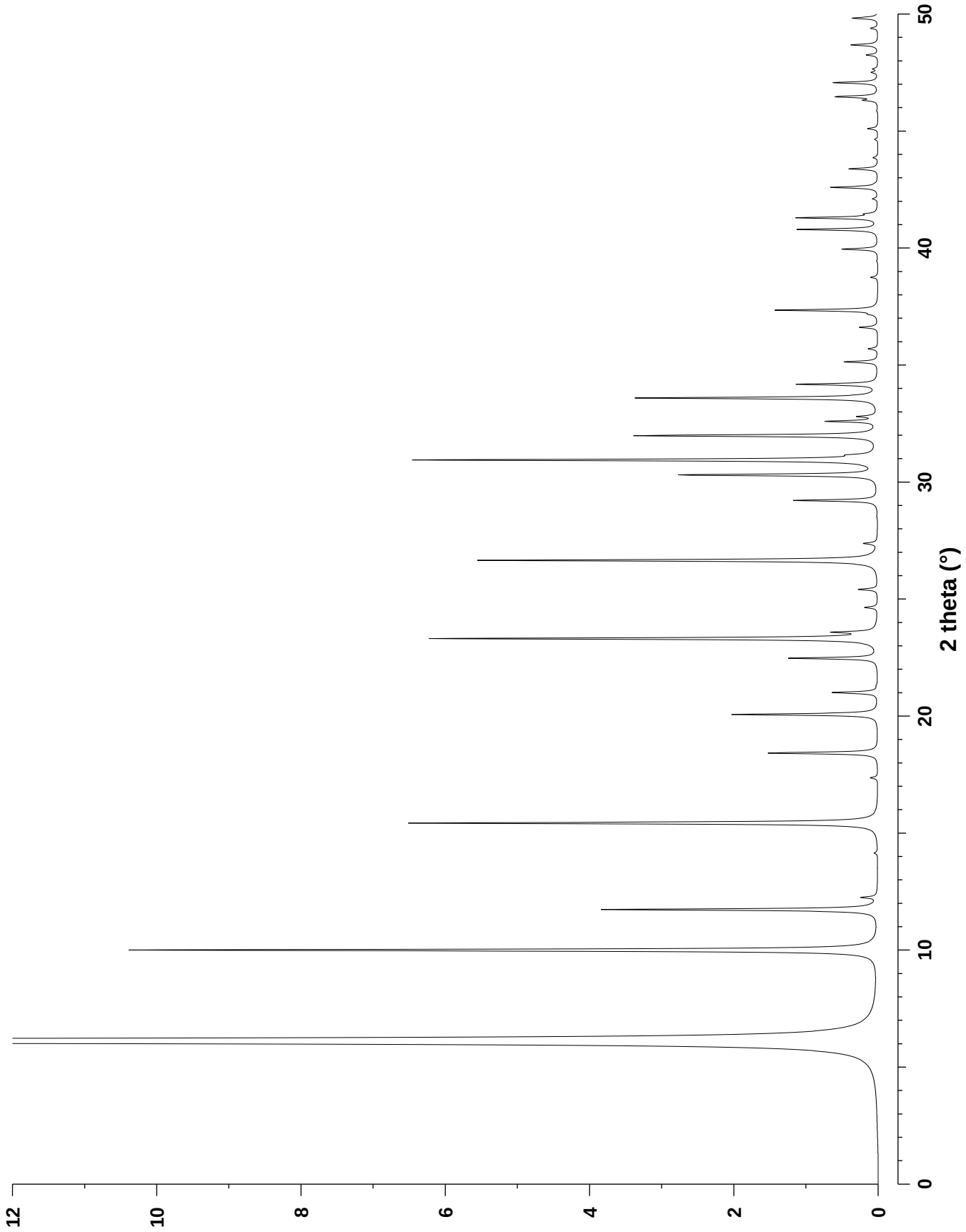
CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre $(\overline{3})$
$a = 25.028$ Å $b = 25.028$ Å $c = 25.028$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.09$

REFERENCE: D. H. Olson,
J. Phys. Chem. **74** 2758–2764 (1970).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	6.12	14.450	8	100.0	6	6	0	30.30	2.950	12	1.0	11	1	1	39.95	2.257	24	0.2
2	2	0	10.00	8.849	12	10.4	8	2	2	30.30	2.950	24	1.7	7	7	5	39.95	2.257	24	0.3
3	1	1	11.73	7.546	24	3.8	7	1	5	30.94	2.890	24	0.4	8	8	0	40.79	2.212	12	1.1
2	2	2	12.25	7.225	8	0.2	7	5	1	30.94	2.890	24	0.4	11	1	3	41.29	2.187	24	0.3
3	3	1	15.43	5.742	24	6.5	5	5	5	30.94	2.890	8	5.7	11	3	1	41.29	2.187	24	0.3
4	2	2	17.36	5.109	24	0.1	6	6	2	31.15	2.871	24	0.2	9	5	5	41.29	2.187	24	0.1
3	3	3	18.42	4.817	8	0.3	8	0	4	31.98	2.798	12	1.6	9	7	1	41.29	2.187	24	0.2
5	1	1	18.42	4.817	24	1.3	8	4	0	31.98	2.798	12	1.8	9	1	7	41.29	2.187	24	0.2
4	4	0	20.07	4.424	12	2.0	7	3	5	32.59	2.747	24	0.1	8	8	2	41.45	2.178	24	0.1
5	3	1	21.00	4.231	24	0.6	9	1	1	32.59	2.747	24	0.1	11	3	3	42.59	2.123	24	0.6
6	2	0	22.47	3.957	12	1.1	7	5	3	32.59	2.747	24	0.4	8	8	4	43.38	2.086	24	0.3
6	0	2	22.47	3.957	12	0.2	8	4	2	32.80	2.731	24	0.1	9	9	1	46.31	1.960	24	0.2
5	3	3	23.31	3.817	24	6.2	8	2	4	32.80	2.731	24	0.1	12	4	2	46.46	1.954	24	0.3
6	2	2	23.58	3.773	24	0.5	6	6	4	33.59	2.668	24	3.4	12	2	4	46.46	1.954	24	0.2
4	4	4	24.64	3.612	8	0.2	9	3	1	34.17	2.624	24	0.5	10	8	2	47.06	1.931	24	0.4
5	5	1	25.41	3.505	24	0.2	9	1	3	34.17	2.624	24	0.6	10	2	8	47.06	1.931	24	0.2
6	2	4	26.65	3.345	24	2.4	8	4	4	35.13	2.554	24	0.5	12	4	4	48.24	1.887	24	0.2
6	4	2	26.65	3.345	24	3.2	8	2	6	36.61	2.454	24	0.1	9	7	7	48.67	1.871	24	0.2
7	3	1	27.37	3.258	24	0.1	10	2	2	37.34	2.408	24	0.2	13	3	3	49.82	1.830	24	0.1
7	3	3	29.21	3.058	24	1.2	6	6	6	37.34	2.408	8	1.2	9	9	5	49.82	1.830	24	0.2

Na-X, Hydrated

FAU



FAU Ultrastable Y, Dehydrated Dealuminated

CHEMICAL COMPOSITION: $|H_{18.9}|\ [Si_{173.1}Al_{18.9}O_{384}]$

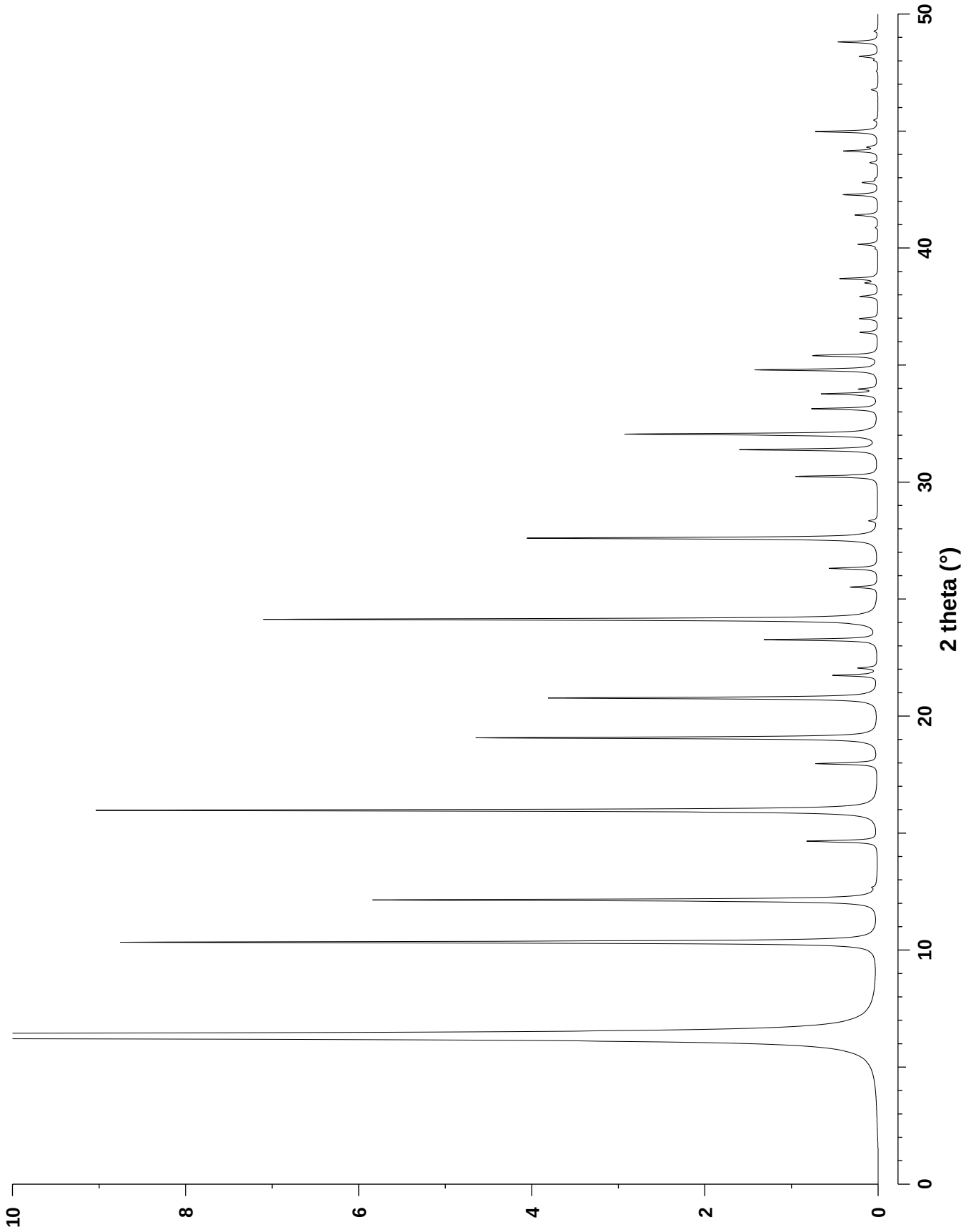
REFINED COMPOSITION: $|Al_{5.6}O_{22.4}|\ [Si_{175.7}Al_{16.3}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}m$ (No. 227) origin at centre ($\overline{3}m$)
$a = 24.188$ Å $b = 24.188$ Å $c = 24.188$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.1041$, $R_I = 0.0561$

REFERENCE: J. B. Parise, D. R. Corbin, L. Abrams and D. E. Cox, *Acta Cryst.* **C40** 1493–1497 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	6.33	13.965	8	100.0	5	5	1	26.31	3.387	24	0.5	8	6	2	37.93	2.372	48	0.2
2	2	0	10.34	8.552	12	8.7	6	4	2	27.60	3.232	48	4.1	9	5	1	38.50	2.338	48	0.1
3	1	1	12.14	7.293	24	5.8	7	3	3	30.24	2.955	24	0.9	6	6	6	38.69	2.327	8	0.4
4	0	0	14.65	6.047	6	0.8	8	2	2	31.38	2.851	24	0.5	8	6	4	40.15	2.246	48	0.2
3	3	1	15.97	5.549	24	9.0	6	6	0	31.38	2.851	12	1.1	11	1	1	41.40	2.181	24	0.2
4	2	2	17.97	4.937	24	0.7	7	5	1	32.04	2.793	48	0.4	8	8	0	42.27	2.138	12	0.4
5	1	1	19.07	4.655	24	4.4	5	5	5	32.04	2.793	8	2.5	9	7	3	44.14	2.052	48	0.2
3	3	3	19.07	4.655	8	0.3	8	4	0	33.13	2.704	24	0.8	11	3	3	44.14	2.052	24	0.2
4	4	0	20.77	4.276	12	3.8	7	5	3	33.76	2.655	48	0.6	10	6	2	44.31	2.044	48	0.1
5	3	1	21.74	4.089	48	0.5	8	4	2	33.97	2.639	48	0.2	8	8	4	44.97	2.016	24	0.5
4	4	2	22.05	4.031	24	0.2	6	6	4	34.79	2.578	24	1.4	12	0	0	44.97	2.016	6	0.2
6	2	0	23.26	3.824	24	1.3	9	3	1	35.40	2.536	48	0.7	8	8	6	48.18	1.889	24	0.2
5	3	3	24.13	3.689	24	7.1	8	4	4	36.39	2.469	24	0.2	10	8	2	48.80	1.866	48	0.5
4	4	4	25.51	3.491	8	0.3	7	5	5	36.98	2.431	24	0.2							

Ultrastable Y, Dehydrated Dealuminated FAU



FAU

Na-Y, Siliceous

CHEMICAL COMPOSITION: $[Si_{192}O_{384}]$

REFINED COMPOSITION: $[Si_{188.16}O_{384}]$

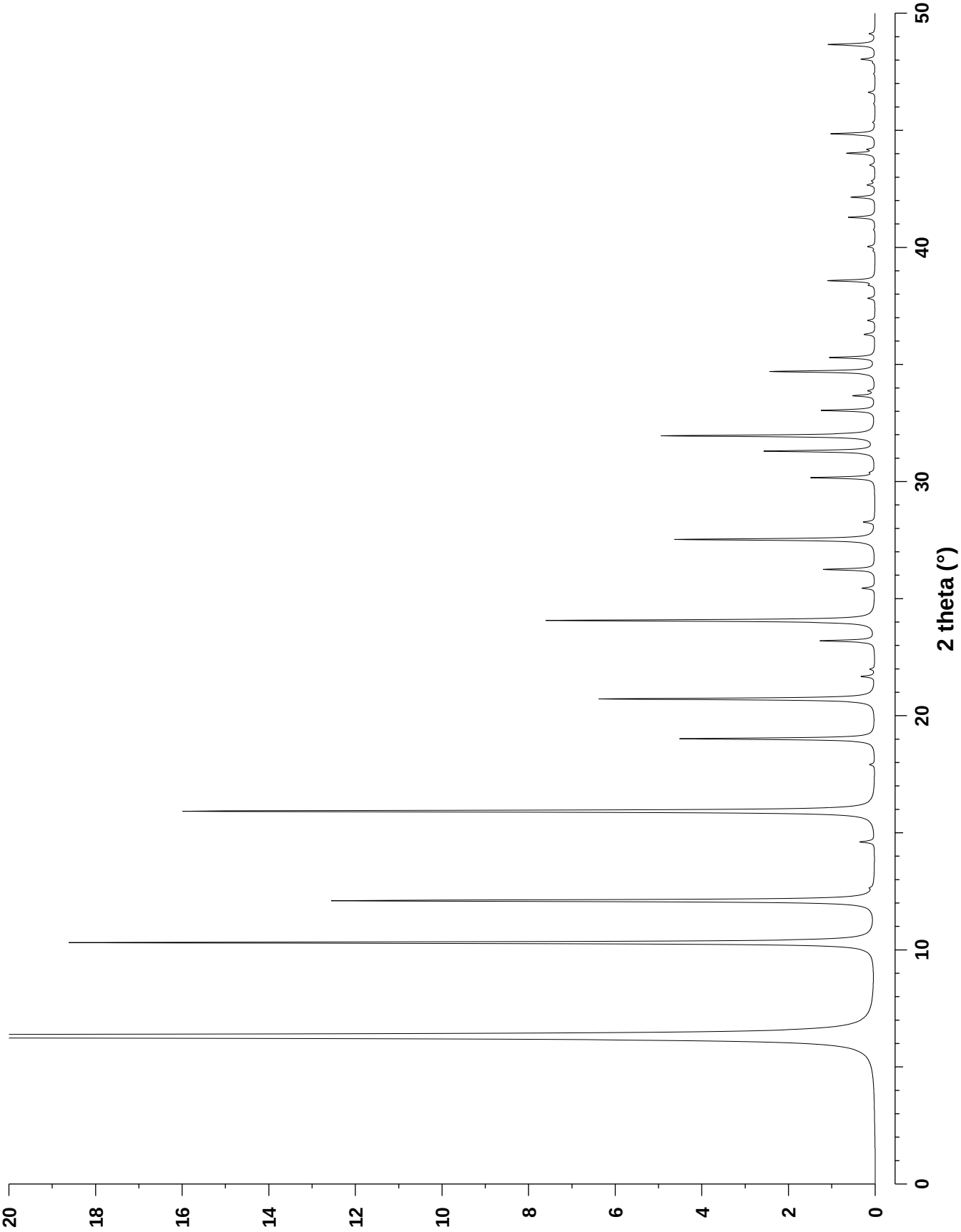
CRYSTAL DATA: $Fd\overline{3}m$ (No. 227) origin at centre ($\overline{3}m$)
$a = 24.2576$ Å $b = 24.2576$ Å $c = 24.2576$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{exp} = 0.022$, $R_{wp} = 0.031$

REFERENCE: J. J. Hriljac, M. M. Eddy, A. K. Cheetham, J. A. Donohue and G. J. Ray, *J. Solid State Chem.* **106** 66–72 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	6.31	14.005	8	100.0	7	3	1	28.26	3.158	48	0.2	8	6	4	40.03	2.252	48	0.2
2	2	0	10.31	8.576	12	18.6	7	3	3	30.16	2.964	24	1.5	11	1	1	41.28	2.187	24	0.4
3	1	1	12.10	7.314	24	12.5	8	2	2	31.29	2.859	24	0.7	7	7	5	41.28	2.187	24	0.2
4	0	0	14.61	6.064	6	0.3	6	6	0	31.29	2.859	12	1.9	8	8	0	42.14	2.144	12	0.6
3	3	1	15.92	5.565	24	16.0	7	5	1	31.95	2.801	48	0.5	9	7	1	42.66	2.119	48	0.1
4	2	2	17.91	4.952	24	0.1	5	5	5	31.95	2.801	8	4.4	10	6	0	43.51	2.080	24	0.1
5	1	1	19.01	4.668	24	4.3	8	4	0	33.03	2.712	24	1.2	9	7	3	44.01	2.058	48	0.1
3	3	3	19.01	4.668	8	0.2	7	5	3	33.66	2.663	48	0.5	11	3	3	44.01	2.058	24	0.5
4	4	0	20.71	4.288	12	6.4	8	4	2	33.87	2.647	48	0.1	10	6	2	44.18	2.050	48	0.2
5	3	1	21.67	4.100	48	0.3	6	6	4	34.69	2.586	24	2.4	12	0	0	44.84	2.021	6	0.3
4	4	2	21.98	4.043	24	0.1	9	3	1	35.29	2.543	48	1.0	8	8	4	44.84	2.021	24	0.7
6	2	0	23.19	3.835	24	1.3	8	4	4	36.28	2.476	24	0.3	9	7	5	46.61	1.948	48	0.1
5	3	3	24.06	3.699	24	7.6	7	5	5	36.87	2.438	24	0.2	12	4	2	48.03	1.894	48	0.1
4	4	4	25.44	3.501	8	0.3	8	6	2	37.82	2.379	48	0.2	8	8	6	48.03	1.894	24	0.2
5	5	1	26.24	3.397	24	1.2	9	5	1	38.38	2.345	48	0.1	10	8	2	48.65	1.872	48	1.1
6	4	2	27.52	3.242	48	4.6	6	6	6	38.57	2.334	8	1.1							

Na-Y, Siliceous

FAU



CHEMICAL COMPOSITION: $|Li_{96}|\ [Si_{96}Al_{96}O_{384}]$

REFINED COMPOSITION: $|Li_{87.36}|\ [Si_{96}Al_{96}O_{384}]$

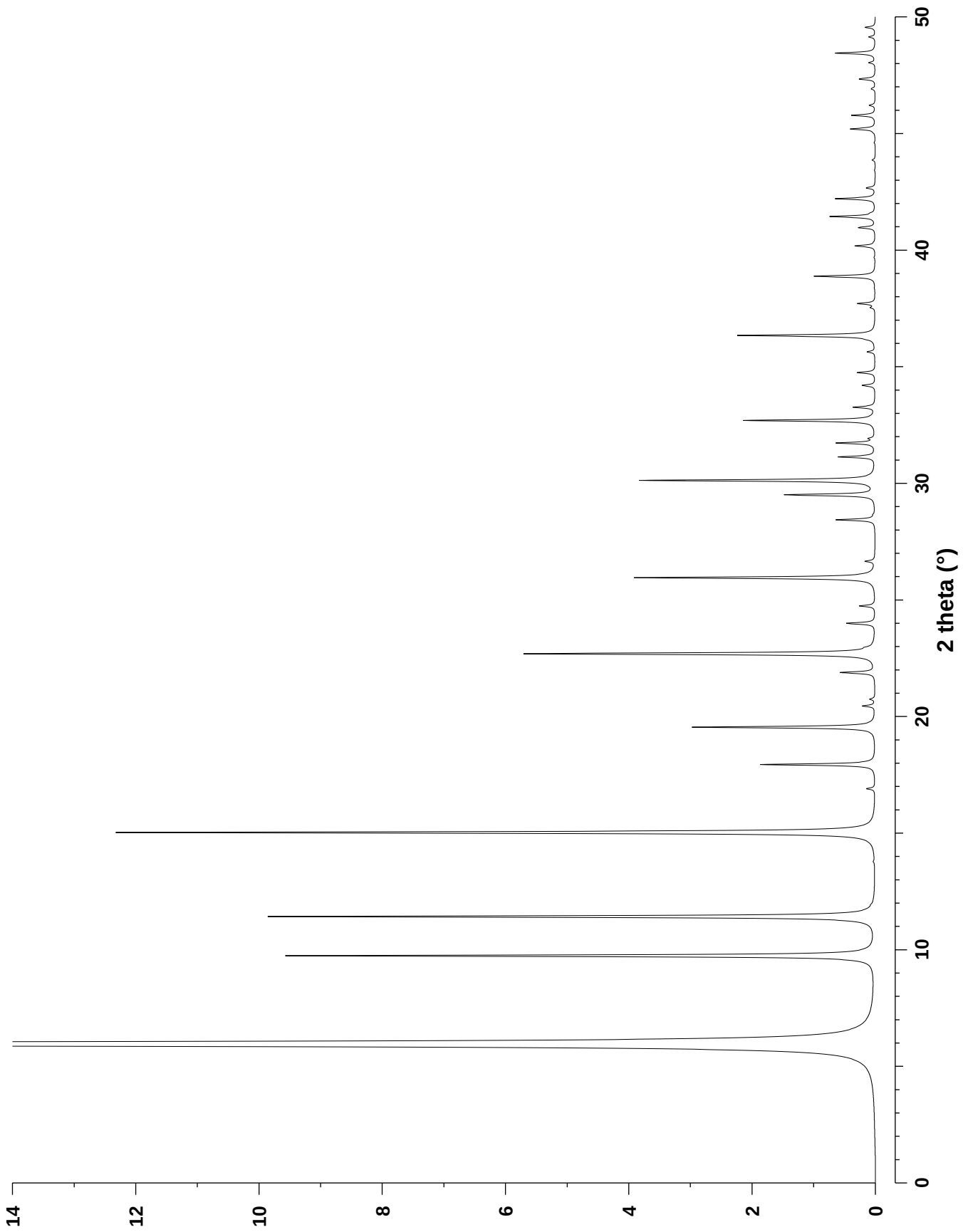
CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre $(\overline{3})$
$a = 25.6957$ Å $b = 25.6957$ Å $c = 25.6957$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray and neutron Rietveld refinement, $R_p = 0.057$, $R_{wp} = 0.069$

REFERENCE: M. Feuerstein and R. F. Lobo,
Chemistry of Materials 2197–2204 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	5.96	14.835	8	100.0	8	2	2	29.50	3.028	24	0.4	11	1	1	38.87	2.317	24	0.2
2	2	0	9.74	9.085	12	9.6	6	6	0	29.50	3.028	12	1.1	9	5	5	40.17	2.245	24	0.1
3	1	1	11.42	7.748	24	9.9	7	1	5	30.12	2.967	24	0.1	8	6	6	40.96	2.203	24	0.1
3	3	1	15.03	5.895	24	12.3	5	5	5	30.12	2.967	8	3.6	11	3	3	41.43	2.179	24	0.3
4	2	2	16.90	5.245	24	0.1	8	0	4	31.13	2.873	12	0.3	9	7	3	41.43	2.179	24	0.2
5	1	1	17.94	4.945	24	1.8	8	4	0	31.13	2.873	12	0.3	9	3	7	41.43	2.179	24	0.2
4	4	0	19.54	4.542	12	3.0	7	3	5	31.72	2.820	24	0.2	8	8	4	42.20	2.141	24	0.6
5	3	1	20.45	4.343	24	0.2	7	5	3	31.72	2.820	24	0.4	12	4	2	45.19	2.006	24	0.2
6	0	2	21.88	4.063	12	0.1	6	6	4	32.69	2.739	24	2.1	12	2	4	45.19	2.006	24	0.1
6	2	0	21.88	4.063	12	0.4	9	1	3	33.26	2.694	24	0.2	10	2	8	45.77	1.982	24	0.1
5	3	3	22.69	3.919	24	5.7	9	3	1	33.26	2.694	24	0.1	10	8	2	45.77	1.982	24	0.3
4	4	4	23.99	3.709	8	0.5	8	4	4	34.19	2.623	24	0.2	9	7	7	47.33	1.921	24	0.2
5	5	1	24.74	3.598	24	0.3	7	7	1	34.74	2.583	24	0.2	9	9	5	48.44	1.879	24	0.6
6	4	2	25.95	3.434	24	2.5	10	2	2	36.33	2.473	24	0.2	8	8	8	49.13	1.854	8	0.1
6	2	4	25.95	3.434	24	1.4	6	6	6	36.33	2.473	8	2.1	11	5	7	49.54	1.840	24	0.1
5	5	3	26.65	3.345	24	0.1	8	6	4	37.70	2.386	24	0.2							
7	3	3	28.43	3.139	24	0.6	7	7	5	38.87	2.317	24	0.8							

Li-LSX

FAU



FER Ferrierite

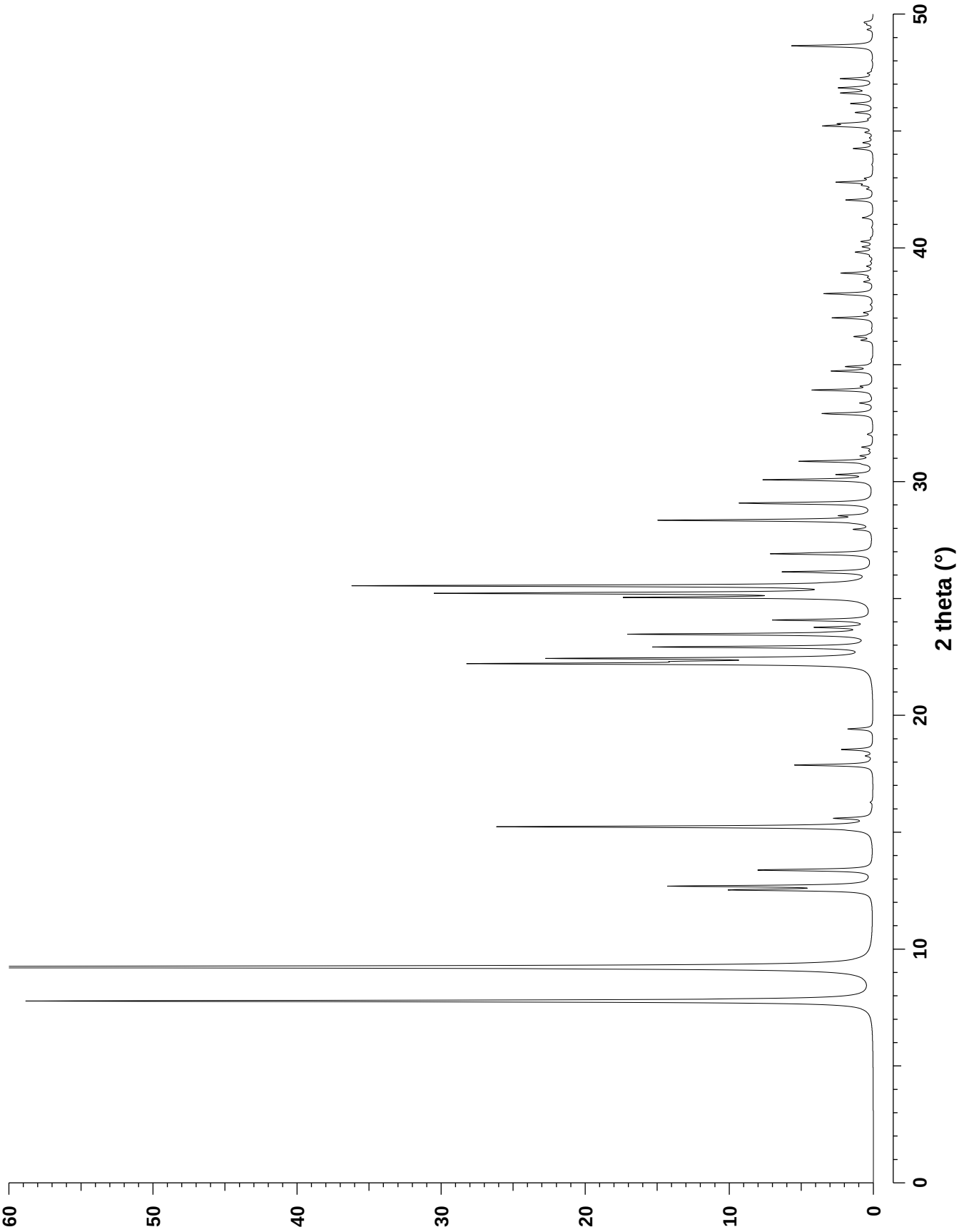
CHEMICAL COMPOSITION: $|Na_{1.5}Mg_2(H_2O)_{18}|\ [Si_{30.5}Al_{5.5}O_{72}]$
Kamloops Lake, British Columbia, Canada

REFINED COMPOSITION: $|Na_{0.96}Mg_2(H_2O)_{12}|\ [Si_{30.24}Al_{5.76}O_{72}]$

CRYSTAL DATA: *Immm* (No. 71)
$a = 19.156$ Å $b = 14.127$ Å $c = 7.489$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.11$

REFERENCE: P. A. Vaughan,
Acta Cryst. **21** 983–990 (1966).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	7.78	11.370	4	58.8	6	2	0	30.73	2.909	4	0.2	7	1	2	41.36	2.183	8	0.2
2	0	0	9.23	9.578	2	100.0	1	3	2	30.86	2.897	8	5.1	2	3	3	42.04	2.149	8	1.9
0	2	0	12.53	7.063	2	9.2	6	1	1	31.10	2.875	8	0.8	3	5	2	42.51	2.127	8	0.4
1	0	1	12.69	6.975	4	13.7	3	4	1	31.31	2.857	8	0.2	3	6	1	42.67	2.119	8	0.6
0	1	1	13.38	6.617	4	7.9	4	4	0	31.47	2.842	4	0.8	4	6	0	42.80	2.113	4	2.5
3	1	0	15.23	5.819	4	26.1	1	5	0	32.02	2.795	4	0.4	9	1	0	42.97	2.105	4	0.5
2	2	0	15.59	5.685	4	2.5	4	2	2	32.90	2.722	8	3.6	9	0	1	44.24	2.047	4	1.4
2	1	1	16.28	5.444	8	0.2	7	1	0	33.35	2.687	4	0.9	6	5	1	44.49	2.036	8	0.7
1	2	1	17.87	4.963	8	5.5	0	5	1	33.91	2.644	4	4.2	1	4	3	44.70	2.027	8	0.2
3	0	1	18.26	4.859	4	0.5	5	1	2	34.08	2.631	8	0.7	8	0	2	44.93	2.017	4	0.5
4	0	0	18.53	4.789	2	2.2	3	5	0	34.72	2.584	4	2.8	1	7	0	45.18	2.007	4	0.2
1	3	0	19.41	4.573	4	1.8	7	0	1	34.91	2.570	4	0.7	5	2	3	45.21	2.005	8	3.1
3	2	1	22.21	4.003	8	26.2	0	4	2	34.92	2.569	4	1.1	6	4	2	45.30	2.002	8	1.8
0	3	1	22.30	3.986	4	7.7	6	3	1	36.04	2.492	8	0.8	7	3	2	45.34	2.000	8	0.3
4	2	0	22.43	3.964	4	21.1	2	4	2	36.20	2.482	8	1.3	0	6	2	45.51	1.993	4	0.2
4	1	1	22.92	3.879	8	15.0	1	0	3	36.29	2.475	4	0.2	8	4	0	45.78	1.982	4	1.2
3	3	0	23.47	3.790	4	16.8	6	0	2	37.00	2.429	4	2.8	9	2	1	46.16	1.966	8	1.5
0	0	2	23.76	3.744	2	3.6	7	2	1	37.22	2.415	8	0.6	0	7	1	46.61	1.949	4	1.7
5	1	0	24.07	3.698	4	6.7	8	0	0	37.56	2.395	2	0.2	6	1	3	46.63	1.948	8	0.6
1	1	2	25.04	3.557	8	15.7	6	4	0	37.99	2.368	4	0.2	5	5	2	46.74	1.944	8	0.2
0	4	0	25.22	3.532	2	29.2	7	3	0	38.03	2.366	4	3.3	3	4	3	46.78	1.942	8	0.2
2	0	2	25.54	3.487	4	35.6	1	2	3	38.54	2.336	8	0.6	8	2	2	46.83	1.940	8	0.1
5	0	1	26.13	3.411	4	6.1	3	0	3	38.73	2.325	4	0.2	9	3	0	46.84	1.940	4	2.0
2	4	0	26.91	3.314	4	6.8	4	5	1	38.91	2.314	8	2.2	5	6	1	46.89	1.938	8	0.2
0	2	2	26.95	3.308	4	0.6	6	2	2	39.21	2.297	8	0.4	3	7	0	47.23	1.924	4	2.3
6	0	0	27.95	3.193	2	1.2	2	6	0	39.41	2.286	4	0.2	10	0	0	47.46	1.916	2	0.3
1	4	1	28.32	3.151	8	1.6	5	5	0	39.63	2.274	4	0.2	0	0	4	48.63	1.872	2	5.7
3	1	2	28.34	3.149	8	13.5	8	2	0	39.75	2.268	4	0.3	1	1	4	49.33	1.847	8	0.4
2	2	2	28.54	3.127	8	1.8	4	4	2	39.81	2.264	8	1.1	4	6	2	49.53	1.840	8	0.3
5	2	1	29.07	3.071	8	9.2	8	1	1	40.04	2.252	8	0.7	2	0	4	49.61	1.837	4	0.3
4	3	1	29.15	3.064	8	0.1	1	5	2	40.26	2.240	8	0.8	2	5	3	49.65	1.836	8	0.4
5	3	0	30.07	2.972	4	7.6	1	6	1	40.43	2.231	8	0.1							
4	0	2	30.30	2.950	4	2.3	4	1	3	41.28	2.187	8	0.7							


0
10
20
30
40
50
2 theta (°)
0
10
20
30
40
50
60

FER Ferrierite, Siliceous

CHEMICAL COMPOSITION: $[Si_{36}O_{72}]$
Dealuminated, synthetic powder.

REFINED COMPOSITION: $[Si_{36}O_{72}]$

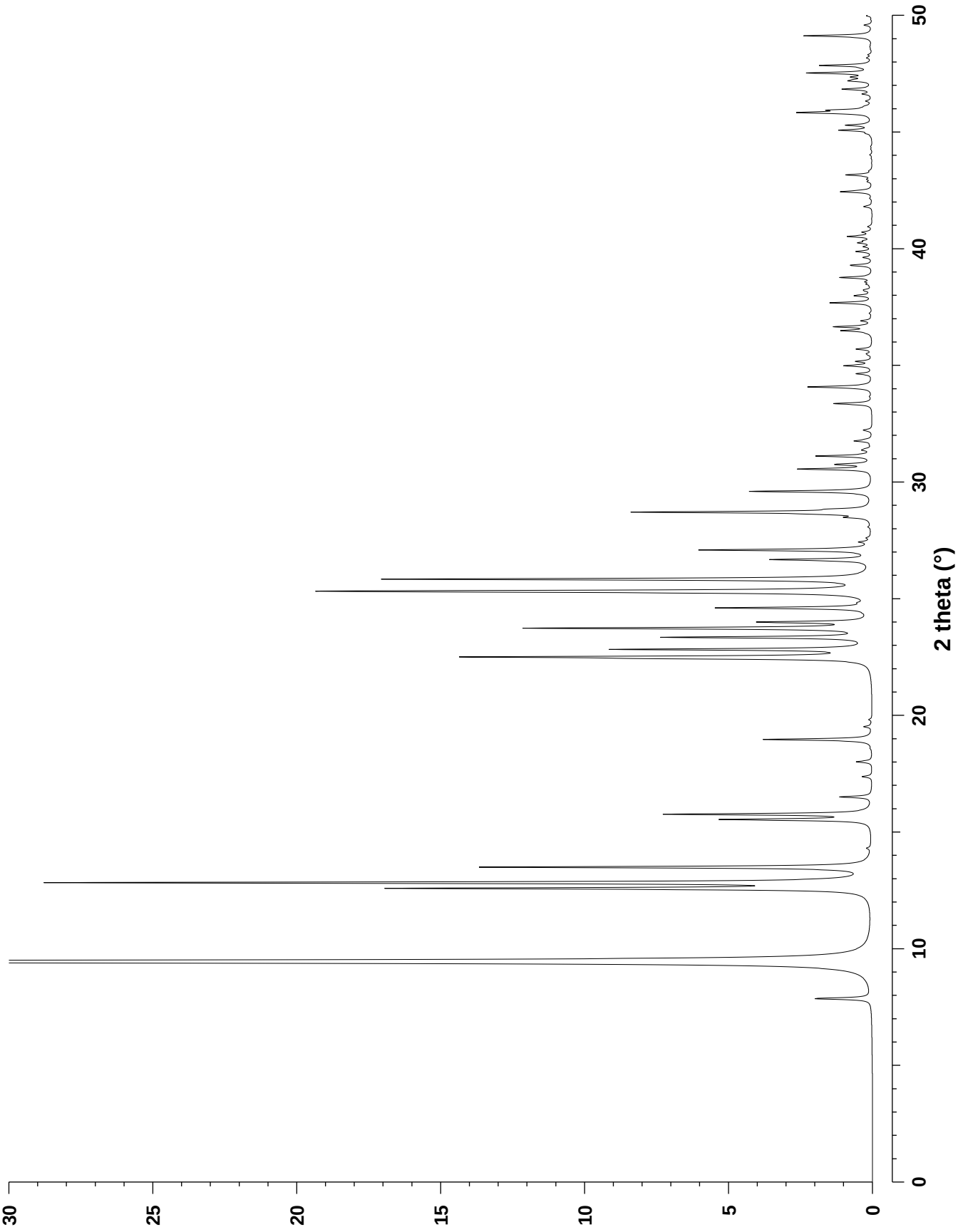
CRYSTAL DATA: *Pnnm* (No. 58)
$a = 14.07025$ Å $b = 7.41971$ Å $c = 18.7202$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Combined X-ray and neutron Rietveld refinement, $R_{wp} = 0.123$

REFERENCE: R. E. Morris, S. J. Weigel, N. J. Henson, L. M. Bull, M. T. Janicke, B. F. Chmelka and A. K. Cheetham,
J. Amer. Chem. Soc. **116** 11849–11855 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	7.86	11.248	4	1.9	2	1	5	29.59	3.019	8	4.2	6	1	0	40.33	2.236	4	0.2
0	0	2	9.45	9.360	2	100.0	4	1	2	29.68	3.010	8	0.1	5	2	1	40.52	2.226	8	0.8
2	0	0	12.58	7.035	2	16.2	3	0	5	30.55	2.926	4	2.5	3	1	7	40.70	2.217	8	0.3
0	1	1	12.83	6.898	4	28.3	3	2	0	30.73	2.910	4	0.2	1	1	8	40.94	2.204	8	0.1
1	1	0	13.49	6.563	4	13.5	0	2	4	30.75	2.907	4	1.0	1	3	4	41.80	2.161	8	0.3
1	1	1	14.30	6.193	8	0.1	3	2	1	31.11	2.875	8	1.9	3	3	2	42.43	2.130	8	1.0
1	0	3	15.53	5.704	4	5.1	2	0	6	31.36	2.852	4	0.3	3	2	6	42.48	2.128	8	0.1
2	0	2	15.76	5.624	4	7.1	1	2	4	31.42	2.847	8	0.1	2	1	8	42.50	2.127	8	0.1
1	1	2	16.50	5.374	8	1.1	1	1	6	31.75	2.818	8	0.6	5	2	3	42.86	2.110	8	0.1
2	1	0	17.37	5.105	4	0.3	4	0	4	31.82	2.812	4	0.1	6	1	3	42.97	2.105	8	0.1
2	1	1	18.01	4.925	8	0.6	3	2	2	32.22	2.778	8	0.3	6	0	4	43.15	2.097	4	0.9
0	0	4	18.96	4.680	2	3.8	2	2	4	33.35	2.687	8	1.3	6	1	4	44.93	2.018	8	0.1
3	0	1	19.51	4.549	4	0.3	3	2	3	34.00	2.637	8	0.1	4	3	1	45.07	2.011	8	0.1
2	1	2	19.81	4.482	8	0.1	5	1	0	34.07	2.631	4	2.1	5	1	6	45.07	2.011	8	1.0
3	1	0	22.43	3.964	4	5.1	4	1	4	34.10	2.629	8	0.2	0	1	9	45.28	2.003	4	0.9
2	1	3	22.50	3.951	8	12.9	1	2	5	34.63	2.590	8	0.5	6	2	0	45.77	1.982	4	0.2
2	0	4	22.82	3.897	4	8.8	5	0	3	34.98	2.565	4	1.0	2	3	5	45.82	1.980	8	2.1
1	1	4	23.34	3.810	8	7.1	4	2	0	35.16	2.553	4	0.5	0	2	8	45.85	1.979	4	0.5
3	0	3	23.73	3.749	4	11.9	4	2	1	35.49	2.529	8	0.1	4	2	6	45.93	1.976	8	1.2
0	2	0	23.99	3.710	2	3.7	0	1	7	35.69	2.516	4	0.6	6	2	1	46.04	1.971	8	0.1
1	0	5	24.60	3.618	4	5.3	4	2	2	36.48	2.463	8	1.0	3	2	7	46.10	1.969	8	0.1
1	2	0	24.82	3.587	4	0.2	0	3	1	36.65	2.452	4	0.5	1	2	8	46.32	1.960	8	0.2
1	2	1	25.28	3.523	8	7.7	3	1	6	36.65	2.452	8	0.8	4	0	8	46.62	1.948	4	0.3
4	0	0	25.32	3.518	2	15.2	1	3	0	36.90	2.436	4	0.4	7	1	0	46.83	1.940	4	1.0
2	1	4	25.82	3.450	8	0.6	0	2	6	37.67	2.388	4	1.5	2	1	9	47.18	1.926	8	0.6
0	2	2	25.83	3.449	4	16.4	2	1	7	37.98	2.369	8	0.6	4	3	3	47.23	1.925	8	0.2
1	2	2	26.61	3.350	8	0.5	1	3	2	38.18	2.357	8	0.1	5	2	5	47.25	1.924	8	0.2
0	1	5	26.67	3.343	4	3.3	1	2	6	38.23	2.354	8	0.2	1	3	6	47.34	1.920	8	0.2
4	0	2	27.08	3.293	4	5.9	0	0	8	38.47	2.340	2	0.2	6	1	5	47.35	1.920	8	0.4
2	2	0	27.17	3.282	4	0.2	4	0	6	38.57	2.334	4	0.2	7	0	3	47.52	1.913	4	2.2
1	1	5	27.42	3.252	8	0.4	3	0	7	38.76	2.323	4	1.1	2	2	8	47.73	1.905	8	0.1
2	2	1	27.60	3.232	8	0.1	5	1	4	39.28	2.294	8	0.8	3	0	9	47.84	1.901	4	1.8
4	1	1	28.48	3.134	8	0.7	6	0	2	39.62	2.275	4	0.3	4	1	8	48.30	1.884	8	0.1
0	0	6	28.61	3.120	2	0.5	2	2	6	39.87	2.261	8	0.5	0	4	0	49.11	1.855	2	2.4
1	2	3	28.70	3.110	8	8.2	5	0	5	40.08	2.250	4	0.3	1	4	0	49.57	1.839	4	0.3
2	2	2	28.83	3.097	8	0.9	4	2	4	40.24	2.241	8	0.4	6	2	4	49.97	1.825	8	0.2

Ferrierite, Siliceous

FER



FRA Franzinite

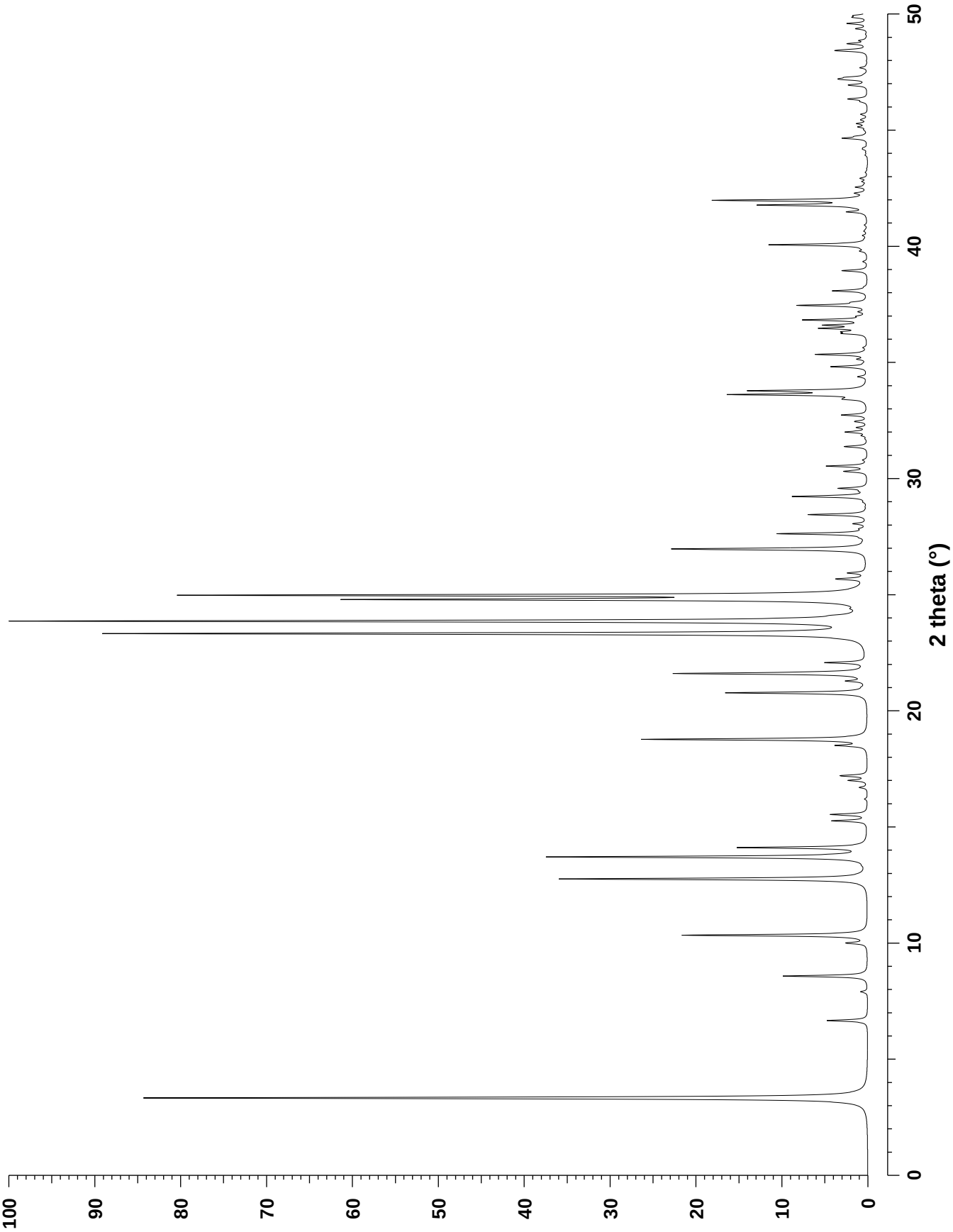
CHEMICAL COMPOSITION: $|(Na,K)_{30}Ca_{10}(SO_4)_{10}(H_2O)_2|\ [Si_{30}Al_{30}O_{120}]$
Sacrofano, Latium, Italy

REFINED COMPOSITION: $|Ca_{30.72}S_{22}O_{70}(H_2O)_6|\ [Si_{30}Al_{30}O_{120}]$

CRYSTAL DATA: $P321$ (No. 150)
$a = 12.916$ Å $b = 12.916$ Å $c = 26.543$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.0596$

REFERENCE: P. Ballirano, E. Bonaccorsi, A. Maras and S. Merlino, *Canadian Mineralogist* **38** 657–668 (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	3.33	26.543	2	85.0	2	2	0	27.62	3.229	6	10.5	3	2	4	37.58	2.393	12	1.1
0	0	2	6.66	13.271	2	4.8	2	2	1	27.83	3.205	12	0.6	4	0	6	38.07	2.364	6	0.6
1	0	0	7.90	11.186	6	0.8	1	0	8	28.05	3.181	6	0.9	0	4	6	38.07	2.364	6	3.5
1	0	1	8.58	10.308	6	9.8	0	1	8	28.05	3.181	6	0.6	3	0	9	38.94	2.313	6	2.9
0	0	3	10.00	8.848	2	2.3	2	0	7	28.44	3.139	6	6.6	1	4	4	39.33	2.291	12	0.5
1	0	2	10.34	8.553	6	13.1	1	2	6	29.22	3.056	12	6.9	1	3	8	39.78	2.266	12	0.5
0	1	2	10.34	8.553	6	8.6	2	1	6	29.22	3.056	12	1.6	0	4	7	40.06	2.251	6	10.9
0	1	3	12.76	6.939	6	0.4	0	3	5	29.27	3.051	6	0.6	4	0	7	40.06	2.251	6	0.6
1	0	3	12.76	6.939	6	35.7	2	2	3	29.45	3.033	12	0.5	2	2	9	41.47	2.178	12	2.2
1	1	0	13.71	6.458	6	37.5	3	1	2	29.57	3.021	12	1.8	3	0	10	41.77	2.162	6	9.7
1	1	1	14.11	6.275	12	15.0	1	3	2	29.57	3.021	12	1.5	0	3	10	41.77	2.162	6	2.6
1	1	2	15.26	5.807	12	4.1	1	1	8	30.28	2.951	12	0.5	3	3	0	41.97	2.153	6	17.8
1	0	4	15.53	5.707	6	4.2	0	0	9	30.31	2.949	2	2.4	2	3	7	42.54	2.125	12	1.3
0	0	5	16.70	5.309	2	0.9	1	3	3	30.53	2.928	12	2.9	4	2	0	42.78	2.114	12	0.5
1	1	3	17.00	5.216	12	2.2	3	1	3	30.53	2.928	12	1.9	2	4	1	42.92	2.107	12	0.8
2	0	2	17.20	5.154	6	1.6	2	2	4	30.79	2.903	12	0.5	2	2	10	44.17	2.050	12	0.5
0	2	2	17.20	5.154	6	1.5	0	2	8	31.35	2.854	6	0.4	2	3	8	44.64	2.030	12	1.1
1	0	5	18.50	4.796	6	0.7	0	1	9	31.37	2.852	6	1.8	0	4	9	44.65	2.029	6	1.4
0	1	5	18.50	4.796	6	2.6	4	0	0	32.00	2.796	6	2.6	0	3	11	44.73	2.026	6	0.8
2	0	3	18.77	4.727	6	0.5	4	0	1	32.19	2.781	6	0.5	5	1	0	45.13	2.009	12	0.8
0	2	3	18.77	4.727	6	26.0	0	4	1	32.19	2.781	6	0.7	5	1	1	45.27	2.003	12	0.8
2	0	4	20.77	4.276	6	1.4	2	2	5	32.45	2.759	12	1.4	5	0	6	45.43	1.996	6	0.6
0	2	4	20.77	4.276	6	15.2	0	4	2	32.73	2.736	6	2.6	5	1	2	45.67	1.986	12	0.8
2	1	1	21.28	4.175	12	1.6	1	1	9	33.40	2.683	12	1.9	2	4	5	46.22	1.964	12	0.4
1	2	1	21.28	4.175	12	0.6	3	1	5	33.45	2.678	12	0.7	2	1	12	46.32	1.960	12	0.6
1	0	6	21.60	4.114	6	5.5	4	0	3	33.61	2.666	6	13.7	5	1	3	46.34	1.959	12	1.6
0	1	6	21.60	4.114	6	16.7	0	4	3	33.61	2.666	6	1.8	3	2	9	46.93	1.936	12	1.4
1	1	5	21.67	4.101	12	2.2	3	0	7	33.71	2.659	6	0.6	2	3	9	46.93	1.936	12	0.6
1	2	2	22.07	4.028	12	0.7	0	0	10	33.77	2.654	2	12.9	5	0	7	47.17	1.927	6	2.0
2	1	2	22.07	4.028	12	4.0	2	0	9	34.38	2.609	6	0.7	4	0	10	47.21	1.925	6	0.7
2	1	3	23.32	3.815	12	85.9	4	0	4	34.81	2.577	6	3.1	0	4	10	47.21	1.925	6	1.1
1	2	3	23.32	3.815	12	3.1	0	4	4	34.81	2.577	6	1.1	5	1	4	47.27	1.923	12	1.8
3	0	0	23.86	3.729	6	100.0	2	3	1	35.13	2.554	12	1.0	4	2	6	47.68	1.907	12	0.8
0	3	1	24.10	3.692	6	1.1	1	3	6	35.34	2.540	12	1.1	4	1	9	48.41	1.880	12	2.2
1	1	6	24.39	3.650	12	0.4	3	1	6	35.34	2.540	12	5.0	1	4	9	48.41	1.880	12	0.8
0	1	7	24.79	3.591	6	55.3	0	3	8	36.24	2.479	6	0.5	1	5	5	48.45	1.879	12	0.7
1	0	7	24.79	3.591	6	1.0	3	0	8	36.24	2.479	6	1.8	5	1	5	48.45	1.879	12	0.9
3	0	2	24.80	3.590	6	1.6	0	4	5	36.31	2.474	6	1.4	1	0	14	48.71	1.869	6	2.3
2	1	4	24.97	3.566	12	69.1	4	0	5	36.31	2.474	6	0.8	6	0	0	48.85	1.864	6	0.9
1	2	4	24.97	3.566	12	9.0	3	2	3	36.46	2.465	12	5.1	4	2	7	49.36	1.846	12	1.0
0	2	6	25.67	3.470	6	0.5	1	1	10	36.60	2.455	12	4.6	1	2	13	49.58	1.839	12	1.0
2	0	6	25.67	3.470	6	2.8	4	1	0	36.82	2.441	12	7.3	2	1	13	49.58	1.839	12	1.3
0	3	3	25.93	3.436	6	1.9	1	4	1	36.98	2.431	12	0.8	1	5	6	49.85	1.829	12	1.4
1	2	5	26.96	3.307	12	10.5	1	2	9	37.17	2.419	12	0.6	0	4	11	49.92	1.827	6	0.7
2	1	5	26.96	3.307	12	12.3	3	1	7	37.45	2.401	12	7.6	4	0	11	49.92	1.827	6	0.6


0
10
20
30
40
50
2 theta (°)
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90
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70
60
50
40
30
20
10
0

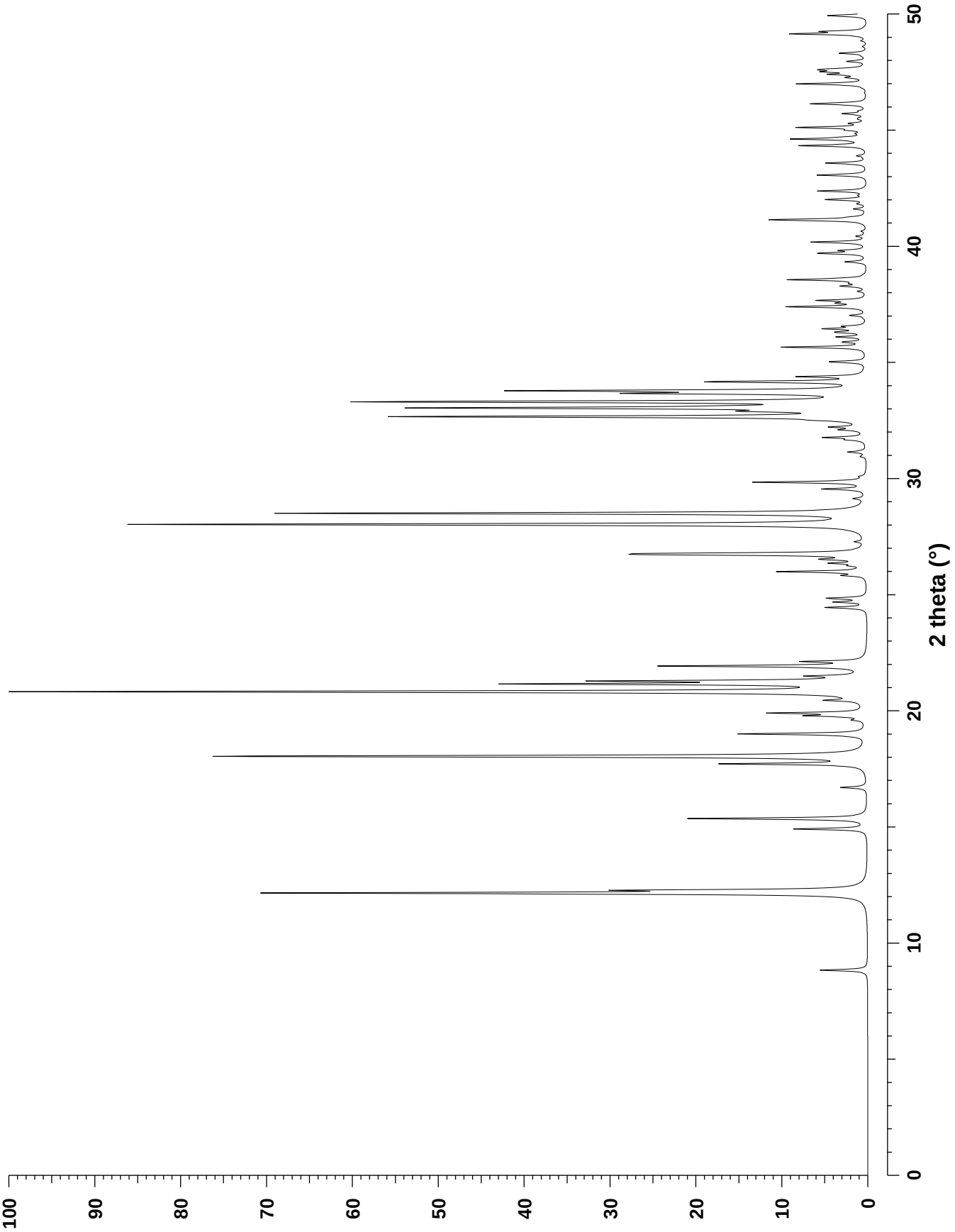
CHEMICAL COMPOSITION: $|Ca_{3.68}(H_2O)_{17.2}|\ [Si_{8.8}Al_{7.2}O_{32}]$
Hohenberg, Buhne, Westfalia

REFINED COMPOSITION: $|Ca_{3.68}(H_2O)_{17.28}|\ [Si_{8.8}Al_{7.2}O_{32}]$

CRYSTAL DATA: $P11\,2_1/a$ (No. 14) unique axis **c**, cell choice 1
$a = 9.843$ Å $b = 10.023$ Å $c = 10.616$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 92.417°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: K. F. Fischer and V. Schramm,
In *Molecular Sieve Zeolites - I* (*ACS Adv. Chem. Ser. No. 101*),
Ed. by E. M. Flanigen and L. B. Sand
(American Chemical Society: Washington, DC) 250–258 (1971).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	8.83	10.014	2	5.6	1	2	3	32.50	2.755	4	2.8	2	3	3	42.00	2.151	4	4.5
0	1	1	12.15	7.285	4	69.0	2	1	3	32.64	2.743	4	6.7	2	4	1	42.05	2.149	4	0.9
1	0	1	12.27	7.214	4	23.5	1	-3	2	32.66	2.742	4	49.6	3	2	3	42.19	2.142	4	0.6
1	-1	1	14.91	5.941	4	8.5	2	-3	1	32.89	2.723	4	9.1	2	-2	4	42.37	2.133	4	5.8
1	1	1	15.36	5.770	4	21.1	3	-1	2	33.03	2.712	4	47.6	2	2	4	43.06	2.101	4	5.9
0	0	2	16.70	5.308	2	3.1	2	3	0	33.06	2.709	2	4.5	0	1	5	43.57	2.077	4	4.7
0	2	0	17.71	5.007	2	16.4	3	-2	1	33.12	2.705	4	6.2	1	0	5	43.61	2.075	4	0.3
2	0	0	18.04	4.917	2	76.7	1	3	2	33.30	2.690	4	58.4	3	0	4	43.89	2.063	4	1.1
0	1	2	18.92	4.690	4	0.7	3	1	2	33.66	2.662	4	23.3	0	4	3	44.32	2.044	4	2.1
1	0	2	19.00	4.671	4	14.9	0	0	4	33.77	2.654	2	39.1	1	-3	4	44.33	2.043	4	5.9
0	2	1	19.60	4.529	4	1.2	2	3	1	34.16	2.625	4	18.2	1	-1	5	44.50	2.036	4	0.4
2	-1	0	19.78	4.489	2	6.2	3	2	1	34.38	2.609	4	7.5	3	-1	4	44.61	2.031	4	8.4
2	0	1	19.90	4.462	4	10.9	1	0	4	35.02	2.562	4	4.2	2	4	2	44.69	2.028	4	1.4
2	1	0	20.45	4.342	2	3.8	2	-2	3	35.65	2.518	4	9.9	1	3	4	44.83	2.022	4	0.4
1	-1	2	20.82	4.266	4	100.0	0	4	0	35.87	2.504	2	2.5	4	-3	0	44.85	2.021	2	0.4
1	1	2	21.15	4.201	4	39.3	1	-1	4	36.09	2.489	4	2.9	1	-4	3	44.99	2.015	4	1.7
1	-2	1	21.28	4.174	4	28.7	2	-3	2	36.09	2.489	4	0.4	3	1	4	45.11	2.010	4	8.0
2	-1	1	21.49	4.135	4	5.4	1	1	4	36.28	2.476	4	1.0	0	5	0	45.28	2.003	2	1.7
1	2	1	21.92	4.055	4	24.0	3	-2	2	36.30	2.475	4	2.5	3	-4	1	45.46	1.995	4	0.6
2	1	1	22.12	4.019	4	6.9	2	2	3	36.44	2.465	4	4.7	4	-1	3	45.52	1.993	4	0.6
0	2	2	24.44	3.642	4	4.9	4	0	0	36.55	2.459	2	2.3	4	-3	1	45.70	1.985	4	2.7
2	0	2	24.68	3.607	4	3.7	0	3	3	37.02	2.428	4	1.9	3	-3	3	45.82	1.980	4	0.7
2	-2	0	24.84	3.585	2	4.6	3	0	3	37.39	2.405	4	9.3	0	5	1	46.12	1.968	4	6.2
1	-2	2	25.82	3.450	4	2.5	4	0	1	37.55	2.395	4	2.6	4	1	3	46.17	1.966	4	1.2
2	2	0	25.93	3.437	2	0.4	1	-4	1	37.66	2.388	4	5.6	5	0	1	46.98	1.934	4	8.1
2	-1	2	25.99	3.428	4	10.2	4	1	0	38.05	2.365	2	0.9	2	-3	4	47.04	1.932	4	0.3
2	-2	1	26.24	3.396	4	1.4	4	-1	1	38.28	2.351	4	2.8	1	-2	5	47.26	1.923	4	1.4
1	2	2	26.35	3.382	4	3.7	0	2	4	38.39	2.345	4	1.1	3	3	3	47.26	1.923	4	0.5
2	1	2	26.52	3.361	4	4.2	1	3	3	38.46	2.341	4	0.4	3	4	1	47.39	1.918	4	3.8
0	3	0	26.71	3.338	2	0.4	2	0	4	38.55	2.336	4	8.9	1	5	1	47.49	1.915	4	1.2
0	1	3	26.72	3.336	4	19.1	3	-3	1	38.62	2.331	4	1.4	5	-1	1	47.51	1.914	4	3.2
1	0	3	26.77	3.330	4	18.8	1	-2	4	39.32	2.291	4	2.5	1	2	5	47.58	1.911	4	1.0
2	2	1	27.28	3.270	4	1.0	1	2	4	39.69	2.271	4	4.9	2	-4	3	47.59	1.911	4	2.7
0	3	1	28.02	3.184	4	86.4	2	-4	0	39.70	2.270	2	0.7	4	3	1	47.63	1.909	4	2.3
3	0	1	28.50	3.132	4	69.1	0	4	2	39.81	2.264	4	2.8	2	1	5	47.68	1.907	4	0.4
1	-3	1	29.13	3.066	4	1.3	4	-2	0	40.17	2.245	2	6.5	3	-4	2	47.95	1.897	4	2.2
3	-1	1	29.54	3.024	4	5.0	4	0	2	40.43	2.231	4	1.1	5	1	1	48.30	1.884	4	3.1
1	3	1	29.84	2.994	4	13.3	2	-4	1	40.64	2.220	4	0.6	0	5	2	48.59	1.874	4	0.4
2	-2	2	30.08	2.971	4	0.6	4	-2	1	41.10	2.196	4	1.2	2	4	3	48.84	1.865	4	0.6
0	2	3	30.94	2.890	4	0.6	4	-1	2	41.11	2.195	4	2.7	1	-5	2	49.13	1.854	4	6.5
2	0	3	31.14	2.872	4	2.2	3	-2	3	41.13	2.194	4	0.4	2	-5	1	49.14	1.854	4	2.3
0	3	2	31.66	2.826	4	1.8	2	4	0	41.14	2.194	2	8.6	4	2	3	49.24	1.850	4	4.6
2	-3	0	31.76	2.818	2	4.8	1	4	2	41.25	2.188	4	1.1	1	5	2	49.90	1.828	4	0.4
3	0	2	32.09	2.789	4	2.5	4	2	0	41.60	2.171	2	1.5	2	-2	5	49.92	1.827	4	0.3
2	-1	3	32.21	2.779	4	3.6	4	1	2	41.82	2.160	4	0.9	5	-1	2	49.92	1.827	4	4.1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2 theta (°)
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30
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10
0

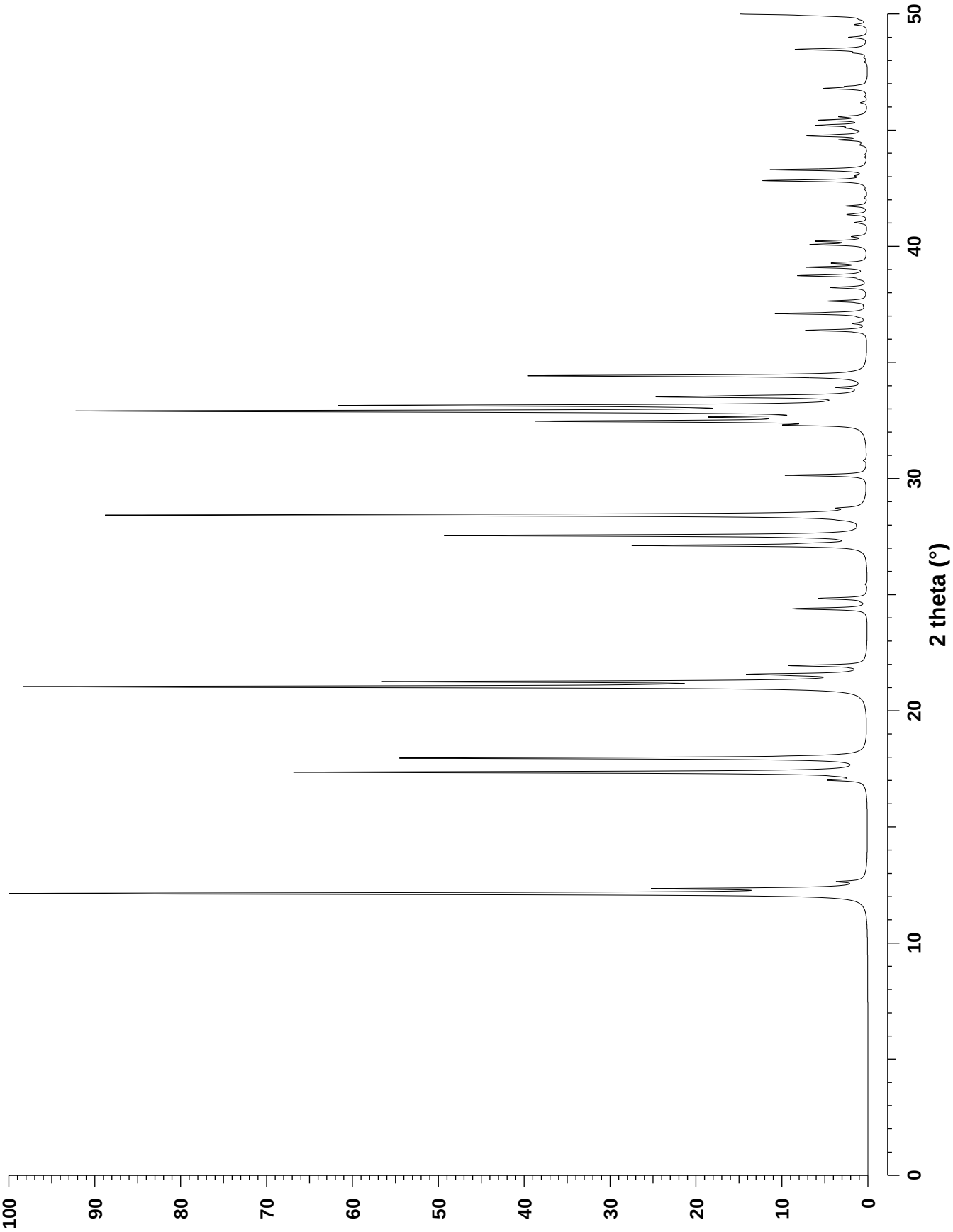
CHEMICAL COMPOSITION: $|Na_{3.6}K_{3.76}(H_2O)_{9.86}|\ [Si_8Al_8O_{32}]$
Hoewenneg, Hegau, Germany

REFINED COMPOSITION: $|Na_{3.6}K_{3.76}(H_2O)_{9.86}|\ [Si_8Al_8O_{32}]$

CRYSTAL DATA: $I121$ (No. 5) unique axis **b**, cell choice 3
$a = 10.226$ Å $b = 10.422$ Å $c = 9.884$ Å
$\alpha = 90°$ $\beta = 88.315°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.033$

REFERENCE: A. Alberti and G. Vezzalini,
Acta Cryst. **B35** 2866–2869 (1979).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	12.13	7.298	4	100.0	-1	3	2	32.85	2.726	4	11.5	-2	4	2	43.29	2.090	4	11.4
1	0	1	12.27	7.211	2	0.8	-3	2	1	32.90	2.722	4	85.8	2	2	4	43.83	2.066	4	0.2
0	1	1	12.34	7.170	4	21.7	2	1	3	33.06	2.710	4	5.3	-4	2	2	43.95	2.060	4	0.2
-1	0	1	12.64	7.002	2	2.7	1	2	3	33.14	2.703	4	58.0	1	5	0	44.35	2.042	4	0.7
0	2	0	17.01	5.211	2	3.8	-3	1	2	33.51	2.674	4	21.2	0	5	1	44.42	2.040	4	0.3
2	0	0	17.35	5.111	2	67.1	-1	2	3	33.57	2.669	4	7.6	3	4	1	44.57	2.033	4	3.0
0	0	2	17.96	4.940	2	54.7	-2	1	3	33.92	2.643	4	2.9	-2	2	4	44.74	2.026	4	2.0
1	2	1	21.03	4.224	4	96.4	0	4	0	34.42	2.605	2	39.7	4	3	1	44.76	2.025	4	5.3
2	1	1	21.13	4.204	4	6.9	0	0	4	36.37	2.470	2	7.2	-3	4	1	44.90	2.019	4	0.4
-1	2	1	21.25	4.180	4	53.0	1	4	1	36.67	2.450	4	1.6	5	0	1	45.02	2.014	2	0.7
1	1	2	21.51	4.131	4	3.6	3	3	0	36.95	2.433	4	0.4	1	4	3	45.09	2.011	4	1.6
-2	1	1	21.57	4.120	4	11.7	4	1	1	37.10	2.424	4	10.8	5	1	0	45.20	2.006	4	4.9
-1	1	2	21.94	4.051	4	8.8	3	0	3	37.42	2.404	2	0.2	-4	3	1	45.21	2.006	4	0.8
2	2	0	24.39	3.649	4	8.7	-4	1	1	37.62	2.391	4	0.5	-1	4	3	45.42	1.997	4	5.3
2	0	2	24.69	3.605	2	0.3	0	3	3	37.63	2.390	4	4.1	3	1	4	45.56	1.991	4	0.9
0	2	2	24.83	3.585	4	5.7	1	1	4	38.22	2.355	4	4.3	-5	0	1	45.58	1.990	2	2.3
-2	0	2	25.44	3.501	2	0.2	-3	0	3	38.57	2.334	2	0.6	-1	3	4	46.17	1.966	4	0.8
1	3	0	27.11	3.289	4	26.8	-1	1	4	38.73	2.325	4	7.9	-4	1	3	46.44	1.955	4	0.2
0	3	1	27.21	3.277	4	2.9	2	4	0	38.79	2.321	4	0.5	0	1	5	46.79	1.941	4	4.9
3	0	1	27.44	3.251	2	1.0	0	4	2	39.09	2.305	4	7.0	-3	1	4	46.88	1.938	4	1.9
3	1	0	27.54	3.239	4	49.2	4	2	0	39.27	2.294	4	3.9	2	5	1	47.92	1.898	4	0.4
-3	0	1	27.95	3.192	2	0.2	2	0	4	40.07	2.250	2	6.3	1	5	2	48.11	1.891	4	0.2
1	0	3	28.22	3.162	2	0.2	-4	0	2	40.21	2.243	2	5.6	-1	5	2	48.32	1.884	4	1.2
0	1	3	28.42	3.140	4	89.4	0	2	4	40.41	2.232	4	1.6	5	2	1	48.46	1.878	4	5.3
-1	0	3	28.72	3.108	2	2.1	3	3	2	41.01	2.201	4	1.4	5	1	2	48.48	1.878	4	3.6
2	2	2	30.14	2.965	4	9.6	2	3	3	41.36	2.183	4	1.9	-5	2	1	48.99	1.859	4	2.2
-2	2	2	30.77	2.906	4	0.4	3	2	3	41.37	2.183	4	0.5	-5	1	2	49.53	1.840	4	1.4
2	3	1	32.30	2.771	4	7.0	-3	3	2	41.73	2.164	4	2.5	2	1	5	49.76	1.832	4	0.4
3	2	1	32.46	2.758	4	36.6	-2	3	3	42.08	2.147	4	0.3	1	2	5	49.92	1.827	4	3.9
1	3	2	32.56	2.750	4	1.7	-3	2	3	42.44	2.130	4	0.2	4	4	0	49.99	1.824	4	14.0
-2	3	1	32.60	2.747	4	0.7	2	4	2	42.82	2.112	4	12.2							
3	1	2	32.64	2.744	4	13.4	4	2	2	43.03	2.102	4	0.9							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2 theta (°)

CHEMICAL COMPOSITION: $|Na_{0.8}Ca_{2.82}(H_2O)_{12.08}|\ [Si_{10.4}Al_{5.6}O_{32}]$
Goble, Oregon, U.S.A.

REFINED COMPOSITION: $|Na_{0.8}Ca_{2.82}(H_2O)_{12.08}|\ [Si_{10.4}Al_{5.6}O_{32}]$

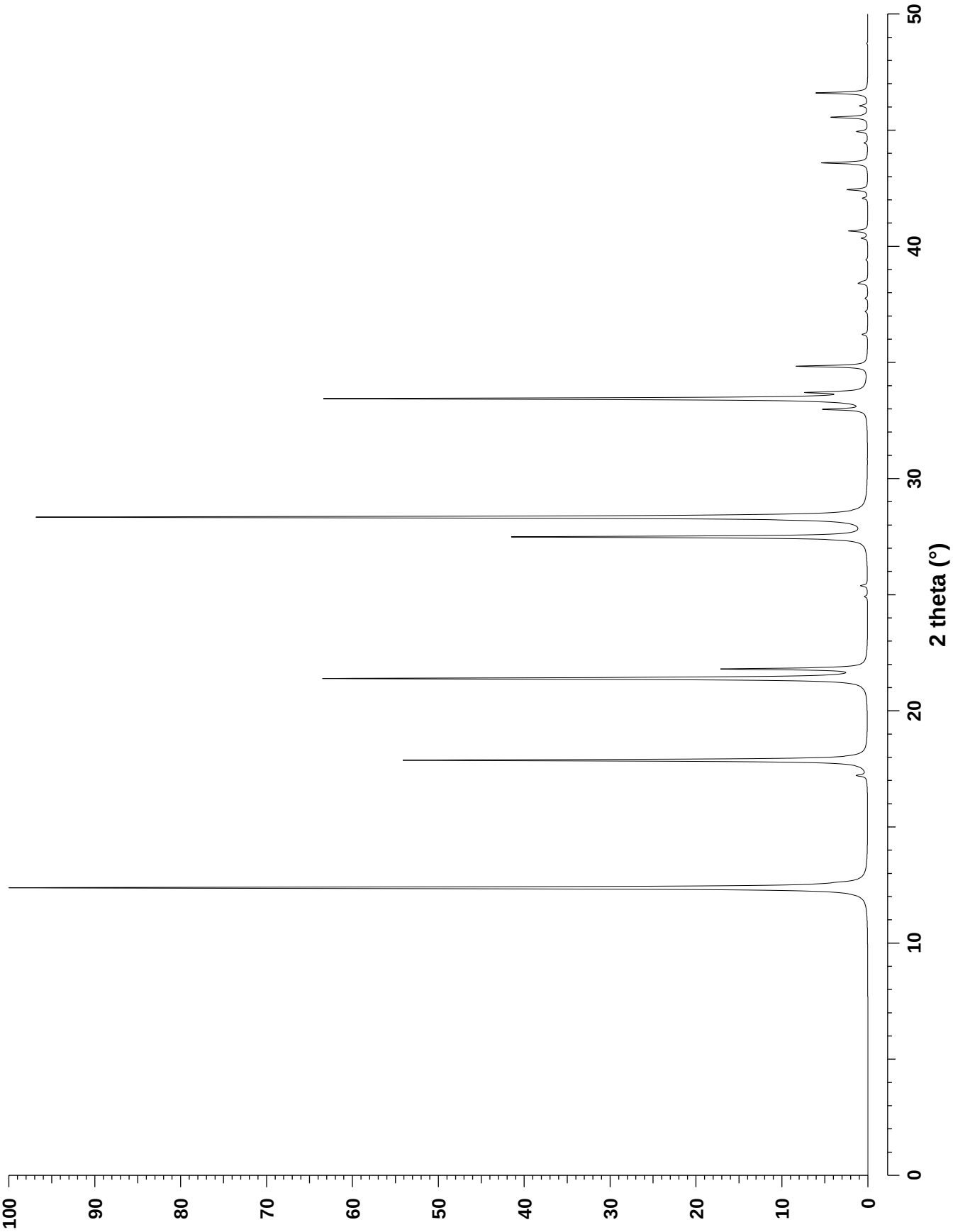
CRYSTAL DATA: $I\bar{4}m2$ (No. 119)
$a = 9.9266$ Å $b = 9.9266$ Å $c = 10.3031$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.047$, $R_{wp} = 0.127$, $R_{F^2} = 0.111$

REFERENCE: G. Artioli,
American Mineralogist **77** 189–196 (1992).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	12.38	7.149	8	100.0	3	1	2	33.43	2.681	16	63.2	3	3	2	42.43	2.130	8	2.4
1	1	0	12.61	7.019	4	0.9	3	2	1	33.70	2.660	16	6.0	2	2	4	43.58	2.077	8	5.4
0	0	2	17.21	5.152	2	1.2	0	0	4	34.83	2.576	2	8.3	4	2	2	44.44	2.038	16	0.4
2	0	0	17.87	4.963	4	54.1	4	0	0	36.20	2.482	4	0.7	1	0	5	44.93	2.018	8	1.3
1	1	2	21.39	4.153	8	63.4	1	1	4	37.18	2.418	8	0.3	3	1	4	45.55	1.991	16	4.3
2	1	1	21.80	4.077	16	16.6	3	0	3	37.75	2.383	8	0.3	4	1	3	46.04	1.971	16	0.9
2	0	2	24.91	3.574	8	0.4	4	1	1	38.40	2.344	16	1.0	4	3	1	46.59	1.949	16	0.3
2	2	0	25.38	3.510	4	0.8	3	3	0	38.47	2.340	4	0.5	5	0	1	46.59	1.949	8	5.7
1	0	3	27.48	3.246	8	41.3	2	0	4	39.41	2.286	8	0.2	5	1	0	46.66	1.947	8	0.2
3	0	1	28.33	3.150	8	96.3	4	0	2	40.34	2.236	8	0.7	2	1	5	48.72	1.869	16	0.1
3	1	0	28.43	3.139	8	3.5	4	2	0	40.65	2.220	8	2.2							
2	1	3	32.97	2.716	16	4.8	3	2	3	42.06	2.148	16	0.6							

Garronite

GIS



Gobbinsite

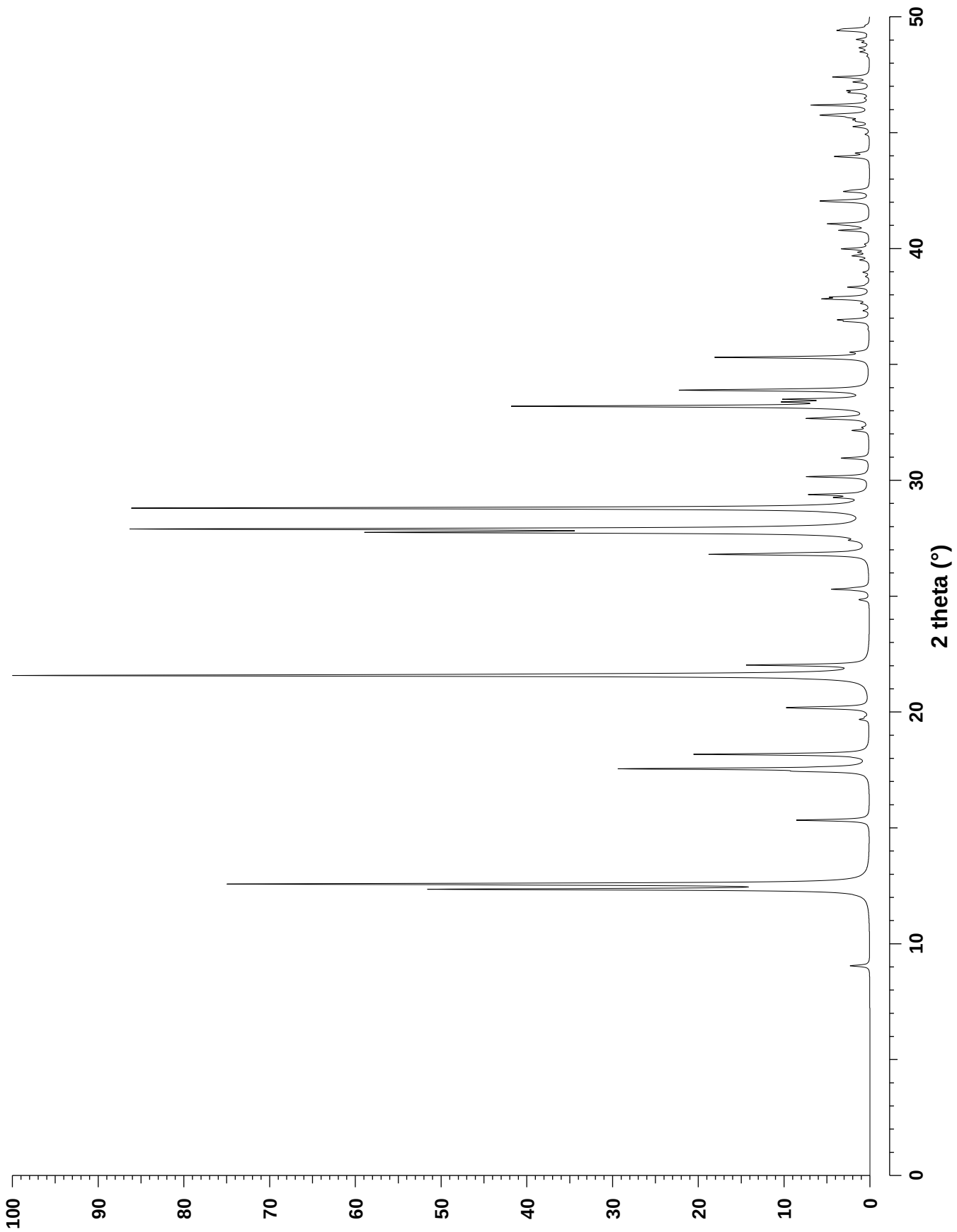
CHEMICAL COMPOSITION: $|Ca_{0.6}Na_{2.6}K_{2.2}(H_2O)_{12}|\ [Si_{10}Al_6O_{32}]$
Antrim District, Northern Ireland

REFINED COMPOSITION: $|Na_{2.6}K_{1.7}(H_2O)_{14.9}|\ [Si_{10}Al_6O_{32}]$

CRYSTAL DATA: $Pmn2_1$ (No. 31)
$a = 10.108$ Å $b = 9.766$ Å $c = 10.171$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.136$, $R_F = 0.126$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
Z. Kristallogr. **171** 281–289 (1985).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	9.05	9.766	2	2.4	0	3	2	32.66	2.742	4	6.6	2	4	1	42.05	2.149	8	4.6
1	0	1	12.35	7.170	4	51.0	2	3	0	32.72	2.737	4	2.5	3	2	3	42.09	2.147	8	0.6
0	1	1	12.57	7.044	4	72.1	2	1	3	33.11	2.705	8	0.8	2	3	3	42.45	2.130	8	2.7
1	1	0	12.60	7.023	4	6.3	3	1	2	33.19	2.699	8	42.5	3	3	2	42.51	2.127	8	1.5
1	1	1	15.33	5.779	8	8.8	1	2	3	33.37	2.685	8	7.7	2	2	4	43.96	2.060	8	4.2
0	0	2	17.44	5.085	2	5.8	3	2	1	33.49	2.676	8	8.8	4	2	2	44.11	2.053	8	1.5
2	0	0	17.55	5.054	2	29.7	1	3	2	33.88	2.646	8	21.3	2	4	2	44.92	2.018	8	0.5
0	2	0	18.17	4.883	2	21.1	2	3	1	33.92	2.643	8	2.9	0	3	4	45.25	2.004	4	1.9
0	1	2	19.68	4.511	4	1.1	0	0	4	35.30	2.543	2	18.7	1	0	5	45.48	1.994	4	1.1
2	1	0	19.78	4.489	4	0.3	4	0	0	35.52	2.527	2	1.8	0	1	5	45.55	1.991	4	1.3
0	2	1	20.17	4.402	4	6.9	0	1	4	36.51	2.461	4	0.1	3	1	4	45.65	1.987	8	1.5
1	2	0	20.20	4.397	4	4.4	2	2	3	36.85	2.439	8	2.3	4	1	3	45.73	1.984	8	3.2
1	1	2	21.57	4.119	8	100.0	3	2	2	36.92	2.435	8	3.3	5	0	1	45.76	1.983	4	2.7
2	1	1	21.64	4.106	8	14.4	2	3	2	37.31	2.410	8	0.7	0	4	3	45.80	1.981	4	1.5
1	2	1	22.02	4.036	8	14.0	1	1	4	37.62	2.391	8	0.7	1	3	4	46.18	1.966	8	7.0
2	0	2	24.84	3.585	4	1.2	4	1	1	37.82	2.379	8	5.0	1	1	5	46.48	1.954	8	0.2
0	2	2	25.29	3.522	4	4.4	0	4	1	37.90	2.374	4	3.9	0	5	0	46.49	1.953	2	0.2
2	2	0	25.36	3.512	4	0.9	0	3	3	38.33	2.348	4	2.6	1	4	3	46.72	1.944	8	1.9
1	2	2	26.80	3.326	8	17.8	3	3	0	38.45	2.341	4	0.2	5	1	1	46.75	1.943	8	0.4
2	2	1	26.86	3.319	8	4.7	3	1	3	38.79	2.321	8	0.4	3	4	1	46.81	1.941	8	2.3
0	3	0	27.40	3.255	2	1.1	1	4	1	38.97	2.311	8	0.8	3	3	3	47.18	1.926	8	1.8
1	0	3	27.75	3.214	4	54.0	3	3	1	39.50	2.281	8	1.1	0	5	1	47.39	1.918	4	4.4
0	1	3	27.85	3.203	4	4.4	2	0	4	39.68	2.271	4	2.0	1	5	1	48.29	1.885	8	0.3
3	0	1	27.89	3.198	4	82.8	4	0	2	39.83	2.263	4	1.1	0	2	5	48.48	1.878	4	1.1
3	1	0	28.01	3.185	4	1.7	0	2	4	39.98	2.255	4	3.3	3	2	4	48.58	1.874	8	0.1
0	3	1	28.79	3.100	4	84.1	4	2	0	40.18	2.244	4	0.5	4	2	3	48.65	1.871	8	1.1
1	3	0	28.81	3.099	4	6.1	2	1	4	40.78	2.212	8	3.6	5	2	0	48.75	1.868	4	0.1
1	1	3	29.25	3.053	8	3.1	4	1	2	40.94	2.205	8	0.4	2	3	4	48.89	1.863	8	0.8
3	1	1	29.38	3.040	8	6.7	1	2	4	41.00	2.201	8	1.0	4	3	2	49.02	1.858	8	1.5
1	3	1	30.15	2.964	8	7.5	0	4	2	41.01	2.201	4	0.6	2	1	5	49.17	1.853	8	0.2
2	2	2	30.95	2.890	8	3.4	2	4	0	41.06	2.198	4	4.4	5	1	2	49.40	1.845	8	3.1
0	2	3	32.14	2.785	4	2.0	4	2	1	41.19	2.192	8	0.3	3	4	2	49.46	1.843	8	2.5
3	2	0	32.28	2.773	4	0.6	1	4	2	42.01	2.151	8	2.3	5	2	1	49.62	1.837	8	0.3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2 theta (°)
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Di-n-propylamine MAPO–43

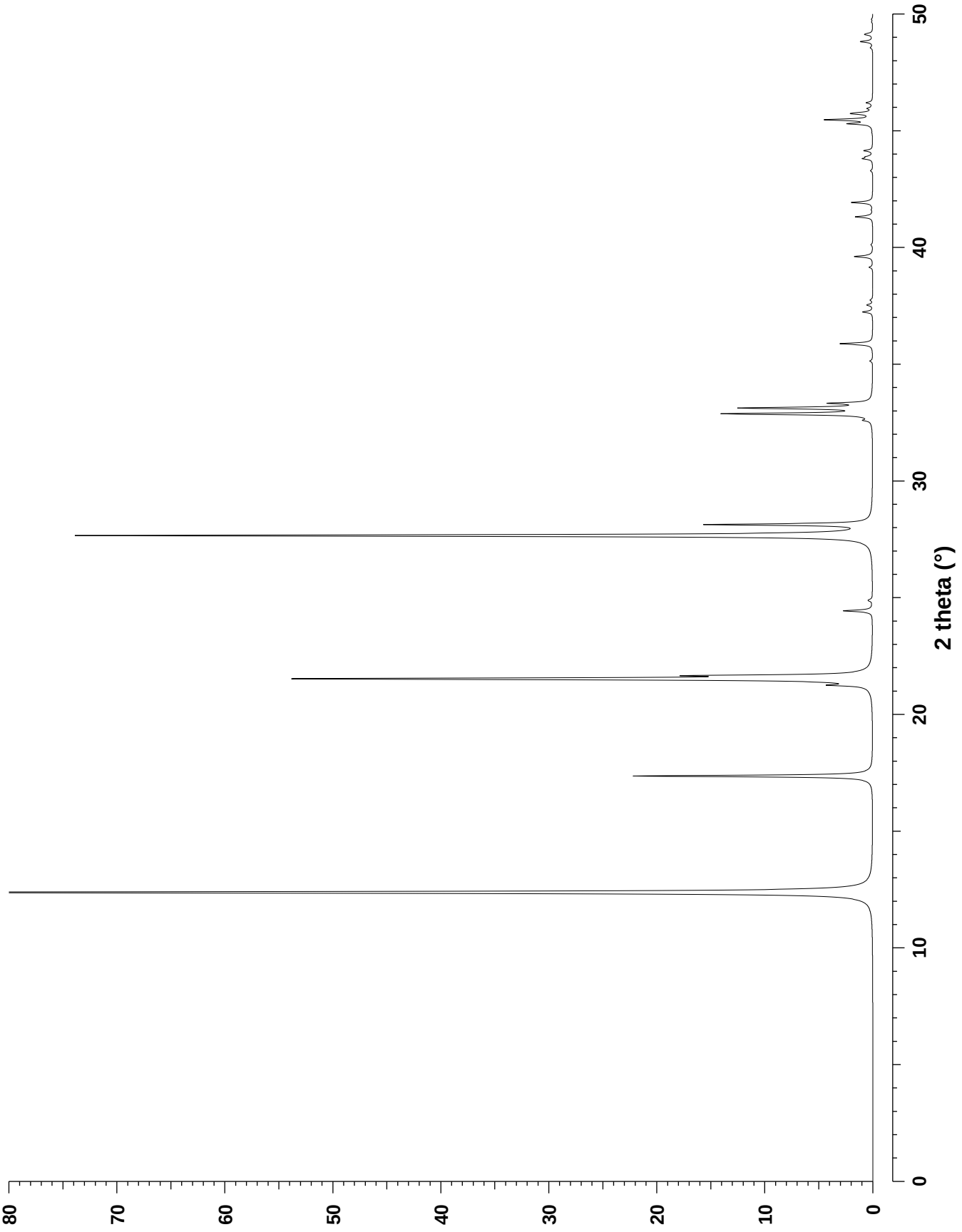
CHEMICAL COMPOSITION: $|(C_6H_{16}N)_2|\ [Al_6Mg_2P_8O_{32}]$
$C_6H_{16}N$ = di-n-propylamine

REFINED COMPOSITION: $|(C_6H_{16}N)_2|\ [Al_8P_8O_{32}]$

CRYSTAL DATA: $I11\,2/b$ (No. 15) unique axis **c**, cell choice 3
$a = 10.2192$ Å $b = 10.2198$ Å $c = 10.0126$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90.987°$
X-ray single crystal refinement, $R_w = 0.049$

REFERENCE: J. J. Pluth, J. V. Smith and J. M. Bennett,
J. Am. Chem. Soc. **111** 1692–1698 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	1	12.38	7.152	4	100.0	1	-2	3	33.16	2.702	4	0.9	2	2	4	44.14	2.052	4	1.6
1	0	1	12.38	7.151	4	98.8	2	-1	3	33.16	2.702	4	0.9	0	5	1	45.29	2.002	4	2.2
0	2	0	17.36	5.109	2	22.4	1	2	3	33.32	2.689	4	3.7	5	0	1	45.29	2.002	4	2.2
2	0	0	17.36	5.109	2	21.7	2	1	3	33.32	2.689	4	3.6	1	-4	3	45.46	1.995	4	4.5
1	-2	1	21.25	4.181	4	2.8	0	4	0	35.13	2.555	2	0.3	4	-1	3	45.47	1.995	4	4.4
2	-1	1	21.25	4.181	4	3.0	4	0	0	35.13	2.554	2	0.3	4	3	1	45.67	1.987	4	0.1
1	2	1	21.50	4.134	4	17.2	0	0	4	35.87	2.503	2	6.0	1	4	3	45.72	1.985	4	1.5
2	1	1	21.50	4.134	4	17.6	1	-4	1	37.23	2.415	4	1.0	4	1	3	45.72	1.984	4	1.5
1	-1	2	21.53	4.127	4	81.9	4	-1	1	37.23	2.415	4	0.9	1	-3	4	45.76	1.983	4	0.8
1	1	2	21.66	4.104	4	26.4	1	4	1	37.53	2.397	4	0.5	3	-1	4	45.76	1.983	4	0.8
2	-2	0	24.43	3.644	2	5.4	4	1	1	37.53	2.396	4	0.5	1	3	4	45.95	1.975	4	0.4
2	2	0	24.86	3.582	2	0.5	0	3	3	37.74	2.384	4	0.2	3	1	4	45.95	1.975	4	0.4
0	2	2	24.90	3.576	4	0.3	3	0	3	37.74	2.384	4	0.2	0	1	5	46.19	1.965	4	0.6
2	0	2	24.90	3.576	4	0.2	2	-4	0	39.15	2.301	2	0.3	1	0	5	46.19	1.965	4	0.5
0	3	1	27.66	3.225	4	72.8	4	-2	0	39.15	2.301	2	0.4	2	-5	1	48.55	1.875	4	0.2
3	0	1	27.66	3.224	4	73.9	0	4	2	39.61	2.275	4	1.8	5	-2	1	48.55	1.875	4	0.2
0	1	3	28.13	3.173	4	14.8	4	0	2	39.61	2.275	4	1.6	1	-5	2	48.81	1.866	4	1.2
1	0	3	28.13	3.173	4	15.3	0	2	4	40.11	2.248	4	0.1	5	-1	2	48.81	1.866	4	1.1
2	-3	1	32.59	2.747	4	0.6	2	0	4	40.11	2.248	4	0.2	1	5	2	49.11	1.855	4	0.7
3	-2	1	32.59	2.747	4	0.6	3	-3	2	41.31	2.186	4	3.3	5	1	2	49.11	1.855	4	0.6
1	-3	2	32.87	2.725	4	13.8	3	3	2	41.92	2.155	4	3.9	2	5	1	49.15	1.854	4	0.3
3	-1	2	32.87	2.725	4	13.5	2	-4	2	43.28	2.091	4	0.2	5	2	1	49.15	1.854	4	0.2
2	3	1	33.09	2.707	4	1.1	4	-2	2	43.28	2.090	4	0.2	1	-2	5	49.65	1.836	4	0.1
3	2	1	33.09	2.707	4	1.2	2	4	2	43.80	2.067	4	0.9	1	2	5	49.77	1.832	4	0.1
1	3	2	33.12	2.705	4	10.9	4	2	2	43.80	2.067	4	0.8	2	1	5	49.77	1.832	4	0.1
3	1	2	33.12	2.705	4	10.6	2	-2	4	43.88	2.063	4	1.1							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2 theta (°)
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70
80

CHEMICAL COMPOSITION: $|Na_6(H_2O)_{12}|\ [Si_{10}Al_6O_{32}]$

REFINED COMPOSITION: $|Na_{5.92}(H_2O)_{11.28}|\ [Si_{9.92}Al_{6.08}O_{32}]$

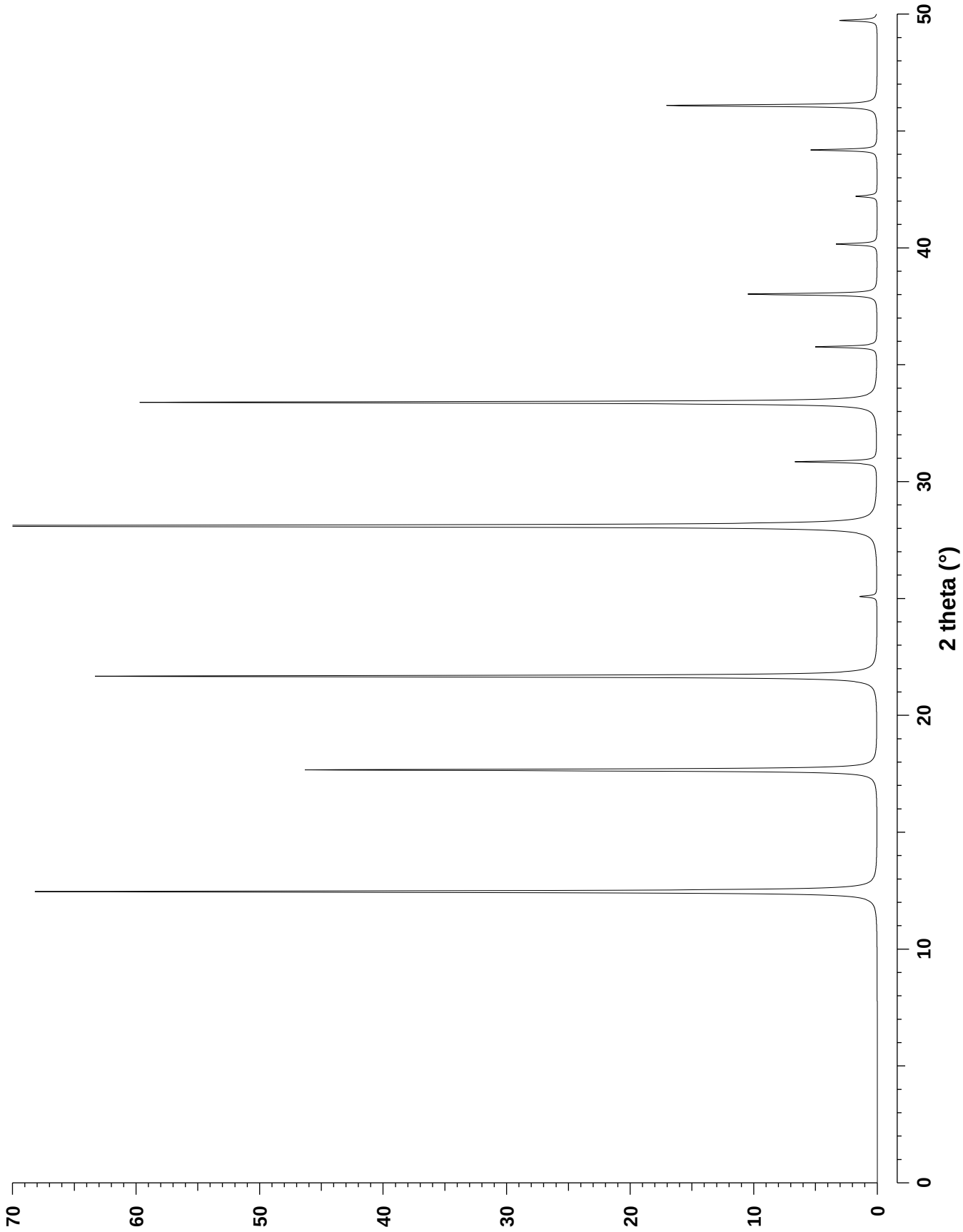
CRYSTAL DATA: $I\bar{4}$ (No. 82)
$a = 10.043$ Å $b = 10.043$ Å $c = 10.043$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray twinned crystal refinement, $R = 0.05$

REFERENCE: Ch. Baerlocher and W. M. Meier,
Z. Kristallogr. **135** 339–354 (1972).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	12.46	7.101	8	92.1	2	3	1	33.38	2.684	8	11.5	2	4	2	44.18	2.050	8	0.5
1	1	0	12.46	7.101	4	1.0	1	3	2	33.38	2.684	8	12.7	2	2	4	44.18	2.050	8	0.4
2	0	0	17.66	5.022	4	60.6	1	2	3	33.38	2.684	8	7.5	1	4	3	46.08	1.970	8	0.2
0	0	2	17.66	5.022	2	2.7	0	0	4	35.76	2.511	2	6.8	3	1	4	46.08	1.970	8	0.1
2	1	1	21.67	4.100	8	13.3	3	0	3	38.01	2.367	8	0.4	5	0	1	46.08	1.970	8	3.3
1	1	2	21.67	4.100	8	66.1	4	1	1	38.01	2.367	8	0.6	5	1	0	46.08	1.970	4	2.2
1	2	1	21.67	4.100	8	7.0	1	1	4	38.01	2.367	8	1.0	1	3	4	46.08	1.970	8	11.1
2	0	2	25.08	3.551	8	0.8	3	3	0	38.01	2.367	4	0.3	4	3	1	46.08	1.970	8	0.9
2	2	0	25.08	3.551	4	1.1	1	4	1	38.01	2.367	8	12.0	1	0	5	46.08	1.970	8	1.6
3	1	0	28.10	3.176	4	1.6	4	0	2	40.15	2.246	8	1.4	4	1	3	46.08	1.970	8	2.0
3	0	1	28.10	3.176	8	100.0	2	0	4	40.15	2.246	8	0.9	3	4	1	46.08	1.970	8	1.8
1	0	3	28.10	3.176	8	34.9	4	2	0	40.15	2.246	4	2.3	2	5	1	49.72	1.834	8	0.2
2	2	2	30.84	2.899	8	9.0	3	2	3	42.20	2.141	8	1.0	5	1	2	49.72	1.834	8	2.9
2	1	3	33.38	2.684	8	3.5	2	3	3	42.20	2.141	8	0.3	2	1	5	49.72	1.834	8	0.7
3	1	2	33.38	2.684	8	45.0	3	3	2	42.20	2.141	8	1.0	1	5	2	49.72	1.834	8	0.3
3	2	1	33.38	2.684	8	1.2	4	2	2	44.18	2.050	8	6.5							

Na-P1

GIS



CHEMICAL COMPOSITION: $|(Na_2, Ca)_4(H_2O)_{24}|\ [Si_{16}Al_8O_{48}]$
Nova Scotia, Canada

REFINED COMPOSITION: $|Ca_4(H_2O)_{26.4}|\ [Si_{16}Al_8O_{48}]$

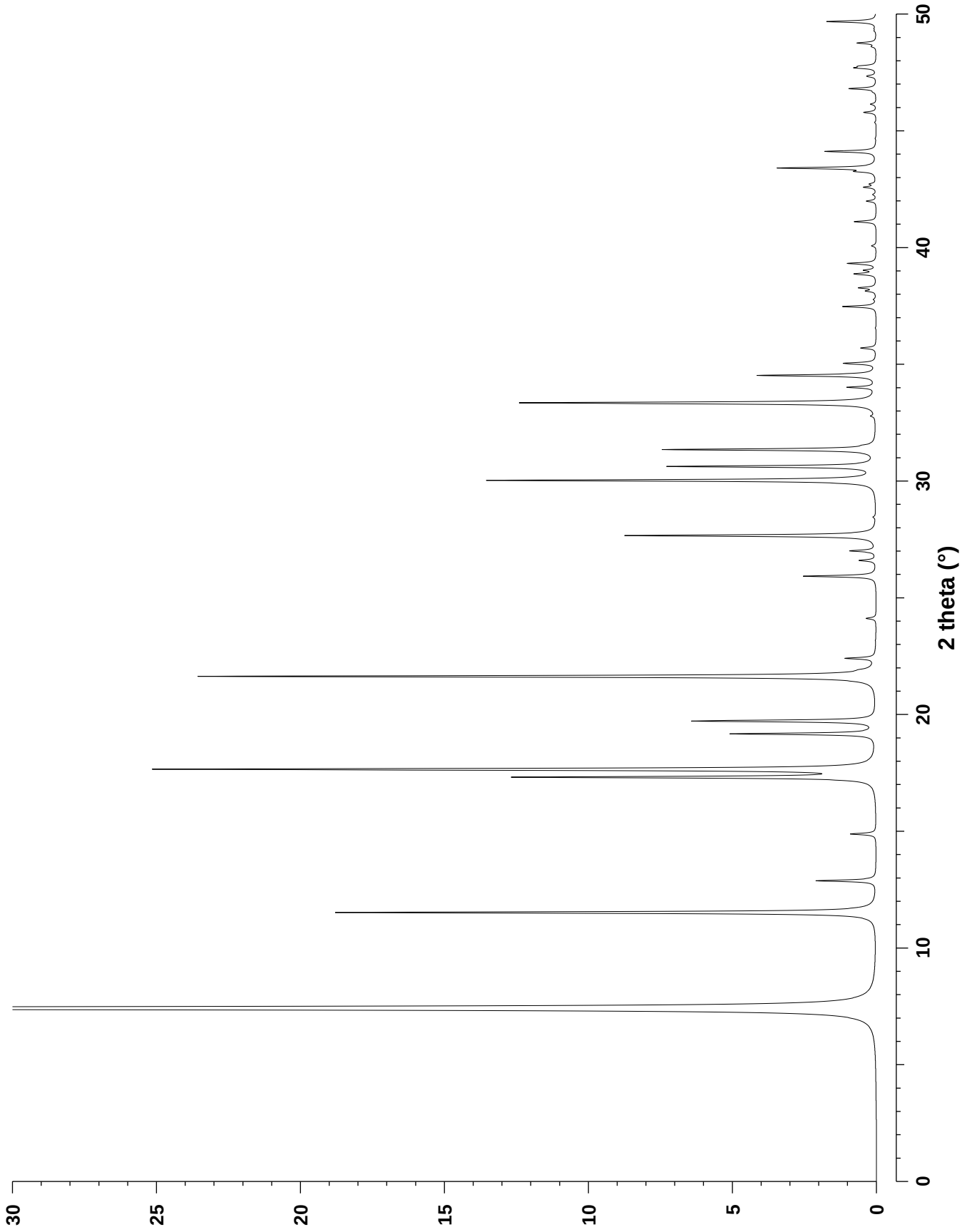
CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.75$ Å $b = 13.75$ Å $c = 10.05$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.17$

REFERENCE: K. Fischer,
Neues Jahrbuch für Mineralogie Monatshefte **1** 1–13 (1966).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.42	11.908	6	100.0	2	0	3	30.62	2.920	12	7.2	5	0	2	41.98	2.152	12	0.3
1	0	1	11.52	7.680	12	18.8	4	0	1	31.34	2.854	12	7.4	5	1	0	42.26	2.139	12	0.1
1	1	0	12.88	6.875	6	2.1	2	2	2	31.53	2.837	12	0.2	3	0	4	42.58	2.123	12	0.4
2	0	0	14.88	5.954	6	0.9	3	2	0	32.78	2.732	12	0.1	3	2	3	42.71	2.117	24	0.2
2	0	1	17.31	5.122	12	12.3	2	1	3	33.34	2.687	24	12.4	5	1	1	43.25	2.092	24	0.6
0	0	2	17.65	5.025	2	25.0	3	2	1	34.01	2.636	24	1.0	3	3	2	43.40	2.085	12	3.4
1	0	2	19.17	4.630	12	5.0	4	1	0	34.52	2.599	12	4.1	4	2	2	44.09	2.054	24	0.2
2	1	0	19.72	4.501	12	6.4	4	0	2	35.03	2.561	12	1.1	4	1	3	44.11	2.053	24	1.7
2	1	1	21.63	4.108	24	23.5	4	1	1	35.69	2.516	24	0.5	1	0	5	45.78	1.982	12	0.4
1	1	2	21.91	4.057	12	0.2	3	2	2	37.47	2.400	24	1.2	5	1	2	46.13	1.968	24	0.2
3	0	0	22.40	3.969	6	1.0	1	1	4	38.13	2.360	12	0.3	5	0	3	46.80	1.941	12	1.0
3	0	1	24.11	3.692	12	0.4	3	1	3	38.27	2.352	24	0.6	4	0	4	47.34	1.920	12	0.3
2	2	0	25.92	3.437	6	2.5	5	0	1	38.86	2.317	12	0.7	5	2	0	47.69	1.907	12	0.7
2	1	2	26.59	3.353	24	0.6	4	1	2	39.02	2.308	24	0.4	2	0	5	47.76	1.904	12	0.5
3	1	0	27.00	3.303	12	0.9	3	3	0	39.31	2.292	6	1.0	5	2	1	48.60	1.873	24	0.1
1	0	3	27.66	3.225	12	8.7	4	2	0	40.07	2.250	12	0.2	4	2	3	48.75	1.868	24	0.7
4	0	0	30.02	2.977	6	13.5	4	2	1	41.10	2.196	24	0.8	2	1	5	49.67	1.835	24	1.7

Gmelinite

GME



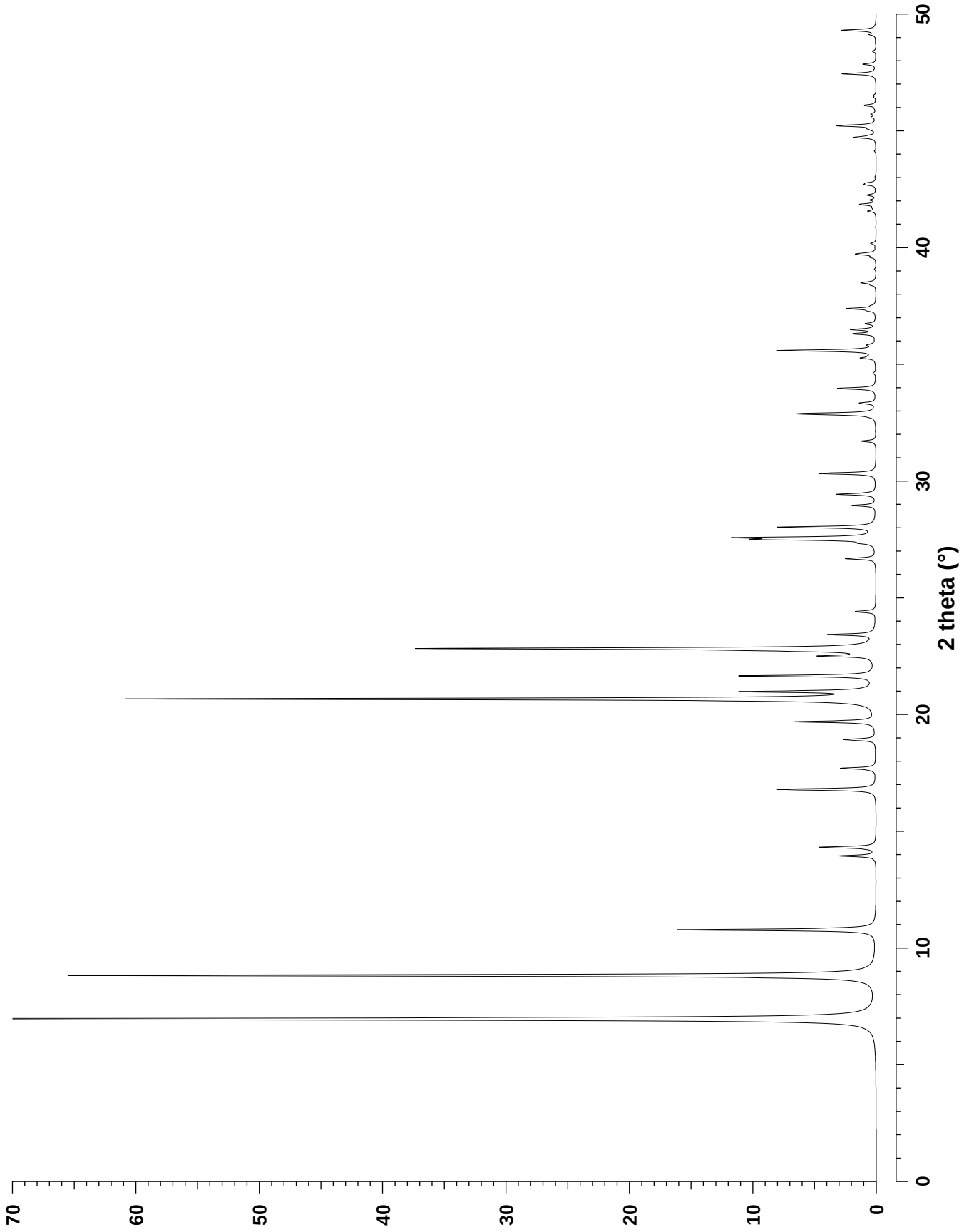
CHEMICAL COMPOSITION: $[Si_{32}O_{64}]$

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: $C222$ (No. 21)
$a = 16.4206$ Å $b = 20.0540$ Å $c = 5.0464$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray powder diffraction.

REFERENCE: J. Plevert, Y. Kubota, T. Honda, T. Okubo and Y. Sugi, *J. Chem. Soc., Chem. Commun.* 2363–2364 (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.96	12.705	4	100.0	1	7	0	31.70	2.822	4	1.2	0	8	1	40.17	2.245	4	0.4
0	2	0	8.82	10.027	2	65.5	6	0	0	32.72	2.737	2	0.2	2	4	2	41.55	2.173	8	0.7
2	0	0	10.78	8.210	2	16.1	5	1	1	32.84	2.727	8	1.7	2	8	1	41.71	2.166	8	0.2
2	2	0	13.94	6.352	4	3.0	3	5	1	32.88	2.724	8	5.5	5	7	0	41.84	2.159	4	1.3
1	3	0	14.31	6.191	4	4.6	4	4	1	33.33	2.688	8	1.3	4	0	2	42.03	2.150	4	0.4
3	1	0	16.79	5.280	4	8.0	6	2	0	33.95	2.640	4	1.8	4	8	0	42.24	2.139	4	0.7
0	4	0	17.69	5.014	2	2.9	2	6	1	33.97	2.639	8	1.6	1	5	2	42.69	2.118	8	0.8
1	1	1	18.92	4.690	8	2.6	4	6	0	34.61	2.592	4	0.2	7	1	1	42.75	2.115	8	0.7
0	2	1	19.69	4.508	4	6.5	5	3	1	35.26	2.545	8	1.1	8	0	0	44.12	2.053	2	0.1
2	0	1	20.66	4.299	4	60.7	5	5	0	35.32	2.541	4	0.1	7	3	1	44.71	2.027	8	1.7
3	3	0	20.98	4.235	4	10.2	3	7	0	35.36	2.538	4	0.2	7	5	0	44.76	2.025	4	0.3
4	0	0	21.65	4.105	2	11.0	0	0	2	35.58	2.523	2	8.0	1	9	1	44.80	2.023	8	0.1
2	2	1	22.50	3.951	8	4.1	0	8	0	35.82	2.507	2	0.6	0	6	2	45.02	2.014	4	0.2
1	3	1	22.73	3.912	8	4.5	1	1	2	36.30	2.475	8	1.8	8	2	0	45.08	2.011	4	0.4
1	5	0	22.82	3.896	4	36.5	1	7	1	36.48	2.463	8	2.0	0	10	0	45.21	2.005	2	3.1
4	2	0	23.42	3.799	4	3.8	0	2	2	36.73	2.447	4	0.8	5	1	2	45.56	1.991	8	0.2
3	1	1	24.40	3.648	8	1.7	2	0	2	37.28	2.412	4	0.4	3	5	2	45.59	1.990	8	0.2
0	6	0	26.67	3.342	2	2.5	6	0	1	37.38	2.406	4	2.3	5	7	1	45.71	1.985	8	0.4
2	4	1	27.33	3.264	8	0.7	2	8	0	37.51	2.397	4	0.3	4	8	1	46.08	1.970	8	0.9
3	3	1	27.49	3.244	8	8.1	2	2	2	38.39	2.345	8	0.3	2	6	2	46.43	1.956	8	0.1
5	1	0	27.52	3.241	4	0.1	6	2	1	38.48	2.339	8	1.2	6	6	1	46.51	1.953	8	0.2
3	5	0	27.57	3.235	4	10.0	1	3	2	38.53	2.337	8	0.1	5	3	2	47.43	1.917	8	2.8
4	0	1	28.02	3.185	4	7.9	4	6	1	39.07	2.306	8	0.1	8	0	1	47.84	1.901	4	1.1
1	5	1	28.95	3.084	8	1.9	3	1	2	39.58	2.277	8	0.4	1	7	2	48.39	1.881	8	0.3
4	2	1	29.43	3.035	8	3.2	5	5	1	39.71	2.270	8	1.4	6	0	2	49.11	1.855	4	0.5
5	3	0	30.32	2.948	4	4.6	3	7	1	39.75	2.268	8	0.4	6	8	0	49.30	1.849	4	2.8


0
10
20
30
40
50
2 theta (°)
0
10
20
30
40
50
60
70

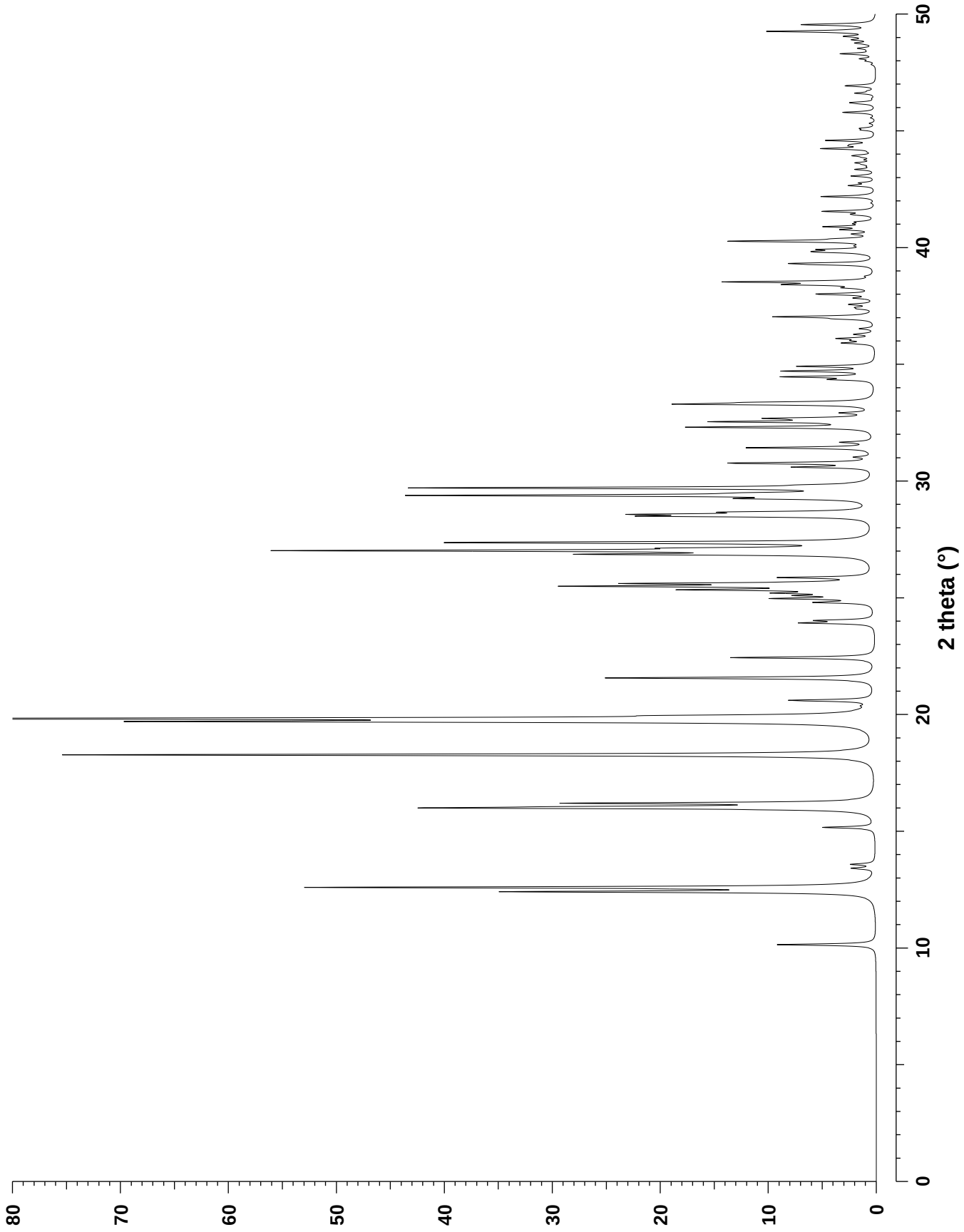
CHEMICAL COMPOSITION: $|Ca_2(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$
Loudon County, Virginia, U.S.A.

REFINED COMPOSITION: $|Ca_2(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$

CRYSTAL DATA: $P12_11$ (No. 4) unique axis **b**
$a = 7.401$ Å $b = 17.439$ Å $c = 7.293$ Å
$\alpha = 90°$ $\beta = 105.44°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.049$

REFERENCE: R. C. Rouse and D. R. Peacor,
American Mineralogist **71** 1494–1501 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	10.14	8.719	2	9.9	1	1	2	31.65	2.827	4	3.1	-3	2	2	41.09	2.197	4	1.6
1	0	0	12.41	7.134	2	35.0	-2	4	1	32.30	2.771	4	10.0	-2	2	3	41.39	2.181	4	0.8
0	0	1	12.59	7.030	2	55.4	-2	2	2	32.30	2.771	4	8.3	0	8	0	41.42	2.180	2	1.5
1	1	0	13.41	6.603	4	2.2	2	4	0	32.43	2.761	4	0.5	1	7	1	41.54	2.174	4	3.9
0	1	1	13.58	6.520	4	2.3	-1	4	2	32.53	2.753	4	15.0	0	3	3	41.55	2.173	4	1.3
-1	0	1	15.16	5.845	2	5.2	1	5	1	32.62	2.745	4	2.9	-3	4	1	42.18	2.143	4	5.4
-1	1	1	15.99	5.542	4	38.9	2	2	1	32.68	2.740	4	9.0	-1	4	3	42.65	2.120	4	2.6
1	2	0	16.05	5.521	4	18.8	1	2	2	32.91	2.722	4	2.9	-3	3	2	42.76	2.114	4	1.4
0	2	1	16.20	5.473	4	28.9	1	6	0	33.29	2.692	4	18.1	-2	3	3	43.06	2.101	4	2.4
-1	2	1	18.27	4.855	4	81.0	0	6	1	33.36	2.686	4	8.7	3	4	0	43.34	2.088	4	1.9
1	3	0	19.70	4.506	4	64.6	-2	3	2	34.34	2.611	4	3.8	0	8	1	43.46	2.082	4	0.5
0	3	1	19.82	4.480	4	100.0	-1	6	1	34.46	2.603	4	8.9	2	3	2	43.55	2.078	4	0.8
1	0	1	19.95	4.450	2	12.8	2	3	1	34.70	2.585	4	8.9	3	1	1	43.62	2.075	4	1.7
0	4	0	20.37	4.360	2	0.4	1	3	2	34.91	2.570	4	7.5	1	0	3	43.75	2.069	2	0.8
1	1	1	20.60	4.312	4	8.2	-2	5	1	35.90	2.502	4	3.1	0	4	3	43.86	2.064	4	0.7
-1	3	1	21.56	4.122	4	26.9	2	5	0	36.01	2.494	4	1.6	-2	6	2	43.93	2.061	4	2.0
1	2	1	22.43	3.964	4	14.4	-1	5	2	36.10	2.488	4	3.5	2	6	1	44.23	2.048	4	4.9
1	4	0	23.92	3.720	4	6.9	0	5	2	36.28	2.476	4	1.9	2	7	0	44.35	2.042	4	1.4
0	4	1	24.02	3.705	4	5.2	-3	0	1	36.52	2.460	2	1.5	1	6	2	44.40	2.040	4	1.2
-2	0	1	24.80	3.590	2	5.3	1	6	1	36.94	2.433	4	2.7	-1	7	2	44.42	2.039	4	0.5
2	0	0	24.96	3.567	2	9.2	-2	4	2	37.03	2.428	4	9.4	0	7	2	44.58	2.033	4	2.3
-1	0	2	25.09	3.550	2	5.7	-1	0	3	37.06	2.426	2	0.6	3	2	1	44.58	2.032	4	2.6
1	3	1	25.20	3.533	4	7.4	2	4	1	37.37	2.406	4	1.2	1	2	3	45.03	2.013	4	1.0
-2	1	1	25.33	3.516	4	11.1	-1	1	3	37.43	2.403	4	1.4	-3	5	1	45.10	2.010	4	1.3
0	0	2	25.34	3.515	2	6.1	1	4	2	37.56	2.394	4	2.4	-2	4	3	45.31	2.002	4	0.6
-1	4	1	25.49	3.495	4	11.4	3	0	0	37.83	2.378	2	1.8	2	4	2	45.78	1.982	4	3.3
2	1	0	25.49	3.495	4	16.6	-3	2	1	38.00	2.368	4	5.6	3	3	1	46.15	1.967	4	1.0
-1	1	2	25.61	3.478	4	22.1	1	7	0	38.27	2.352	4	2.2	3	5	0	46.20	1.965	4	2.2
0	1	2	25.86	3.446	4	8.7	0	0	3	38.41	2.343	2	7.4	1	3	3	46.60	1.949	4	1.7
-2	2	1	26.86	3.320	4	25.8	-1	2	3	38.52	2.337	4	14.3	0	5	3	46.70	1.945	4	0.5
2	2	0	27.01	3.301	4	56.4	0	1	3	38.77	2.322	4	0.6	-3	1	3	46.92	1.936	4	3.0
-1	2	2	27.12	3.288	4	13.3	3	2	0	39.27	2.294	4	3.1	-2	7	2	47.98	1.896	4	0.8
0	2	2	27.36	3.260	4	41.7	-1	7	1	39.31	2.292	4	7.0	-2	5	3	48.08	1.892	4	1.4
1	5	0	28.49	3.133	4	19.3	-3	3	1	39.79	2.266	4	3.3	3	4	1	48.29	1.885	4	3.2
0	5	1	28.57	3.124	4	18.9	0	2	3	39.83	2.263	4	3.5	2	5	2	48.53	1.876	4	1.5
1	4	1	28.66	3.114	4	11.3	-2	6	1	39.91	2.259	4	4.6	0	9	1	48.75	1.868	4	1.7
-2	3	1	29.24	3.054	4	10.2	-3	1	2	40.06	2.251	4	0.7	-2	8	1	48.88	1.863	4	0.9
2	3	0	29.38	3.040	4	44.4	-2	5	2	40.26	2.240	4	6.5	-1	6	3	48.90	1.862	4	1.1
-1	3	2	29.48	3.030	4	6.6	0	6	2	40.26	2.240	4	5.2	-1	8	2	49.04	1.858	4	2.6
0	3	2	29.70	3.008	4	45.2	-1	3	3	40.28	2.239	4	3.3	0	8	2	49.18	1.853	4	0.5
-1	5	1	29.83	2.995	4	3.6	-2	1	3	40.37	2.234	4	2.4	-4	0	1	49.25	1.850	2	10.4
-2	0	2	30.59	2.923	2	7.5	2	5	1	40.57	2.223	4	1.9	-3	3	3	49.33	1.847	4	0.4
0	6	0	30.76	2.906	2	14.1	1	5	2	40.76	2.214	4	2.9	3	6	0	49.53	1.840	4	6.0
-2	1	2	31.02	2.882	4	1.6	2	1	2	40.89	2.207	4	4.7	-4	1	1	49.55	1.840	4	0.5
2	1	1	31.42	2.847	4	12.7	3	3	0	41.01	2.201	4	1.4	-1	9	1	49.56	1.839	4	1.4


0
10
20
30
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50
2 theta (°)
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30
40
50
60
70
80

HEU Heulandite

CHEMICAL COMPOSITION: $|Na_{0.1}K_{8.57}Ba_{0.04}(H_2O)_{19.56}|\ [Si_{26.83}Al_{9.31}O_{72}]$
Mossyrock Dam, Washington, U.S.A.

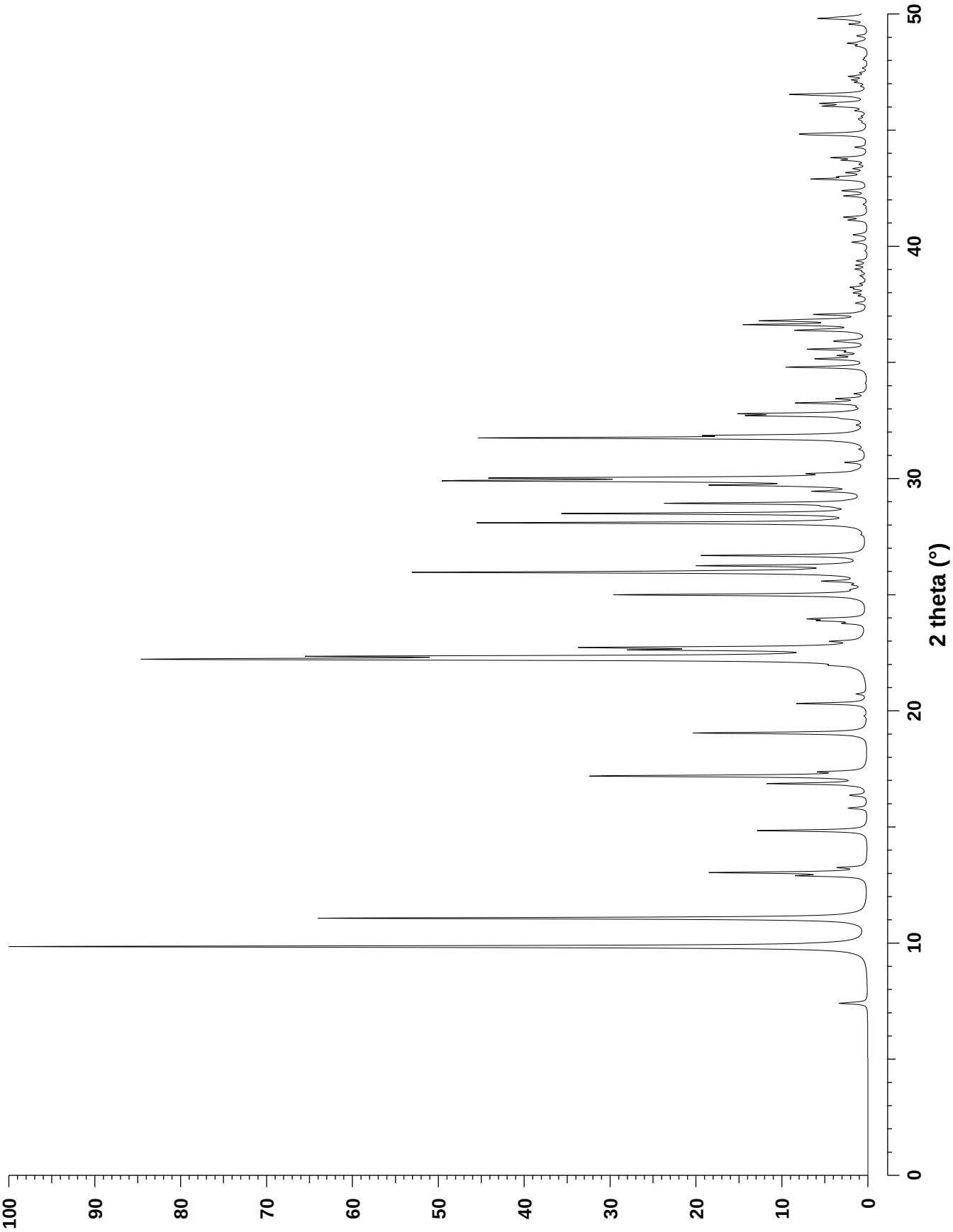
REFINED COMPOSITION: $|K_{8.48}(H_2O)_{18}|\ [Si_{26.64}Al_{9.36}O_{72}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 17.767$ Å $b = 17.958$ Å $c = 7.431$ Å
$\alpha = 90°$ $\beta = 115.93°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.07$

REFERENCE: E. Galli, G. Gottardi, H. Mayer, A. Preisinger and E. Passaglia, *Acta Cryst.* **B39** 189–197 (1983).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	7.41	11.937	4	3.3	3	5	0	30.01	2.978	4	27.8	0	8	0	40.17	2.245	2	0.9
0	2	0	9.85	8.979	2	100.0	1	1	2	30.03	2.975	4	12.7	0	0	3	40.49	2.228	2	1.4
2	0	0	11.07	7.989	2	64.0	-6	0	1	30.21	2.958	2	4.5	-6	2	3	41.12	2.195	4	2.0
-1	1	1	12.90	6.865	4	6.8	4	0	1	30.69	2.913	2	2.3	-1	3	3	41.25	2.189	4	2.6
-2	0	1	13.03	6.792	2	17.8	-2	4	2	31.25	2.862	4	0.5	2	8	0	41.80	2.161	4	0.4
0	0	1	13.25	6.683	2	2.9	5	3	0	31.74	2.819	4	43.6	-2	4	3	42.16	2.143	4	1.9
2	2	0	14.84	5.969	4	12.9	-6	2	1	31.85	2.810	4	14.0	4	0	2	42.17	2.143	2	0.8
1	3	0	15.81	5.606	4	2.2	4	2	1	32.30	2.771	4	0.7	7	3	0	42.38	2.133	4	2.4
-2	2	1	16.36	5.417	4	1.9	-6	0	2	32.57	2.749	2	1.5	-2	8	1	42.41	2.131	4	0.8
-3	1	1	16.86	5.258	4	11.3	-2	6	1	32.70	2.739	4	10.6	-7	1	3	42.85	2.110	4	0.6
1	1	1	17.19	5.157	4	32.0	-5	3	2	32.72	2.737	4	1.6	6	2	1	42.89	2.108	4	5.9
3	1	0	17.37	5.106	4	4.3	0	6	1	32.79	2.732	4	12.8	-6	6	1	42.99	2.104	4	2.6
-1	3	1	19.04	4.661	4	20.3	-4	4	2	33.07	2.708	4	0.5	-3	7	2	43.16	2.096	4	2.2
-4	0	1	20.31	4.373	2	8.2	1	3	2	33.25	2.694	4	7.7	4	6	1	43.34	2.088	4	1.3
2	0	1	20.72	4.286	2	1.1	2	0	2	33.28	2.692	2	0.5	-5	7	1	43.52	2.079	4	0.7
-3	3	1	21.95	4.050	4	1.9	0	4	2	33.43	2.681	4	3.2	1	1	3	43.70	2.071	4	2.6
1	3	1	22.21	4.003	4	60.2	6	0	0	33.65	2.663	2	1.3	3	7	1	43.81	2.067	4	3.9
4	0	0	22.25	3.995	2	34.7	2	2	2	34.79	2.579	4	9.4	5	5	1	44.26	2.046	4	1.4
3	3	0	22.34	3.979	4	53.8	-3	5	2	35.12	2.555	4	1.4	-7	5	2	44.80	2.023	4	5.2
-4	2	1	22.62	3.931	4	21.9	6	2	0	35.15	2.553	4	4.8	-6	4	3	44.84	2.021	4	4.7
2	4	0	22.72	3.914	4	29.4	-1	5	2	35.29	2.543	4	2.8	3	5	2	45.48	1.994	4	0.7
2	2	1	22.99	3.868	4	3.1	1	7	0	35.44	2.533	4	1.7	6	6	0	45.60	1.990	4	0.5
-2	4	1	23.76	3.745	4	2.2	-5	5	1	35.56	2.525	4	6.7	1	9	0	45.83	1.980	4	1.1
0	4	1	23.88	3.727	4	4.4	3	5	1	35.89	2.502	4	2.5	-8	4	1	46.03	1.972	4	4.4
-2	0	2	23.96	3.715	2	5.9	-7	1	1	35.93	2.499	4	2.1	-5	7	2	46.06	1.971	4	0.4
-3	1	2	24.99	3.563	4	29.4	-6	4	1	36.37	2.470	4	3.2	-1	5	3	46.14	1.967	4	4.3
-1	1	2	25.22	3.531	4	0.9	-4	6	1	36.37	2.470	4	3.9	-8	4	2	46.18	1.966	4	1.1
1	5	0	25.42	3.504	4	0.9	5	1	1	36.42	2.467	4	2.4	6	4	1	46.50	1.953	4	2.6
-5	1	1	25.58	3.482	4	4.5	2	6	1	36.62	2.454	4	11.3	-9	1	2	46.53	1.952	4	7.1
-2	2	2	25.96	3.433	4	50.8	-3	1	3	36.63	2.453	4	2.3	8	2	0	46.58	1.950	4	0.5
3	1	1	26.03	3.424	4	6.8	4	4	1	36.78	2.444	4	10.4	2	0	3	46.89	1.938	2	0.6
-4	0	2	26.24	3.396	2	18.5	-2	0	3	36.84	2.439	2	3.9	-8	2	3	47.05	1.932	4	1.2
0	0	2	26.68	3.341	2	19.0	-7	1	2	37.06	2.426	4	5.6	-1	9	1	47.16	1.927	4	1.3
-4	2	2	28.09	3.176	4	45.1	4	6	0	37.55	2.395	4	1.3	-2	8	2	47.31	1.921	4	2.1
-4	4	1	28.49	3.132	4	34.1	3	1	2	37.86	2.377	4	0.9	5	1	2	47.46	1.916	4	0.8
0	2	2	28.50	3.132	4	0.8	-4	2	3	37.99	2.368	4	1.5	7	1	1	47.67	1.908	4	0.5
-3	3	2	28.73	3.107	4	1.0	-5	1	3	38.15	2.359	4	1.1	2	2	3	48.03	1.894	4	0.5
2	4	1	28.80	3.100	4	2.4	-2	2	3	38.23	2.354	4	1.7	-4	8	2	48.62	1.873	4	1.1
-1	3	2	28.93	3.086	4	22.8	-6	4	2	38.39	2.345	4	0.7	3	9	0	48.73	1.869	4	2.1
-5	1	2	29.45	3.033	4	5.3	-3	7	1	38.73	2.325	4	0.5	-9	3	2	48.81	1.866	4	0.5
3	3	1	29.64	3.013	4	1.6	1	7	1	38.89	2.316	4	0.4	-4	0	4	49.05	1.857	2	1.2
-3	5	1	29.71	3.007	4	15.0	2	4	2	39.01	2.309	4	1.3	-5	1	4	49.55	1.840	4	2.0
0	6	0	29.85	2.993	2	4.1	5	3	1	39.18	2.299	4	1.3	5	3	2	49.71	1.834	4	0.7
1	5	1	29.90	2.988	4	41.6	-3	3	3	39.37	2.288	4	1.1	-3	1	4	49.80	1.831	4	5.0
4	4	0	29.94	2.984	4	2.2	-4	6	2	40.16	2.245	4	1.0	-7	5	3	49.86	1.829	4	2.0

Heulandite HEU



HEU Clinoptilolite

CHEMICAL COMPOSITION: $|Na_{1.84}K_{1.76}Mg_{0.2}Ca_{1.24}(H_2O)_{21.36}|\ [Si_{29.84}Al_{6.16}O_{72}]$
Agoura, California, U.S.A.

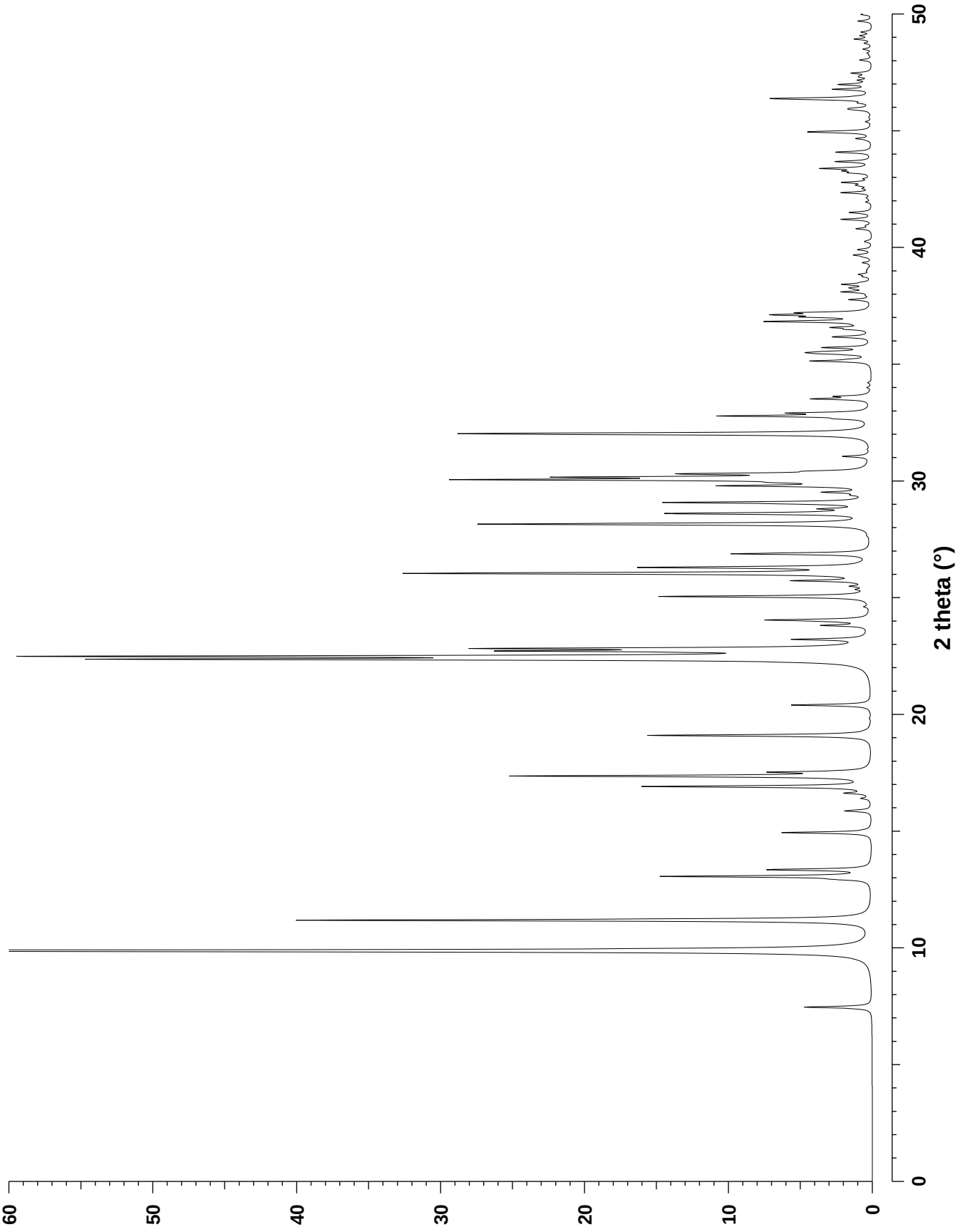
REFINED COMPOSITION: $|Na_{1.84}K_{1.76}Mg_{0.2}Ca_{1.24}(H_2O)_{21.36}|\ [Si_{29.84}Al_{6.16}O_{72}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 17.662$ Å $b = 17.911$ Å $c = 7.407$ Å
$\alpha = 90°$ $\beta = 116.40°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.088$

REFERENCE: K. Koyama and Y. Takeuchi,
Z. Kristallogr. **145** 216–239 (1977).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	7.46	11.857	4	4.7	4	4	0	30.15	2.964	4	0.4	-7	3	2	39.92	2.258	4	0.4
0	2	0	9.88	8.955	2	100.0	3	5	0	30.16	2.963	4	17.8	-4	6	2	40.25	2.240	4	0.3
2	0	0	11.19	7.910	2	40.0	1	1	2	30.30	2.950	4	11.2	0	0	3	40.80	2.212	2	1.1
-1	1	1	12.94	6.842	4	1.4	-6	0	1	30.41	2.940	2	2.7	3	3	2	40.93	2.205	4	0.3
-2	0	1	13.06	6.780	2	14.5	4	0	1	31.05	2.880	2	1.9	-6	2	3	41.20	2.191	4	2.1
0	0	1	13.35	6.635	2	7.0	5	3	0	32.01	2.796	4	23.1	-1	3	3	41.49	2.176	4	1.5
2	2	0	14.94	5.929	4	6.3	-6	2	1	32.04	2.793	4	8.7	2	8	0	41.94	2.154	4	0.4
1	3	0	15.87	5.586	4	1.9	4	2	1	32.66	2.742	4	0.6	6	0	1	42.13	2.145	2	0.3
-2	2	1	16.40	5.405	4	0.6	-6	0	2	32.66	2.742	2	0.8	-2	4	3	42.34	2.134	4	2.1
0	2	1	16.63	5.331	4	1.6	-2	6	1	32.78	2.732	4	9.7	-2	8	1	42.52	2.126	4	0.5
-3	1	1	16.91	5.243	4	15.8	-5	3	2	32.79	2.731	4	0.4	4	0	2	42.66	2.120	2	0.8
1	1	1	17.36	5.110	4	24.8	0	6	1	32.90	2.722	4	4.9	7	3	0	42.78	2.114	4	1.9
3	1	0	17.53	5.059	4	6.0	1	3	2	33.51	2.674	4	4.0	-7	1	3	42.94	2.106	4	0.4
-1	3	1	19.10	4.648	4	15.6	2	0	2	33.62	2.666	2	1.0	-6	6	1	43.19	2.095	4	1.3
-4	0	1	20.40	4.354	2	5.6	0	4	2	33.62	2.665	4	1.2	-3	7	2	43.27	2.091	4	1.4
1	3	1	22.36	3.976	4	49.2	6	0	0	34.00	2.637	2	0.3	6	2	1	43.38	2.086	4	3.4
4	0	0	22.48	3.955	2	18.1	2	2	2	35.13	2.555	4	4.1	4	6	1	43.67	2.073	4	2.3
3	3	0	22.49	3.952	4	37.2	-3	5	2	35.21	2.549	4	0.7	3	7	1	44.07	2.055	4	1.5
-4	2	1	22.71	3.916	4	21.0	-1	5	2	35.44	2.533	4	2.3	1	1	3	44.08	2.054	4	0.9
2	4	0	22.82	3.897	4	24.4	6	2	0	35.49	2.529	4	2.9	5	5	1	44.66	2.029	4	1.0
2	2	1	23.21	3.832	4	4.9	1	7	0	35.54	2.526	4	1.8	-6	4	3	44.93	2.018	4	2.7
-2	4	1	23.81	3.736	4	3.1	-5	5	1	35.71	2.514	4	3.2	-7	5	2	44.96	2.016	4	2.3
0	4	1	23.98	3.712	4	1.5	3	5	1	36.16	2.484	4	2.0	-7	3	3	45.38	1.998	4	0.4
-2	0	2	24.04	3.702	2	6.8	-7	1	1	36.19	2.482	4	0.9	8	0	0	45.89	1.978	2	0.4
4	2	0	24.61	3.618	4	0.3	-4	6	1	36.49	2.462	4	1.3	6	6	0	45.92	1.976	4	0.8
-3	1	2	25.05	3.555	4	14.7	-6	4	1	36.57	2.457	4	2.4	1	9	0	45.96	1.975	4	0.9
-1	1	2	25.35	3.513	4	0.6	-4	0	3	36.69	2.449	2	0.4	-5	7	2	46.18	1.966	4	0.6
1	5	0	25.49	3.494	4	1.0	2	6	1	36.82	2.441	4	6.2	-8	4	1	46.34	1.959	4	2.6
-5	1	1	25.72	3.463	4	5.0	5	1	1	36.85	2.439	4	1.3	-8	4	2	46.38	1.958	4	1.2
-2	2	2	26.04	3.421	4	32.1	-2	0	3	37.02	2.428	2	3.6	-1	5	3	46.38	1.958	4	4.5
-4	0	2	26.29	3.390	2	13.6	4	4	1	37.11	2.422	4	5.7	-9	1	2	46.77	1.942	4	2.6
3	1	1	26.32	3.386	4	2.8	-7	1	2	37.20	2.417	4	4.1	6	4	1	46.97	1.934	4	2.2
0	0	2	26.88	3.317	2	9.6	4	6	0	37.76	2.383	4	1.5	-8	2	3	47.16	1.927	4	0.8
-4	2	2	28.15	3.170	4	27.2	-4	2	3	38.09	2.362	4	2.0	-1	9	1	47.30	1.922	4	0.6
-4	4	1	28.60	3.121	4	13.8	-5	1	3	38.22	2.355	4	0.6	2	0	3	47.35	1.920	2	0.4
0	2	2	28.70	3.111	4	0.5	3	1	2	38.27	2.352	4	1.1	-2	8	2	47.46	1.916	4	1.3
-3	3	2	28.80	3.100	4	2.7	-2	2	3	38.41	2.344	4	1.9	5	1	2	48.02	1.895	4	0.8
2	4	1	29.00	3.078	4	1.0	-6	4	2	38.50	2.338	4	0.4	-2	6	3	48.32	1.884	4	0.3
-1	3	2	29.07	3.072	4	14.0	-2	6	2	38.75	2.324	4	0.5	2	2	3	48.49	1.877	4	0.6
-5	3	1	29.39	3.039	4	0.7	-3	7	1	38.84	2.319	4	0.8	-4	8	2	48.74	1.868	4	0.5
-5	1	2	29.51	3.027	4	2.8	-7	3	1	38.97	2.311	4	0.2	3	9	0	48.92	1.862	4	1.2
-3	5	1	29.79	2.999	4	9.5	2	4	2	39.34	2.290	4	0.6	-9	3	2	49.06	1.857	4	0.6
3	3	1	29.92	2.986	4	1.3	5	3	1	39.59	2.276	4	0.4	-4	0	4	49.22	1.851	2	0.7
0	6	0	29.93	2.985	2	2.0	6	4	0	39.67	2.272	4	1.2	-5	1	4	49.69	1.835	4	1.0
1	5	1	30.05	2.973	4	26.4	-6	0	3	39.89	2.260	2	0.7	-7	5	3	49.97	1.825	4	0.8

Clinoptilolite HEU



IFR ITQ-4, Calcined

CHEMICAL COMPOSITION: $[Si_{32}O_{64}]$

REFINED COMPOSITION: $[Si_{32}O_{64}]$

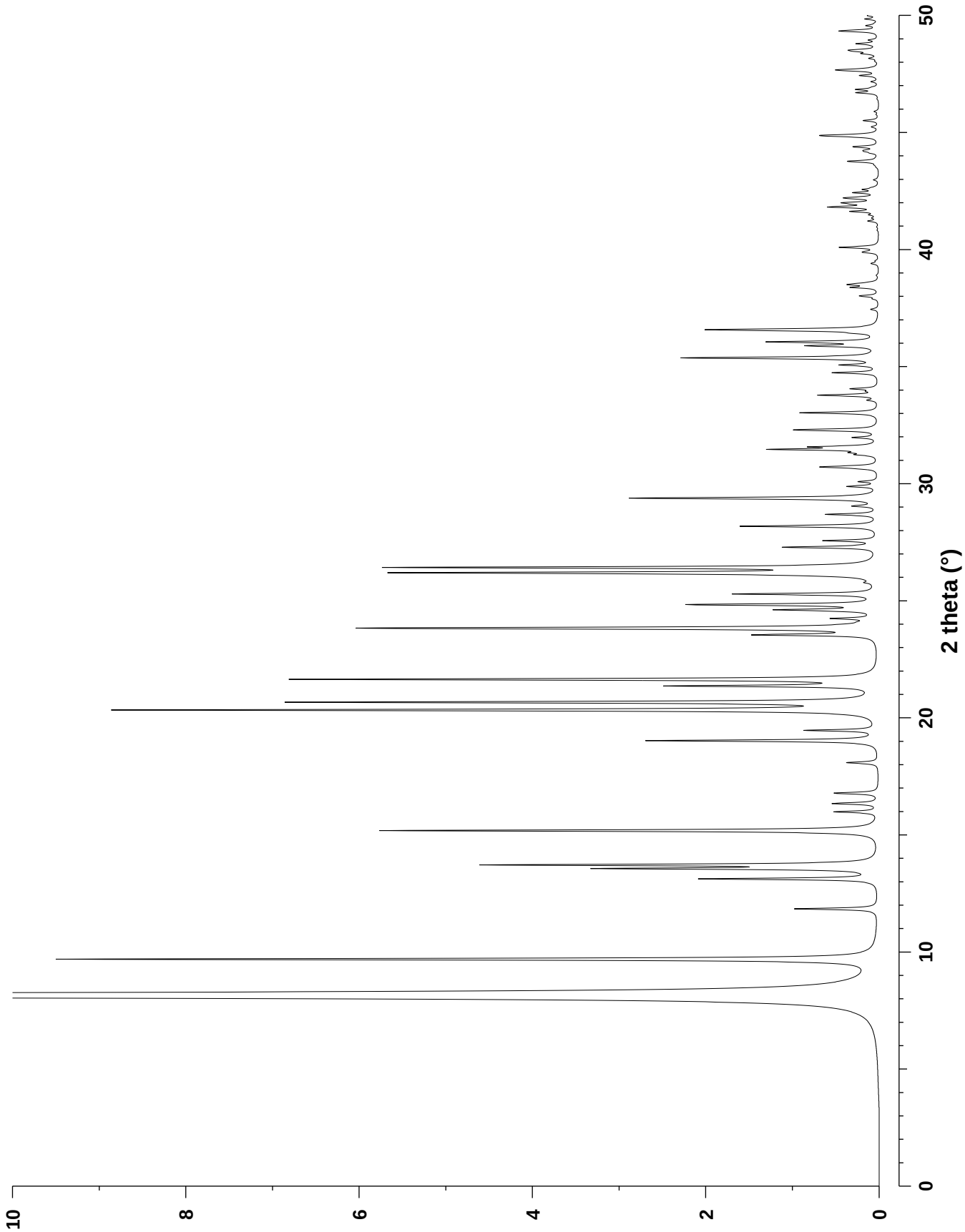
CRYSTAL DATA: $I1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 3
$a = 18.65243$ Å $b = 13.49597$ Å $c = 7.63109$ Å
$\alpha = 90.0°$ $\beta = 101.9781°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_{wp} = 0.0767$, $R_p = 0.0558$, $R_b = 0.0644$

REFERENCE: P. A. Barrett, M. A. Camblor, A. Corma, R. H. Jones and L. A. Villaescusa, *Chemistry of Materials* **9** 1713–1715 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.15	10.850	4	100.0	6	0	0	29.37	3.041	2	1.7	1	2	3	39.87	2.261	4	0.1
2	0	0	9.69	9.123	2	9.4	5	0	1	29.39	3.039	2	1.4	0	6	0	40.09	2.249	2	0.4
-1	0	1	11.84	7.474	2	1.0	1	4	1	29.88	2.990	4	0.3	7	2	1	41.21	2.190	4	0.1
0	2	0	13.12	6.748	2	2.0	-6	1	1	30.08	2.971	4	0.2	5	5	0	41.62	2.170	4	0.3
0	1	1	13.56	6.532	4	3.0	2	2	2	30.70	2.912	4	0.4	8	2	0	41.81	2.161	4	0.5
1	0	1	13.72	6.455	2	4.4	-1	3	2	30.73	2.910	4	0.3	4	5	1	41.93	2.154	4	0.1
-2	1	1	15.18	5.837	4	5.8	-5	1	2	31.23	2.864	4	0.2	3	0	3	41.99	2.152	2	0.3
3	1	0	15.98	5.545	4	0.5	3	1	2	31.32	2.856	4	0.2	-3	5	2	42.17	2.143	4	0.2
2	2	0	16.34	5.425	4	0.5	-3	4	1	31.46	2.843	4	1.2	1	5	2	42.21	2.141	4	0.3
-3	0	1	16.78	5.283	2	0.5	5	3	0	31.57	2.834	4	0.7	-6	1	3	42.42	2.131	4	0.3
2	1	1	18.08	4.906	4	0.4	4	3	1	31.97	2.799	4	0.3	1	6	1	42.56	2.124	4	0.2
1	2	1	19.02	4.665	4	2.7	-3	3	2	32.27	2.774	4	0.4	-3	6	1	43.74	2.070	4	0.1
4	0	0	19.46	4.562	2	0.8	6	2	0	32.29	2.773	4	0.3	-9	0	1	43.77	2.068	2	0.3
1	3	0	20.33	4.368	4	8.8	5	2	1	32.31	2.771	4	0.3	6	2	2	44.23	2.048	4	0.1
3	0	1	20.66	4.299	2	6.7	1	3	2	32.31	2.770	4	0.1	8	1	1	44.38	2.041	4	0.3
-3	2	1	21.36	4.160	4	2.3	4	4	0	33.02	2.713	4	0.9	-7	0	3	44.83	2.022	2	0.4
-4	1	1	21.64	4.106	4	6.7	1	5	0	33.56	2.670	4	0.1	-6	5	1	44.87	2.020	4	0.5
4	2	0	23.54	3.779	4	1.3	3	4	1	33.77	2.654	4	0.7	4	1	3	45.50	1.994	4	0.2
-2	0	2	23.81	3.737	2	3.0	4	0	2	34.05	2.633	2	0.3	-6	3	3	46.69	1.946	4	0.2
0	0	2	23.84	3.732	2	3.8	6	1	1	34.73	2.583	4	0.5	-9	1	2	46.83	1.940	4	0.2
-1	1	2	24.24	3.672	4	0.5	7	1	0	35.06	2.559	4	0.4	1	7	0	47.42	1.917	4	0.2
3	2	1	24.55	3.625	4	0.2	0	5	1	35.36	2.538	4	1.3	7	4	1	47.63	1.909	4	0.2
3	3	0	24.61	3.617	4	1.1	-1	0	3	35.38	2.537	2	1.1	-2	0	4	47.67	1.908	2	0.4
-5	0	1	24.83	3.585	2	2.2	0	4	2	35.88	2.503	4	0.7	8	4	0	48.16	1.890	4	0.1
5	1	0	25.28	3.523	4	1.6	-2	1	3	36.01	2.494	4	0.1	5	0	3	48.36	1.882	2	0.2
2	3	1	26.05	3.421	4	0.1	-3	0	3	36.05	2.491	2	0.6	-1	1	4	48.46	1.878	4	0.2
-3	1	2	26.13	3.410	4	0.8	-2	5	1	36.05	2.491	4	0.6	8	3	1	48.51	1.877	4	0.2
1	1	2	26.19	3.403	4	5.3	3	5	0	36.42	2.467	4	0.1	0	7	1	48.78	1.867	4	0.2
0	4	0	26.42	3.374	2	5.6	-6	2	2	36.53	2.460	4	0.5	-2	7	1	49.32	1.848	4	0.4
-2	2	2	27.28	3.269	4	0.9	-5	4	1	36.57	2.457	4	1.4	-10	1	1	49.36	1.846	4	0.1
0	2	2	27.30	3.266	4	0.3	-5	3	2	36.59	2.456	4	0.4	4	3	3	49.55	1.839	4	0.1
-4	0	2	27.56	3.237	2	0.6	-4	1	3	38.01	2.367	4	0.2	0	5	3	49.84	1.830	4	0.1
-5	2	1	28.18	3.166	4	1.5	-7	1	2	38.38	2.345	4	0.3	10	0	0	49.98	1.825	2	0.1
-4	3	1	28.68	3.112	4	0.6	5	1	2	38.49	2.339	4	0.3							
-1	4	1	29.04	3.075	4	0.3	-4	4	2	38.54	2.336	4	0.1							

ITQ-4, Calcined

IFR



ITQ–7, Siliceous, Calcined

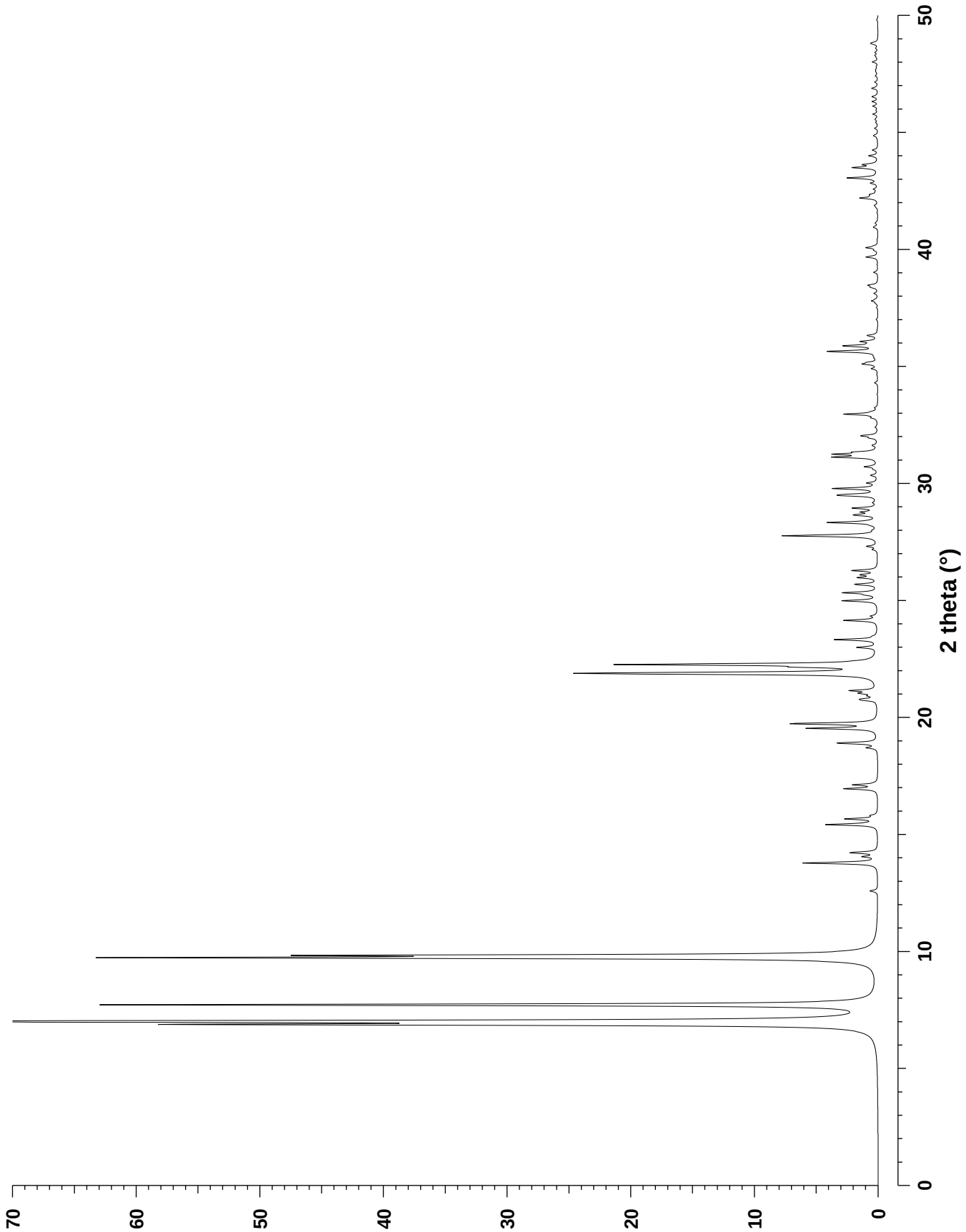
CHEMICAL COMPOSITION: $[Si_{64}O_{128}]$

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: $P\,4_2/m\,mc$ (No. 131)
$a = 12.8528$ Å $b = 12.8528$ Å $c = 25.2136$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0827$, $R_{wp} = 0.1076$, $R_b = 0.0.0626$

REFERENCE: L. A. Villaescusa, P. A. Barrett and M. A. Camblor,
Angew. Chem., Int. ed. **38** 1997–2000 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	6.88	12.853	4	52.2	4	0	1	27.99	3.187	8	0.2	4	3	4	37.79	2.380	16	0.5
0	0	2	7.01	12.607	2	100.0	3	1	5	28.20	3.164	16	0.2	3	2	8	38.11	2.361	16	0.3
1	0	1	7.72	11.451	8	65.5	0	0	8	28.32	3.152	2	4.2	2	0	10	38.35	2.347	8	0.2
1	1	0	9.73	9.088	4	60.5	2	0	7	28.40	3.142	8	0.3	5	2	2	38.38	2.345	16	0.2
1	0	2	9.83	9.000	8	41.4	4	1	0	28.64	3.117	8	1.6	3	0	9	38.39	2.345	8	0.2
1	0	3	12.58	7.034	8	0.7	4	0	2	28.67	3.114	8	0.4	5	1	4	38.46	2.340	16	0.8
2	0	0	13.78	6.426	4	6.3	3	2	4	28.77	3.103	16	1.2	2	1	10	39.01	2.309	16	0.3
0	0	4	14.05	6.303	2	1.1	2	2	6	28.94	3.085	8	2.1	4	4	0	39.67	2.272	4	1.0
2	0	1	14.22	6.227	8	2.3	1	0	8	29.17	3.061	8	0.3	1	0	11	39.95	2.257	8	0.2
2	1	0	15.42	5.748	8	4.3	3	3	0	29.48	3.029	4	2.5	4	0	8	40.07	2.250	8	1.0
2	0	2	15.48	5.725	8	0.3	4	1	2	29.52	3.026	16	1.6	4	2	7	40.14	2.247	16	0.1
1	0	4	15.66	5.659	8	2.7	4	0	3	29.77	3.001	8	0.9	5	3	0	40.94	2.204	8	0.2
2	1	1	15.81	5.604	16	0.5	3	0	6	29.78	3.000	8	2.9	5	3	1	41.11	2.196	16	0.2
2	1	2	16.95	5.230	16	2.8	1	1	8	30.01	2.978	8	0.8	5	2	5	41.87	2.157	16	0.2
1	1	4	17.12	5.180	8	2.0	3	3	2	30.34	2.946	8	0.5	6	0	0	42.19	2.142	4	1.4
2	1	3	18.70	4.744	16	0.9	3	1	6	30.60	2.921	16	0.2	4	4	4	42.28	2.137	8	0.3
1	0	5	18.90	4.694	8	3.4	3	2	5	30.71	2.911	16	1.1	6	0	1	42.34	2.134	8	0.5
2	2	0	19.53	4.544	4	5.8	4	2	0	31.12	2.874	8	3.6	4	2	8	42.57	2.124	16	0.3
2	0	4	19.73	4.500	8	7.2	4	0	4	31.24	2.863	8	3.3	6	0	2	42.82	2.112	8	0.3
3	0	0	20.73	4.284	4	0.9	4	2	1	31.33	2.855	16	1.5	4	0	9	42.82	2.112	8	0.2
2	2	2	20.78	4.275	8	1.0	2	0	8	31.62	2.830	8	0.4	0	0	12	43.05	2.101	2	2.6
2	1	4	20.92	4.247	16	0.6	4	2	2	31.94	2.802	16	0.6	5	3	4	43.49	2.081	16	2.1
3	0	1	21.03	4.224	8	1.3	4	1	4	32.03	2.794	16	1.3	5	2	6	43.61	2.075	16	1.1
0	0	6	21.14	4.202	2	2.2	2	1	8	32.40	2.764	16	0.2	1	0	12	43.65	2.074	8	0.1
3	1	0	21.87	4.064	8	21.3	3	3	4	32.80	2.730	8	0.4	3	2	10	43.99	2.058	16	0.8
3	0	2	21.91	4.056	8	8.4	3	2	6	32.95	2.718	16	2.8	1	1	12	44.24	2.047	8	0.4
3	1	1	22.15	4.013	16	4.3	4	0	5	33.06	2.710	8	0.3	3	0	11	44.84	2.021	8	0.3
1	0	6	22.26	3.994	8	21.5	3	1	7	33.23	2.696	16	0.2	5	3	5	44.88	2.020	16	0.1
2	0	5	22.41	3.967	8	0.5	4	2	4	34.29	2.615	16	0.3	5	4	0	45.17	2.007	8	0.3
3	1	2	22.99	3.868	16	1.7	5	0	0	34.90	2.571	4	0.3	5	0	8	45.54	1.992	8	0.2
3	0	3	23.30	3.817	8	0.2	4	3	0	34.90	2.571	8	0.2	5	4	2	45.77	1.982	16	0.4
1	1	6	23.32	3.814	8	3.4	4	3	1	35.09	2.557	16	0.8	5	1	8	46.11	1.969	16	0.4
2	1	5	23.47	3.791	16	0.2	5	0	1	35.09	2.557	8	0.3	4	1	10	46.31	1.960	16	0.5
2	2	4	24.14	3.686	8	2.9	4	0	6	35.16	2.553	8	0.7	5	4	3	46.51	1.952	16	0.2
3	1	3	24.33	3.659	16	0.5	3	0	8	35.35	2.539	8	0.2	5	3	6	46.52	1.952	16	0.3
3	2	0	24.98	3.565	8	3.0	0	0	10	35.61	2.521	2	0.5	3	3	10	46.88	1.938	8	0.5
3	2	1	25.23	3.530	16	0.6	5	1	0	35.62	2.521	8	1.0	3	2	11	47.14	1.928	16	0.3
2	0	6	25.32	3.517	8	2.9	5	0	2	35.64	2.519	8	1.5	1	0	13	47.40	1.918	8	0.2
1	0	7	25.68	3.468	8	1.9	4	3	2	35.64	2.519	16	1.3	2	2	12	47.68	1.907	8	0.2
3	2	2	25.97	3.430	16	1.6	2	1	9	35.65	2.518	16	0.3	4	2	10	48.00	1.895	16	0.4
3	1	4	26.09	3.416	16	1.3	4	1	6	35.87	2.504	16	2.8	6	2	5	48.28	1.885	16	0.2
2	1	6	26.27	3.392	16	2.1	4	2	5	35.97	2.497	16	0.3	5	3	7	48.41	1.880	16	0.2
3	2	3	27.17	3.282	16	0.4	3	1	8	36.06	2.491	16	1.3	5	1	9	48.59	1.874	16	0.2
3	0	5	27.31	3.265	8	0.9	1	0	10	36.31	2.474	8	0.8	3	1	12	48.79	1.866	16	0.3
4	0	0	27.76	3.213	4	8.1	5	2	0	37.69	2.387	8	0.2	5	4	5	48.83	1.865	16	0.2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60
70

ITE ITQ–3, Calcined

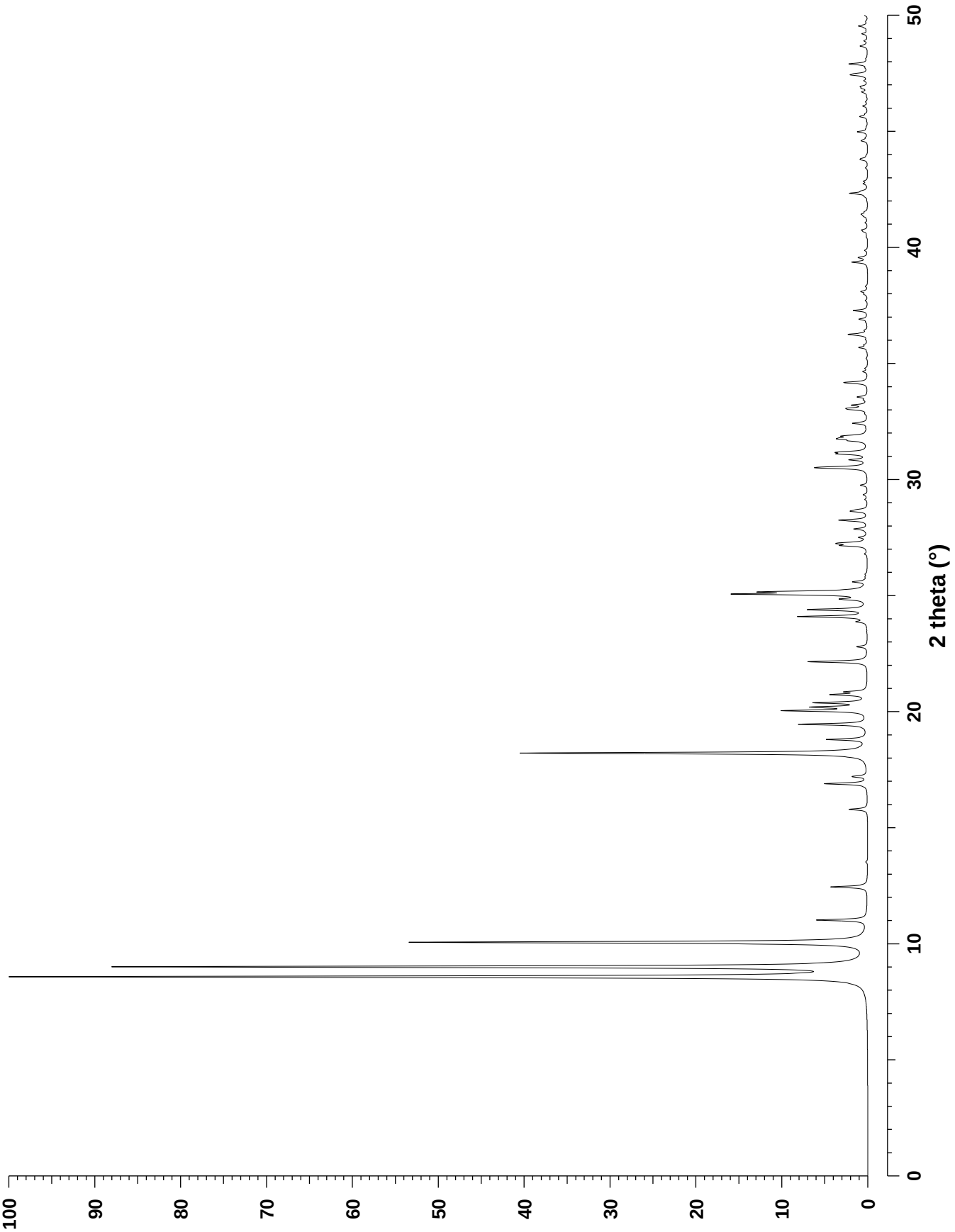
CHEMICAL COMPOSITION: $[Si_{64}O_{128}]$

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 20.622$ Å $b = 9.7242$ Å $c = 19.623$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_{wp} = 0.086$, $R_p = 0.062$

REFERENCE: M.A. Camblor, A. Corma, P. Lightfoot, L.A. Villaescusa and P.A. Wright, *Angew. Chem., Int. ed.* **36** 2659–2661 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	8.58	10.311	2	100.0	3	3	1	30.84	2.900	8	2.0	3	3	6	41.36	2.183	8	0.2
0	0	2	9.01	9.811	2	87.8	1	3	3	31.10	2.876	8	2.9	7	3	0	41.42	2.180	4	0.6
1	1	0	10.06	8.795	4	53.6	4	2	4	31.17	2.869	8	3.0	9	1	2	41.52	2.175	8	0.3
1	1	1	11.02	8.026	8	5.9	3	1	6	31.66	2.826	8	1.6	2	2	8	42.18	2.142	8	0.2
2	0	2	12.45	7.108	4	4.3	7	1	0	31.74	2.819	4	2.4	5	3	5	42.28	2.137	8	0.2
1	1	2	13.52	6.549	8	0.2	6	0	4	31.79	2.815	4	1.7	7	1	6	42.32	2.135	8	2.0
3	1	0	15.79	5.613	4	2.2	3	3	2	31.86	2.809	8	1.8	2	4	4	42.41	2.131	8	0.4
1	1	3	16.89	5.249	8	5.0	6	2	0	31.89	2.807	4	1.0	6	2	6	42.44	2.130	8	0.2
4	0	0	17.20	5.155	2	1.7	4	0	6	32.42	2.762	4	1.7	1	1	9	42.73	2.116	8	0.5
0	0	4	18.08	4.906	2	0.4	5	1	5	32.82	2.729	8	0.2	9	1	3	42.84	2.111	8	0.4
3	1	2	18.21	4.872	8	40.7	0	2	6	33.01	2.714	4	1.5	4	4	3	43.42	2.084	8	0.3
0	2	1	18.80	4.719	4	4.6	7	1	2	33.06	2.710	8	1.8	7	3	3	43.77	2.068	8	0.6
4	0	2	19.45	4.564	4	8.0	6	2	2	33.20	2.698	8	1.7	8	2	4	43.82	2.066	8	0.5
2	0	4	20.04	4.430	4	9.6	1	3	4	33.42	2.681	8	0.3	5	1	8	43.94	2.060	8	0.1
2	2	0	20.19	4.398	4	5.9	1	1	7	33.55	2.671	8	1.2	3	1	9	44.58	2.032	8	0.6
0	2	2	20.38	4.357	4	6.0	4	2	5	34.12	2.627	8	0.1	9	1	4	44.63	2.030	8	0.3
2	2	1	20.70	4.291	8	0.5	2	2	6	34.17	2.624	8	2.8	4	2	8	44.97	2.016	8	1.2
1	1	4	20.73	4.284	8	3.8	7	1	3	34.64	2.589	8	0.5	5	3	6	45.10	2.010	8	0.1
3	1	3	20.85	4.260	8	2.3	6	2	3	34.78	2.579	8	0.3	4	4	4	45.19	2.007	8	0.1
2	2	2	22.15	4.013	8	7.0	5	3	0	35.21	2.549	4	0.2	7	1	7	45.63	1.988	8	0.9
0	2	3	22.79	3.902	4	1.3	3	3	4	35.68	2.517	8	1.0	6	2	7	45.74	1.983	8	0.2
5	1	1	23.87	3.728	8	1.1	3	1	7	35.80	2.508	8	0.4	8	2	5	46.08	1.970	8	0.5
3	1	4	24.09	3.694	8	8.0	8	0	2	36.02	2.493	4	0.2	0	0	10	46.26	1.962	2	0.2
2	2	3	24.39	3.650	8	6.9	1	3	5	36.20	2.481	8	0.4	1	3	8	46.64	1.947	8	0.1
1	1	5	24.84	3.584	8	2.7	5	1	6	36.25	2.478	8	2.2	6	4	2	46.69	1.945	8	0.6
4	0	4	25.06	3.554	4	14.2	5	3	2	36.42	2.467	8	0.3	9	1	5	46.85	1.939	8	0.6
5	1	2	25.15	3.541	8	8.1	7	1	4	36.77	2.444	8	0.1	1	5	0	46.92	1.936	4	0.7
4	2	0	25.18	3.537	4	4.0	6	2	4	36.90	2.436	8	1.0	1	5	1	47.17	1.927	8	0.4
4	2	1	25.59	3.481	8	1.6	0	4	1	37.27	2.413	4	1.7	4	4	5	47.39	1.918	8	0.4
0	2	4	25.80	3.453	4	0.1	2	0	8	37.70	2.386	4	0.3	2	4	6	47.42	1.917	8	1.4
6	0	0	25.92	3.437	2	0.2	6	0	6	37.98	2.369	4	0.4	1	1	10	47.47	1.915	8	1.0
4	2	2	26.79	3.328	8	0.3	2	2	7	38.07	2.364	8	0.1	7	3	5	47.72	1.906	8	0.1
5	1	3	27.15	3.284	8	2.7	1	1	8	38.09	2.363	8	0.7	1	5	2	47.89	1.900	8	0.5
2	2	4	27.23	3.275	8	2.2	3	3	5	38.32	2.349	8	0.2	6	4	3	47.89	1.899	8	1.4
0	0	6	27.27	3.270	2	1.9	7	1	5	39.35	2.290	8	1.6	10	2	0	47.91	1.898	4	0.3
6	0	2	27.50	3.244	4	0.9	1	3	6	39.38	2.288	8	0.4	5	1	9	48.12	1.891	8	0.1
1	3	0	27.86	3.202	4	1.6	8	0	4	39.49	2.282	4	0.1	9	3	0	48.66	1.871	4	0.7
1	3	1	28.24	3.160	8	3.4	0	4	3	39.55	2.279	4	0.7	8	2	6	48.72	1.869	8	0.2
2	0	6	28.63	3.117	4	1.8	8	2	0	39.57	2.277	4	0.4	3	5	1	48.89	1.863	8	0.4
4	2	3	28.69	3.111	8	0.8	5	3	4	39.86	2.262	8	0.3	3	1	10	49.19	1.852	8	0.6
1	1	6	29.13	3.065	8	0.3	9	1	0	40.44	2.230	4	0.1	9	1	6	49.46	1.843	8	0.1
1	3	2	29.34	3.044	8	0.5	8	2	2	40.67	2.218	8	0.4	11	1	0	49.52	1.841	4	0.8
5	1	4	29.75	3.003	8	0.8	4	0	8	40.74	2.215	4	0.6	6	4	4	49.54	1.840	8	0.3
3	3	0	30.49	2.932	4	4.4	4	4	0	41.05	2.199	4	0.3	4	0	10	49.71	1.834	4	0.1
2	2	5	30.53	2.928	8	3.3	4	4	1	41.32	2.185	8	0.2	4	4	6	49.98	1.825	8	0.3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2 theta (°)

Nepheline Hydrate

CHEMICAL COMPOSITION: $|Na_3H_2O|\,[Si_3Al_3O_{12}]$

REFINED COMPOSITION: $|Na_3H_2O|\,[Si_3Al_3O_{12}]$

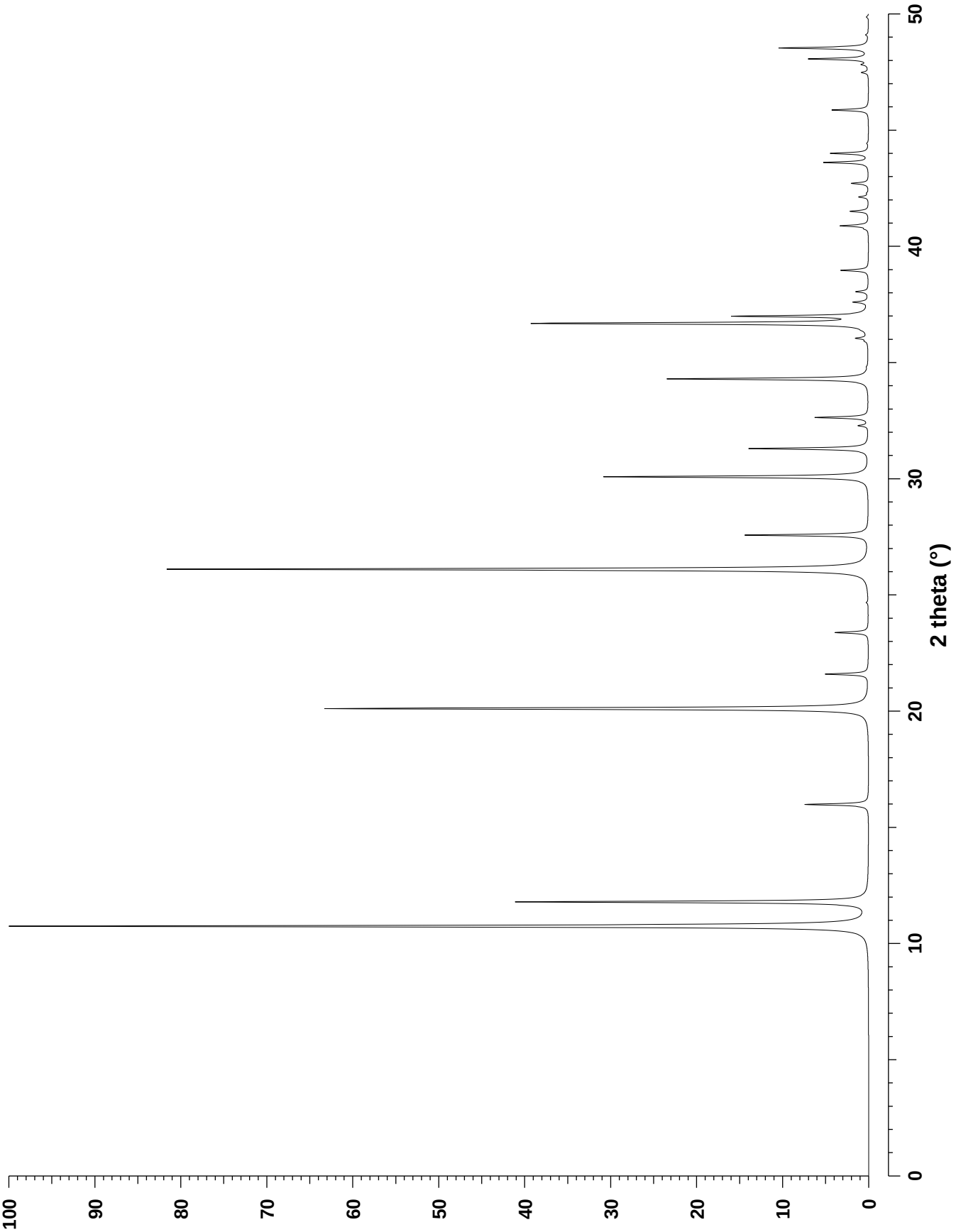
CRYSTAL DATA: $Pmc2_1$ (No. 26)
$a = 7.503$ Å $\quad b = 8.233$ Å $\quad c = 5.230$ Å
$\alpha = 90°$ $\quad \beta = 90°$ $\quad \gamma = 90°$
X-ray single crystal refinement, $R = 0.039$

REFERENCE: A. Rheinhardt, E. Hellner and H. Ahsbahs,
Fortsch. der Mineralogie **60** 175–176 (1982).

h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$
0	1	0	10.75	8.233	2	100.0	0	0	2	34.29	2.615	2	23.4	2	0	2	42.12	2.145	4	1.1
1	0	0	11.79	7.503	2	41.0	1	3	0	34.81	2.577	4	0.1	3	2	0	42.28	2.137	4	0.2
1	1	0	15.98	5.546	4	7.4	3	0	0	35.91	2.501	2	0.3	1	2	2	42.70	2.118	8	2.0
0	1	1	20.11	4.415	4	63.3	0	1	2	36.04	2.492	4	1.4	2	1	2	43.60	2.076	8	5.2
0	2	0	21.59	4.116	2	5.0	1	0	2	36.38	2.469	4	0.2	0	4	0	43.99	2.058	2	4.4
1	1	1	23.38	3.805	8	3.9	2	2	1	36.68	2.450	8	39.1	2	3	1	44.42	2.040	8	0.2
1	2	0	24.67	3.609	4	0.2	0	3	1	36.99	2.430	4	15.3	3	2	1	45.86	1.979	8	4.3
2	1	0	26.10	3.414	4	81.7	3	1	0	37.59	2.393	4	1.7	0	4	1	47.47	1.915	4	0.8
0	2	1	27.57	3.235	4	14.4	1	1	2	38.04	2.365	8	1.4	2	2	2	47.81	1.902	8	0.7
1	2	1	30.08	2.970	8	30.8	1	3	1	38.96	2.312	8	3.2	0	3	2	48.06	1.893	4	6.9
2	1	1	31.29	2.859	8	13.9	2	3	0	40.74	2.215	4	0.3	4	0	0	48.53	1.876	2	10.4
2	2	0	32.28	2.773	4	1.1	0	2	2	40.88	2.207	4	3.3	1	4	1	49.09	1.856	8	0.3
0	3	0	32.63	2.744	2	6.2	3	1	1	41.50	2.176	8	2.2	4	1	0	49.86	1.829	4	0.2

Nepheline Hydrate

JBW



KFI (Cs,K) ZK5, Dehydrated

CHEMICAL COMPOSITION: $|Cs_{9.7}K_{13}|\ [Si_{73.2}Al_{22.8}O_{192}]$

REFINED COMPOSITION: $|Cs_{9.72}K_{12.88}|\ [Si_{72.96}Al_{23.04}O_{192}]$

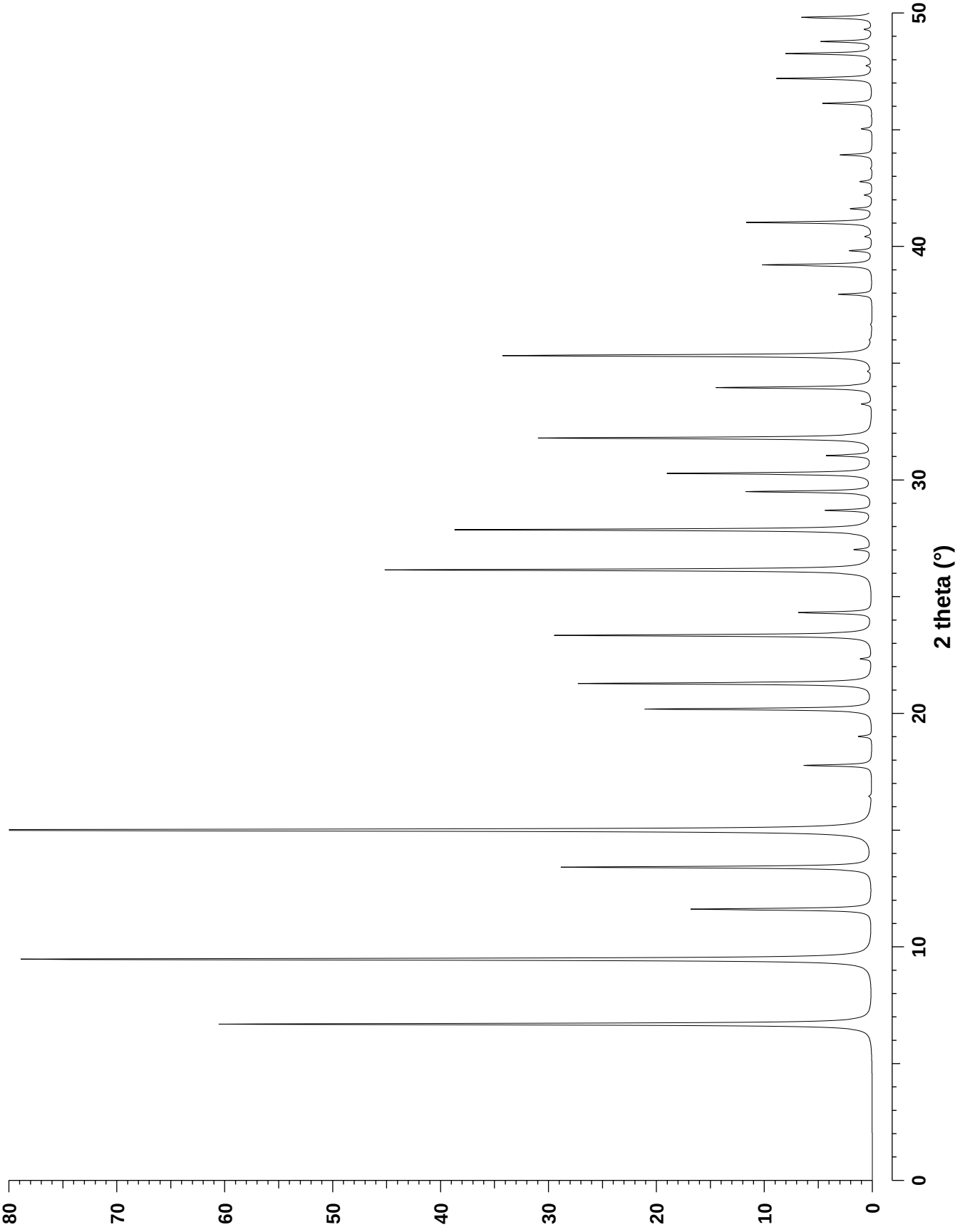
CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 18.671$ Å $\quad b = 18.671$ Å $\quad c = 18.671$ Å
$\alpha = 90°$ $\quad \beta = 90°$ $\quad \gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.09$

REFERENCE: J. B. Parise, R. D. Shannon, E. Prince and D. E. Cox,
Z. Kristallogr. **165** 175–190 (1983).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.69	13.202	12	60.6	6	2	0	30.27	2.952	24	18.9	7	5	0	41.61	2.170	24	0.2
2	0	0	9.47	9.335	6	78.9	5	4	1	31.04	2.881	48	4.1	6	6	2	42.19	2.142	24	0.7
2	1	1	11.61	7.622	24	16.8	6	2	2	31.79	2.815	24	30.9	7	5	2	42.77	2.114	48	1.1
2	2	0	13.41	6.601	12	28.8	4	4	4	33.24	2.695	8	0.9	8	4	0	43.34	2.087	24	0.1
3	1	0	15.00	5.904	24	100.0	7	1	0	33.95	2.640	24	0.2	8	3	3	43.91	2.062	24	0.3
2	2	2	16.45	5.390	8	0.2	5	5	0	33.95	2.640	12	6.2	9	1	0	43.91	2.062	24	2.6
3	2	1	17.77	4.990	48	6.3	5	4	3	33.95	2.640	48	8.0	7	6	1	45.03	2.013	48	0.1
4	0	0	19.01	4.668	6	1.3	6	4	0	34.64	2.589	24	0.3	9	2	1	45.03	2.013	48	0.6
4	1	1	20.18	4.401	24	20.6	6	3	3	35.32	2.541	24	24.1	6	5	5	45.03	2.013	24	0.3
3	3	0	20.18	4.401	12	0.5	5	5	2	35.32	2.541	24	10.1	8	5	1	46.12	1.968	48	3.3
4	2	0	21.28	4.175	24	27.2	6	4	2	36.00	2.495	48	0.2	7	5	4	46.12	1.968	48	0.2
3	3	2	22.33	3.981	24	1.0	7	3	0	36.65	2.452	24	0.1	9	3	0	46.12	1.968	24	1.1
4	2	2	23.34	3.811	24	29.5	6	5	1	37.94	2.371	48	0.1	7	6	3	47.19	1.926	48	8.9
4	3	1	24.31	3.662	48	1.9	7	3	2	37.94	2.371	48	3.0	8	4	4	47.73	1.906	24	0.5
5	1	0	24.31	3.662	24	4.9	7	4	1	39.20	2.298	48	0.4	8	5	3	48.25	1.886	48	5.2
5	2	1	26.14	3.409	48	45.1	8	1	1	39.20	2.298	24	6.2	7	7	0	48.25	1.886	12	2.8
4	4	0	27.01	3.301	12	1.5	5	5	4	39.20	2.298	24	3.6	10	0	0	48.77	1.867	6	4.5
4	3	3	27.86	3.202	24	15.5	8	2	0	39.81	2.264	24	0.3	8	6	0	48.77	1.867	24	0.2
5	3	0	27.86	3.202	24	23.1	6	4	4	39.81	2.264	24	1.8	10	1	1	49.29	1.849	24	0.2
6	0	0	28.69	3.112	6	4.1	6	5	3	40.42	2.232	48	0.6	7	7	2	49.29	1.849	24	0.5
4	4	2	28.69	3.112	24	0.1	8	2	2	41.02	2.200	24	2.5	10	2	0	49.80	1.831	24	0.8
6	1	1	29.49	3.029	24	4.4	6	6	0	41.02	2.200	12	9.2	8	6	2	49.80	1.831	48	5.8
5	3	2	29.49	3.029	48	7.2	7	4	3	41.61	2.170	48	1.8							

(Cs,K) ZK5, Dehydrated

KFI



LAU Laumontite

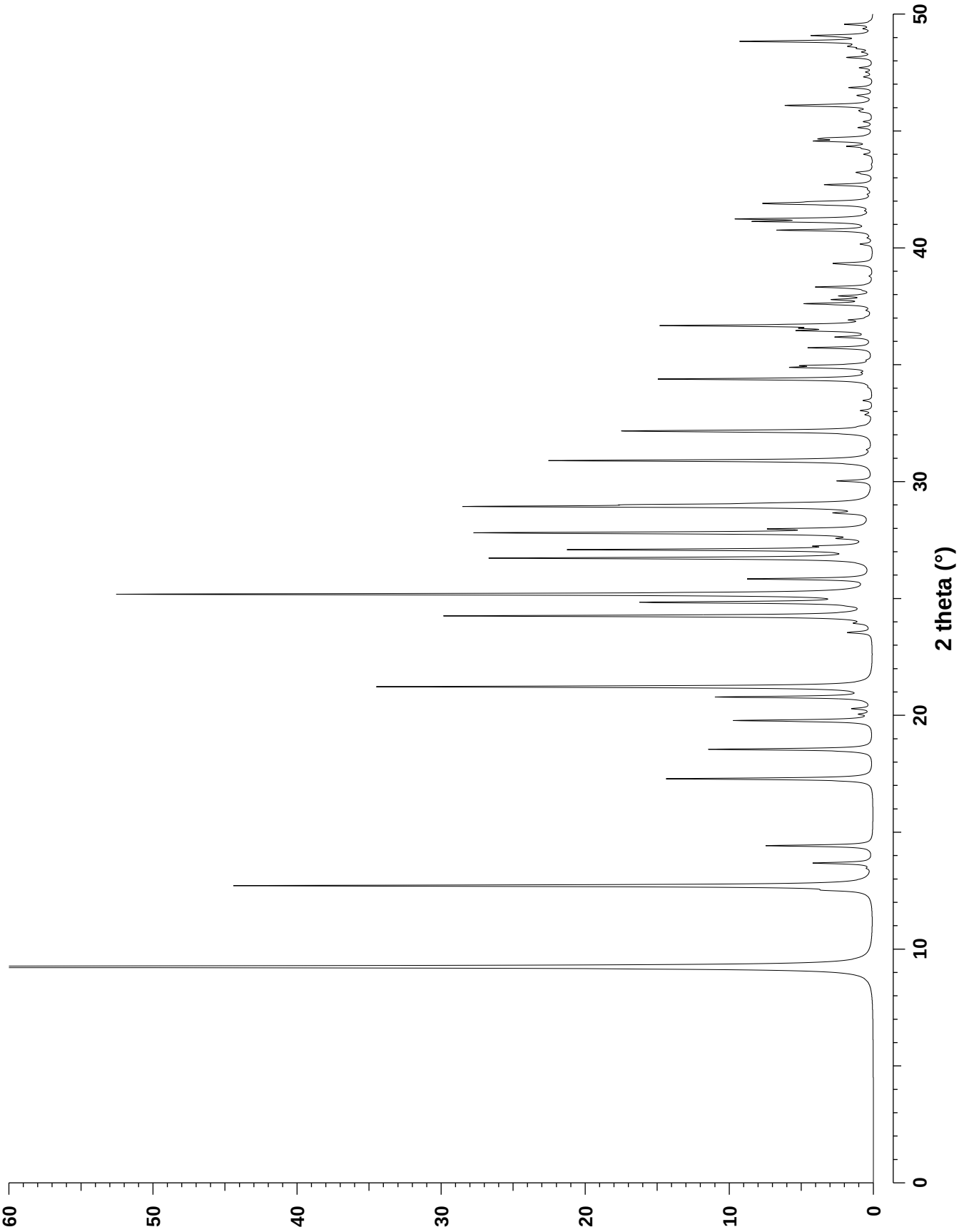
CHEMICAL COMPOSITION: $|Ca_4(H_2O)_{18}|\ [Si_{16}Al_8O_{48}]$
Nasik, India

REFINED COMPOSITION: $|Ca_4(H_2O)_{18}|\ [Si_{16}Al_8O_{48}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.8538$ Å $b = 13.1695$ Å $c = 7.5421$ Å
$\alpha = 90°$ $\beta = 110.323°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.115$, $R_p = 0.090$, $R_{F^2} = 0.046$

REFERENCE: G. Artioli and K. Ståhl,
Zeolites **13** 249–255 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.24	9.570	4	100.0	-4	2	2	32.16	2.783	4	15.2	-1	3	3	41.97	2.153	4	2.8
0	0	1	12.52	7.073	2	1.7	4	0	1	32.36	2.766	2	0.3	4	0	2	42.28	2.138	2	0.2
2	0	0	12.71	6.965	2	44.3	5	1	0	32.86	2.726	4	0.5	2	4	2	42.50	2.127	4	0.2
0	2	0	13.45	6.585	2	0.2	-3	3	2	33.03	2.712	4	0.8	4	4	1	42.69	2.118	4	3.3
-1	1	1	13.68	6.474	4	4.1	3	3	1	33.46	2.678	4	0.6	0	6	1	43.15	2.096	4	0.6
-2	0	1	14.42	6.142	2	7.4	-5	1	2	34.03	2.635	4	0.2	2	6	0	43.22	2.093	4	0.2
1	1	1	17.28	5.132	4	14.4	2	4	1	34.38	2.609	4	14.9	-3	5	2	43.22	2.093	4	0.8
0	2	1	18.41	4.819	4	0.1	1	5	0	34.66	2.588	4	0.3	5	3	1	43.99	2.059	4	0.6
2	2	0	18.54	4.785	4	11.4	1	3	2	34.88	2.572	4	4.9	-6	0	3	44.24	2.047	2	0.5
-2	2	1	19.77	4.492	4	9.6	2	2	2	34.96	2.566	4	4.0	-7	1	2	44.34	2.043	4	1.6
-3	1	1	20.05	4.428	4	0.7	4	2	1	35.19	2.551	4	0.2	4	2	2	44.56	2.033	4	3.5
3	1	0	20.28	4.379	4	1.3	-2	0	3	35.72	2.514	2	4.5	2	0	3	44.65	2.029	2	2.4
2	0	1	20.78	4.275	2	10.7	-1	5	1	36.18	2.483	4	2.4	1	5	2	44.70	2.027	4	2.0
1	3	0	21.22	4.187	4	34.4	-2	4	2	36.45	2.465	4	4.4	6	0	1	45.14	2.009	2	1.0
-1	3	1	23.54	3.780	4	1.6	-5	3	1	36.55	2.458	4	3.1	-2	4	3	45.39	1.998	4	0.6
-2	0	2	23.94	3.717	2	0.8	-4	4	1	36.67	2.451	4	14.3	-5	3	3	45.81	1.981	4	0.6
-4	0	1	24.25	3.670	2	29.6	-3	1	3	36.91	2.435	4	1.2	-6	4	1	45.87	1.978	4	0.6
-1	1	2	24.67	3.609	4	0.4	-1	1	3	37.03	2.428	4	0.2	-5	5	1	46.08	1.970	4	5.6
2	2	1	24.83	3.586	4	15.4	0	4	2	37.32	2.410	4	0.3	1	3	3	46.12	1.968	4	0.8
0	0	2	25.18	3.536	2	52.2	3	1	2	37.56	2.394	4	0.2	7	1	0	46.13	1.968	4	0.2
1	3	1	25.83	3.449	4	8.4	4	4	0	37.60	2.392	4	4.5	-6	2	3	46.44	1.955	4	0.2
-3	1	2	26.72	3.337	4	26.3	1	5	1	37.78	2.381	4	2.5	2	6	1	46.51	1.953	4	1.0
0	4	0	27.08	3.292	2	20.6	-4	0	3	37.94	2.372	2	2.1	2	2	3	46.85	1.939	4	1.7
3	1	1	27.24	3.274	4	2.6	0	0	3	38.17	2.358	2	0.3	6	2	1	47.31	1.921	4	0.6
-2	2	2	27.56	3.237	4	1.5	5	3	0	38.26	2.352	4	0.4	5	5	0	47.51	1.914	4	0.4
-3	3	1	27.80	3.209	4	26.6	-2	2	3	38.32	2.349	4	3.8	-7	3	1	47.70	1.907	4	0.9
-4	2	1	27.83	3.206	4	1.0	6	0	0	38.79	2.322	2	0.2	-2	6	2	48.14	1.890	4	1.8
3	3	0	27.97	3.190	4	5.7	-5	3	2	39.29	2.293	4	1.2	-5	5	2	48.37	1.882	4	0.6
0	2	2	28.65	3.115	4	2.0	3	5	0	39.33	2.291	4	2.1	-2	0	4	48.52	1.876	2	0.7
1	1	2	28.93	3.086	4	26.0	-4	4	2	40.15	2.246	4	0.8	5	1	2	48.61	1.873	4	1.1
4	2	0	29.01	3.078	4	11.4	-4	2	3	40.42	2.231	4	0.3	-7	3	2	48.67	1.871	4	0.5
-4	0	2	29.08	3.071	2	2.4	-6	2	2	40.75	2.214	4	6.5	-3	1	4	48.82	1.865	4	4.5
2	4	0	30.02	2.977	4	2.4	0	6	0	41.12	2.195	2	7.3	0	6	2	48.83	1.865	4	4.8
-2	4	1	30.81	2.902	4	0.4	6	2	0	41.23	2.189	4	8.6	-4	0	4	49.01	1.859	2	0.6
-5	1	1	30.89	2.895	4	22.4	1	1	3	41.58	2.172	4	0.2	-7	1	3	49.07	1.856	4	3.8
-1	3	2	31.36	2.852	4	0.2	-3	3	3	41.86	2.158	4	4.0	-8	0	1	49.37	1.846	2	0.5
2	0	2	32.12	2.787	2	4.6	-1	5	2	41.90	2.156	4	4.8	3	1	3	49.55	1.839	4	1.9


0
10
20
30
40
50
2 theta (°)
60
50
40
30
20
10
0

Leonhardite

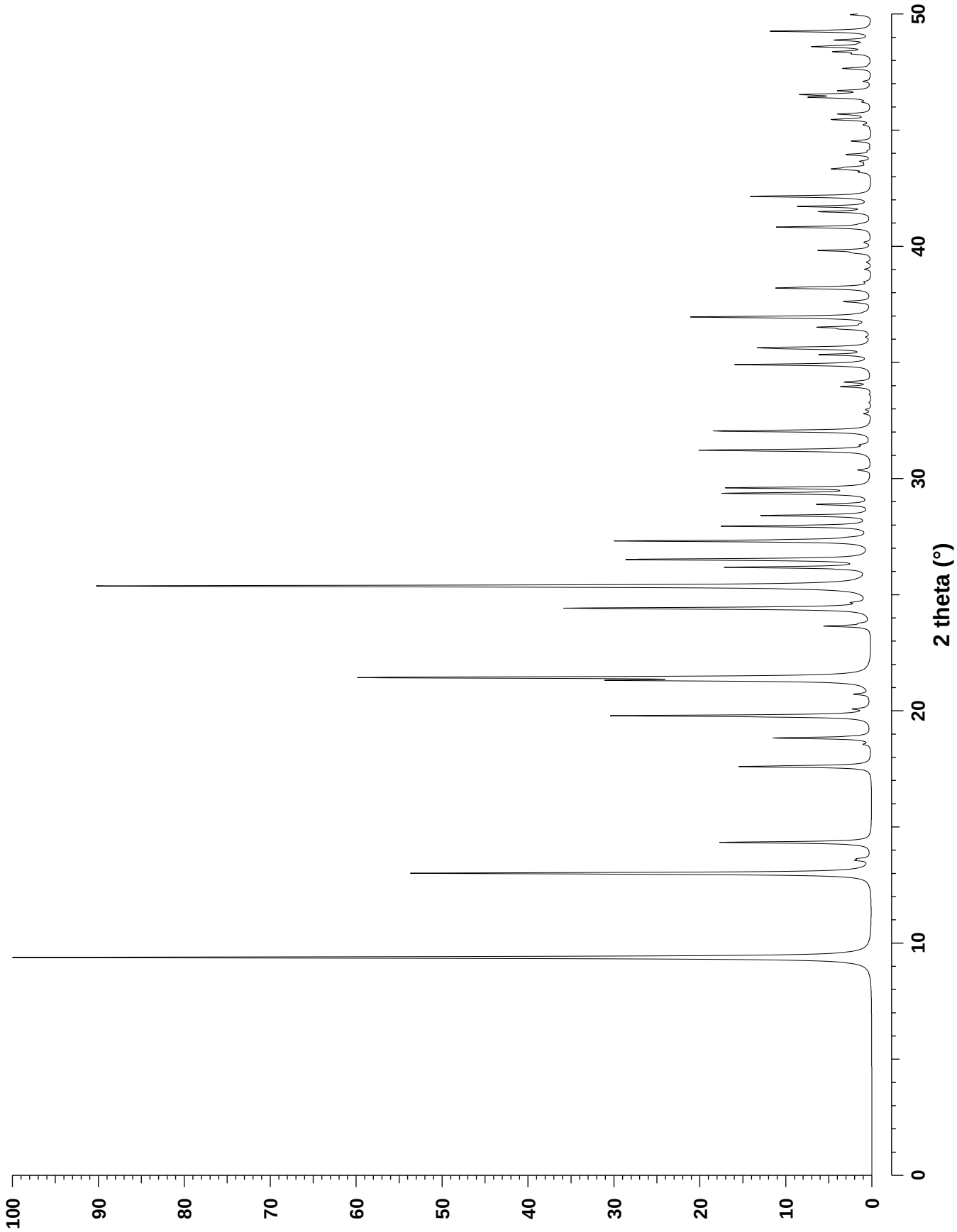
CHEMICAL COMPOSITION: $|K_{0.1}Na_{0.30}Ca_{3.60}(H_2O)_{25.2}|$ $[Si_{16.40}Al_{7.60}O_{48}]$
Teigahorn, Berufjördur, Iceland

REFINED COMPOSITION: $|Ca_4H_{25.184}O_{13.36}|$ $[Si_{16.4}Al_{7.6}O_{48}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.690$ Å $b = 13.061$ Å $c = 7.574$ Å
$\alpha = 90°$ $\beta = 112.01°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{F^2} = 0.084$; At T = 15K.

REFERENCE: G. Artioli, J. V. Smith and Å. Kvick,
Zeolites **9** 377–391 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.38	9.427	4	100.0	5	1	0	33.61	2.667	4	0.2	3	3	2	43.34	2.088	4	1.7
2	0	0	13.00	6.810	2	53.7	-5	1	2	33.95	2.641	4	3.5	4	0	2	43.40	2.085	2	2.0
0	2	0	13.56	6.530	2	1.4	3	3	1	34.15	2.625	4	3.0	0	6	1	43.53	2.079	4	0.2
-1	1	1	13.63	6.496	4	1.2	2	4	1	34.90	2.571	4	15.7	4	4	1	43.56	2.078	4	0.4
-2	0	1	14.33	6.182	2	17.7	1	5	0	34.97	2.565	4	0.6	2	6	0	43.65	2.073	4	1.1
1	1	1	17.60	5.040	4	15.5	1	3	2	35.33	2.540	4	5.7	-6	0	3	43.94	2.061	2	2.8
0	2	1	18.55	4.782	4	0.7	-2	0	3	35.58	2.523	2	6.2	-2	6	1	44.10	2.053	4	0.3
2	2	0	18.83	4.713	4	11.4	2	2	2	35.63	2.520	4	10.7	3	5	1	44.27	2.046	4	0.1
-2	2	1	19.78	4.489	4	30.3	4	2	1	36.08	2.490	4	0.5	-7	1	2	44.52	2.035	4	2.4
-3	1	1	20.08	4.422	4	1.7	-1	5	1	36.43	2.466	4	2.6	5	3	1	45.06	2.012	4	0.1
3	1	0	20.71	4.288	4	1.8	-2	4	2	36.51	2.461	4	5.6	1	5	2	45.22	2.005	4	0.8
2	0	1	21.31	4.170	2	25.3	-3	1	3	36.65	2.452	4	0.6	-2	4	3	45.43	1.997	4	0.6
1	3	0	21.43	4.147	4	57.3	-5	3	1	36.91	2.435	4	2.7	2	0	3	45.45	1.996	2	4.1
-1	3	1	23.64	3.764	4	5.3	-4	4	1	36.95	2.433	4	19.6	-5	3	3	45.58	1.990	4	0.3
-2	0	2	23.76	3.744	2	0.9	-1	1	3	37.10	2.423	4	0.2	4	2	2	45.68	1.986	4	3.8
-4	0	1	24.41	3.647	2	35.6	-4	0	3	37.60	2.392	2	1.9	-6	2	3	46.20	1.965	4	0.7
-1	1	2	24.66	3.611	4	1.3	0	4	2	37.62	2.391	4	1.4	-6	4	1	46.40	1.957	4	3.3
2	2	1	25.34	3.514	4	20.4	4	4	0	38.19	2.357	4	5.0	6	0	1	46.42	1.956	2	3.6
0	0	2	25.37	3.511	2	77.0	1	5	1	38.19	2.357	4	4.7	-5	5	1	46.52	1.952	4	7.4
4	0	0	26.17	3.405	2	1.3	-2	2	3	38.24	2.354	4	3.9	1	3	3	46.69	1.946	4	3.5
1	3	1	26.17	3.405	4	15.2	3	1	2	38.46	2.341	4	0.5	-4	4	3	47.09	1.930	4	0.1
-3	1	2	26.51	3.362	4	28.2	5	3	0	39.00	2.309	4	0.8	2	6	1	47.09	1.930	4	0.8
0	4	0	27.31	3.265	2	29.7	-5	3	2	39.30	2.292	4	0.5	2	2	3	47.65	1.908	4	3.3
-2	2	2	27.46	3.248	4	0.9	6	0	0	39.71	2.270	2	1.6	0	4	3	47.81	1.902	4	0.1
-3	3	1	27.94	3.194	4	16.2	3	5	0	39.81	2.264	4	6.0	5	5	0	48.27	1.885	4	1.6
3	1	1	27.96	3.192	4	1.3	-4	2	3	40.14	2.246	4	0.3	-7	3	1	48.36	1.882	4	0.9
3	3	0	28.40	3.142	4	12.7	-4	4	2	40.17	2.245	4	0.5	-2	6	2	48.37	1.882	4	3.2
0	2	2	28.87	3.092	4	2.6	-6	2	2	40.82	2.211	4	11.0	-5	5	2	48.52	1.876	4	0.5
-4	0	2	28.89	3.091	2	3.9	-5	1	3	40.92	2.205	4	0.1	-3	1	4	48.59	1.874	4	6.0
1	1	2	29.36	3.042	4	16.9	0	2	3	40.96	2.203	4	0.6	6	2	1	48.59	1.874	4	0.3
4	2	0	29.59	3.019	4	16.5	0	6	0	41.48	2.177	2	5.9	-4	0	4	48.64	1.872	2	0.5
2	4	0	30.36	2.944	4	1.5	-3	3	3	41.71	2.165	4	8.3	-4	6	1	48.72	1.869	4	0.6
-5	1	1	31.21	2.866	4	20.0	-1	3	3	42.11	2.146	4	0.5	6	4	0	48.86	1.864	4	0.6
-1	3	2	31.45	2.844	4	0.8	1	1	3	42.12	2.145	4	1.2	-7	1	3	48.87	1.863	4	3.4
-4	2	2	32.04	2.794	4	18.4	-1	5	2	42.13	2.145	4	3.5	-7	3	2	48.91	1.862	4	0.2
2	0	2	32.79	2.731	2	0.8	6	2	0	42.15	2.144	4	10.1	0	6	2	49.25	1.850	4	11.5
-3	3	2	32.96	2.718	4	0.6	2	4	2	43.18	2.095	4	1.1	1	7	0	49.29	1.849	4	0.4
4	0	1	33.27	2.693	2	0.2	-3	5	2	43.31	2.089	4	3.0	5	1	2	49.96	1.825	4	2.5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2 theta (°)
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90
80
70
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20
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0

LAU Cobalt Gallophosphate

CHEMICAL COMPOSITION: $|(C_5H_5NH)_8|\ [Co_8Ga_{16}P_{24}O_{96}]$
C_5H_5NH = pyridinium cation

REFINED COMPOSITION: $|(C_5H_6N)_8|\ [Co_8Ga_{16}P_{24}O_{96}]$

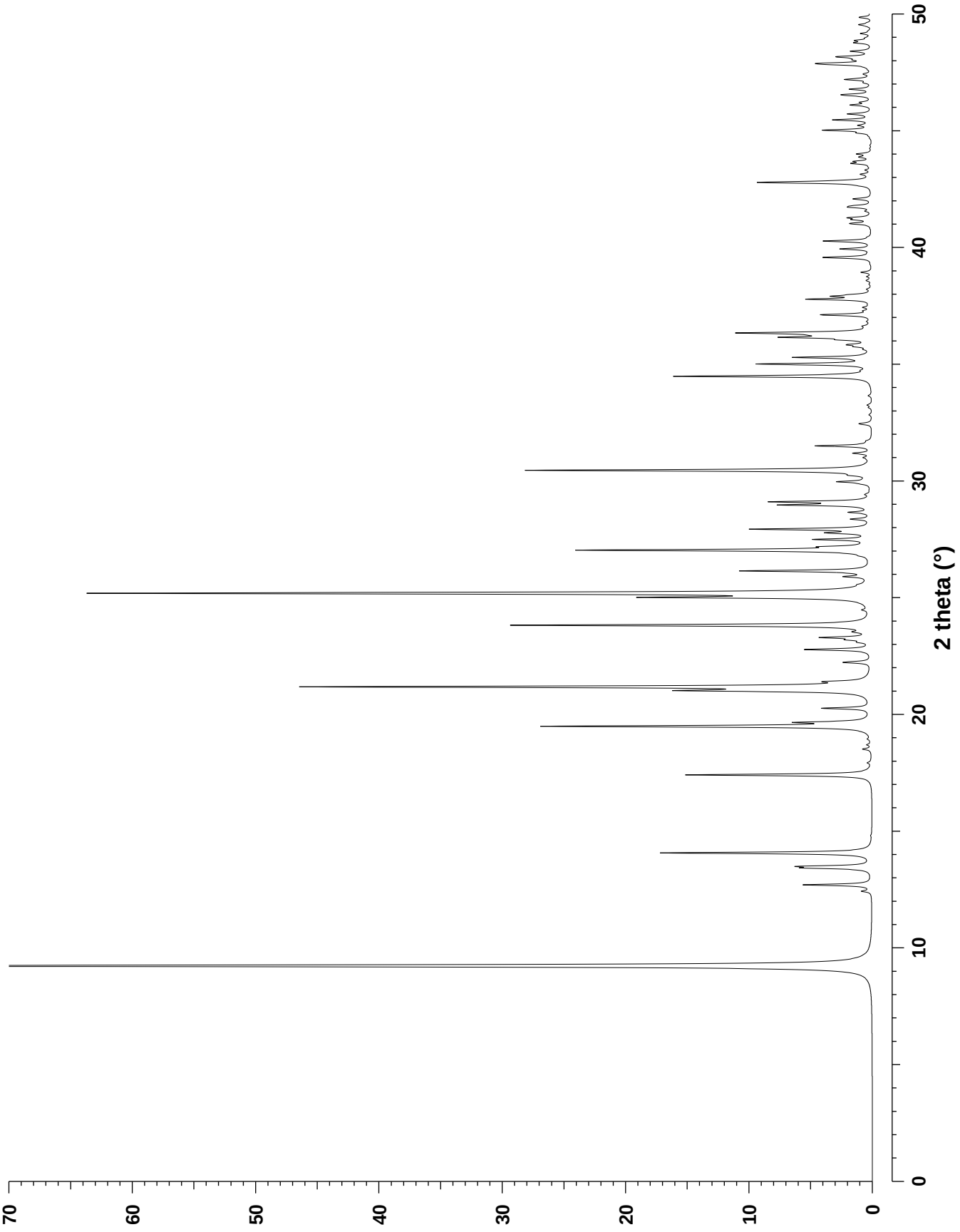
CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 15.058$ Å $b = 13.197$ Å $c = 15.273$ Å
$\alpha = 90°$ $\beta = 112.20°$ $\gamma = 90°$

REFERENCE: A. M. Chippindale and R. I. Walton,
J. Chem. Soc., Chem. Commun. 2453–2454 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.23	9.584	4	100.0	-4	2	4	31.50	2.840	4	4.6	-7	1	2	42.82	2.112	4	0.8
1	1	1	12.43	7.121	4	0.7	2	0	4	32.44	2.760	2	1.0	-2	6	1	42.86	2.110	4	0.7
2	0	0	12.70	6.971	2	5.6	2	4	2	34.48	2.601	4	15.5	2	6	0	43.13	2.098	4	0.6
0	2	0	13.42	6.599	2	4.5	0	2	5	34.50	2.599	4	0.7	-1	1	7	43.31	2.089	4	0.4
-1	1	2	13.49	6.562	4	5.1	1	3	4	35.00	2.564	4	9.2	-2	6	2	43.59	2.076	4	1.5
-2	0	2	14.07	6.293	2	17.2	2	2	4	35.25	2.546	4	0.4	3	5	2	43.68	2.072	4	1.2
1	1	2	17.41	5.093	4	15.1	-2	0	6	35.29	2.543	2	6.0	3	1	5	43.85	2.065	4	0.4
2	2	0	18.51	4.792	4	0.7	1	5	1	35.63	2.520	4	0.4	-2	2	7	43.88	2.063	4	0.6
-2	2	2	19.49	4.554	4	26.6	5	1	1	35.75	2.512	4	0.9	-7	1	1	43.99	2.058	4	0.5
-3	1	2	19.66	4.515	4	5.1	-6	0	2	35.83	2.506	2	1.6	6	2	1	44.00	2.058	4	0.6
3	1	0	20.26	4.383	4	3.9	-1	5	2	36.04	2.492	4	1.8	-5	3	6	44.90	2.019	4	0.7
2	0	2	21.01	4.229	2	12.6	-2	4	4	36.13	2.486	4	0.8	-2	4	6	45.01	2.014	4	0.9
2	2	1	21.06	4.218	4	3.0	-5	3	2	36.15	2.485	4	5.8	2	0	6	45.02	2.014	2	1.6
1	3	0	21.18	4.195	4	45.4	-1	3	5	36.23	2.479	4	1.8	4	2	4	45.02	2.014	4	1.5
-1	3	1	21.40	4.153	4	2.4	-3	1	6	36.28	2.476	4	1.4	-7	1	5	45.22	2.005	4	0.9
-3	1	3	22.23	3.998	4	2.2	-4	4	2	36.33	2.473	4	8.2	6	0	2	45.46	1.995	2	2.8
-2	2	3	22.77	3.906	4	4.4	-5	1	5	36.33	2.473	4	1.1	-5	5	2	45.71	1.985	4	1.8
1	3	1	22.79	3.903	4	1.2	-4	4	1	36.37	2.470	4	1.2	7	1	0	46.09	1.969	4	1.2
1	1	3	23.09	3.852	4	0.7	-5	3	1	36.63	2.453	4	0.5	-5	5	1	46.10	1.969	4	0.5
0	2	3	23.19	3.836	4	1.4	-4	0	6	37.11	2.423	2	4.1	-6	4	1	46.21	1.965	4	0.8
3	1	1	23.29	3.820	4	3.8	0	4	4	37.28	2.412	4	0.5	-4	4	6	46.50	1.953	4	1.2
-2	0	4	23.53	3.782	2	0.9	-6	0	4	37.43	2.403	2	0.4	2	6	2	46.54	1.951	4	1.7
-4	0	2	23.82	3.736	2	29.2	1	5	2	37.78	2.381	4	5.1	-6	4	4	46.77	1.942	4	0.8
-1	1	4	24.47	3.638	4	0.4	-2	2	6	37.91	2.373	4	2.4	4	4	3	46.78	1.942	4	0.9
2	2	2	25.01	3.560	4	16.1	3	1	4	37.97	2.370	4	1.0	2	2	6	47.19	1.926	4	1.9
0	0	4	25.19	3.535	2	62.9	-5	3	4	38.58	2.333	4	0.4	-7	3	2	47.24	1.924	4	0.4
1	3	2	25.90	3.440	4	1.8	-3	5	2	38.93	2.313	4	0.8	5	5	0	47.43	1.917	4	0.4
-3	1	4	26.14	3.409	4	10.5	5	1	2	39.56	2.278	4	2.0	-7	3	4	47.82	1.902	4	1.4
0	4	0	27.03	3.299	2	23.7	-4	4	4	39.58	2.277	4	2.1	-2	6	4	47.84	1.901	4	1.2
-2	2	4	27.18	3.281	4	2.8	-6	2	4	39.93	2.258	4	1.9	-7	1	6	47.86	1.900	4	0.4
-4	2	1	27.48	3.245	4	0.4	4	2	3	39.94	2.257	4	0.7	6	4	0	47.88	1.900	4	2.9
-3	3	2	27.49	3.245	4	4.0	-5	1	6	40.27	2.239	4	3.7	-4	6	1	48.03	1.894	4	0.8
0	4	1	27.77	3.213	4	3.1	3	5	1	41.00	2.201	4	1.0	-2	0	8	48.09	1.892	2	0.6
3	3	0	27.93	3.195	4	9.6	0	6	0	41.03	2.199	2	1.0	-3	1	8	48.16	1.889	4	2.5
-4	0	4	28.36	3.147	2	1.6	6	2	0	41.19	2.192	4	1.3	1	1	7	48.40	1.881	4	1.0
0	2	4	28.65	3.116	4	1.7	-3	3	6	41.27	2.187	4	1.7	5	3	3	48.40	1.880	4	0.6
4	2	0	28.97	3.082	4	7.0	0	6	1	41.55	2.173	4	0.4	0	6	4	48.76	1.868	4	1.0
1	1	4	29.10	3.068	4	7.8	-1	5	4	41.72	2.165	4	1.4	-1	7	1	48.85	1.864	4	0.7
-3	3	3	29.42	3.036	4	0.4	-1	3	6	41.77	2.162	4	0.9	-8	0	2	48.87	1.864	2	0.5
0	4	2	29.88	2.990	4	0.5	1	1	6	41.78	2.162	4	0.4	4	6	0	48.97	1.860	4	0.4
2	4	0	29.96	2.982	4	2.6	0	4	5	42.08	2.147	4	1.3	5	1	4	49.15	1.854	4	0.4
3	3	1	30.24	2.956	4	0.9	-4	4	5	42.65	2.120	4	0.4	-5	3	7	49.16	1.853	4	0.5
-5	1	2	30.45	2.936	4	28.1	4	0	4	42.76	2.114	2	2.4	2	6	3	49.53	1.840	4	0.6
-5	1	1	31.00	2.884	4	0.5	-3	5	4	42.78	2.114	4	5.5	1	7	1	49.54	1.840	4	0.4
-1	3	4	31.18	2.869	4	1.4	3	3	4	42.80	2.113	4	1.6	-1	7	2	49.85	1.829	4	1.0

Cobalt Gallophosphate

LAU



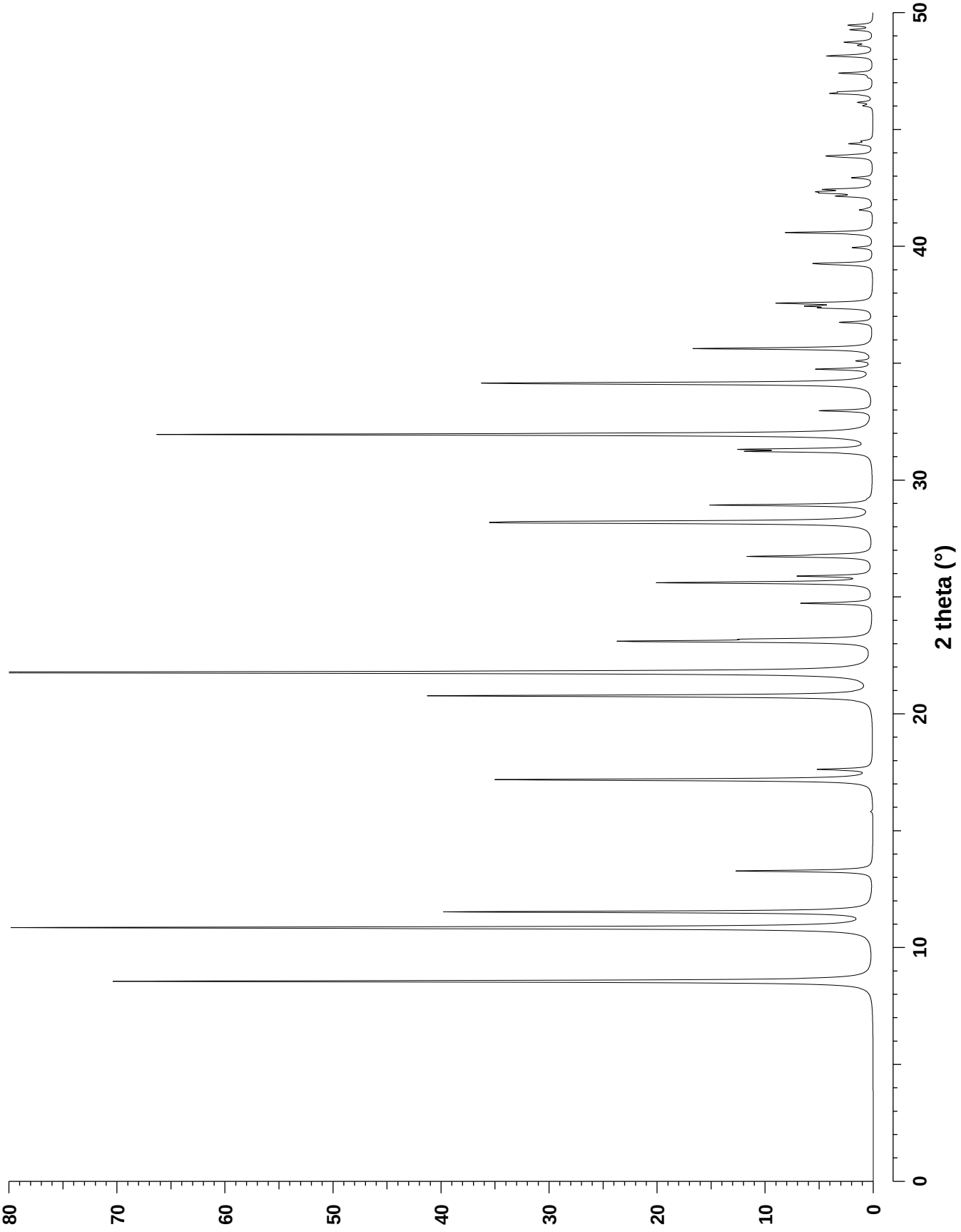
CHEMICAL COMPOSITION: $|Ca_{8.19}Na_{1.95}K_{0.6}(H_2O)_{50}|\ [Si_{35}Al_{19}O_{108}]$
Nurri, Nuoro, Sardinia, Italy

REFINED COMPOSITION: $|Ca_{7.8}Na_{2.16}K_{0.72}(H_2O)_{46.08}|\ [Si_{35.1}Al_{18.9}O_{108}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.338$ Å $b = 13.338$ Å $c = 23.014$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: S. Merlino, E. Galli and A. Alberti,
Tschermaks Mineral. Petrogr. Mitt. **22** 117–129 (1975).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	8.56	10.324	6	73.2	0	4	2	31.95	2.801	6	68.3	0	3	9	42.43	2.130	6	3.2
0	1	2	10.85	8.152	6	83.0	1	3	4	31.97	2.799	12	0.8	3	0	9	42.43	2.130	6	0.9
0	0	3	11.53	7.671	2	41.1	3	0	6	32.96	2.717	6	2.5	1	4	6	42.93	2.107	12	0.9
1	1	0	13.28	6.669	6	13.2	0	3	6	32.96	2.717	6	2.6	4	1	6	42.93	2.107	12	1.1
0	2	1	15.82	5.602	6	0.2	3	1	5	34.10	2.629	12	7.6	5	1	1	43.81	2.066	12	1.5
2	0	2	17.18	5.162	6	36.4	2	1	7	34.14	2.626	12	33.9	5	0	5	43.85	2.065	6	2.0
1	1	3	17.62	5.033	12	5.1	2	3	2	34.74	2.582	12	5.3	3	2	7	43.88	2.063	12	2.5
2	1	1	20.71	4.289	12	4.0	0	0	9	35.09	2.557	2	1.4	1	5	2	44.37	2.042	12	0.6
0	1	5	20.77	4.276	6	41.6	4	1	0	35.62	2.521	12	17.0	2	4	4	44.38	2.041	12	1.6
1	2	2	21.77	4.082	12	100.0	2	2	6	35.68	2.517	12	1.0	0	4	8	44.45	2.038	6	0.2
0	2	4	21.80	4.076	6	6.3	0	4	5	36.74	2.446	6	3.2	2	1	10	44.50	2.036	12	0.9
3	0	0	23.10	3.850	6	23.1	3	2	4	37.36	2.407	12	4.0	4	2	5	46.01	1.972	12	0.9
0	0	6	23.19	3.836	2	8.9	1	2	8	37.44	2.402	12	5.0	2	0	11	46.15	1.967	6	1.4
2	0	5	24.73	3.600	6	6.9	1	4	3	37.56	2.395	12	1.7	5	1	4	46.53	1.952	12	3.6
2	1	4	25.61	3.478	12	20.7	4	1	3	37.56	2.395	12	7.0	2	3	8	46.60	1.949	12	2.5
3	0	3	25.89	3.441	6	4.9	0	5	1	39.19	2.299	6	0.6	6	0	0	47.21	1.925	6	0.3
0	3	3	25.89	3.441	6	1.9	2	3	5	39.23	2.297	12	1.8	3	3	6	47.26	1.923	12	0.2
2	2	0	26.73	3.334	6	11.4	1	3	7	39.26	2.294	12	4.5	0	0	12	47.40	1.918	2	3.3
1	1	6	26.81	3.325	12	3.3	1	0	10	39.94	2.257	6	2.0	0	5	7	48.14	1.890	6	4.4
1	3	1	28.12	3.173	12	0.2	3	3	0	40.58	2.223	6	8.4	1	2	11	48.23	1.887	12	0.3
1	2	5	28.17	3.168	12	26.8	2	4	1	41.55	2.173	12	1.2	3	4	2	48.59	1.874	12	1.2
1	0	7	28.22	3.162	6	23.4	4	0	7	41.62	2.170	6	0.3	1	3	10	48.72	1.869	12	2.5
3	1	2	28.93	3.086	12	15.6	4	2	2	42.13	2.145	12	1.1	0	6	3	48.77	1.867	6	0.1
2	2	3	29.20	3.058	12	0.1	0	5	4	42.15	2.144	6	2.1	6	0	3	48.77	1.867	6	0.3
4	0	1	31.22	2.865	6	10.4	0	2	10	42.27	2.138	6	3.5	5	2	0	49.26	1.850	12	2.2
0	2	7	31.31	2.857	6	11.1	3	3	3	42.33	2.135	12	3.8	1	1	12	49.45	1.843	12	2.4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2 theta (°)
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80

LEV 1-aminoadamantane NU-3

CHEMICAL COMPOSITION: $|(C_{10}H_{15}NH_2)_6|\ [Si_{54}O_{108}]$
$C_{10}H_{15}NH_2$ = 1-aminoadamantane

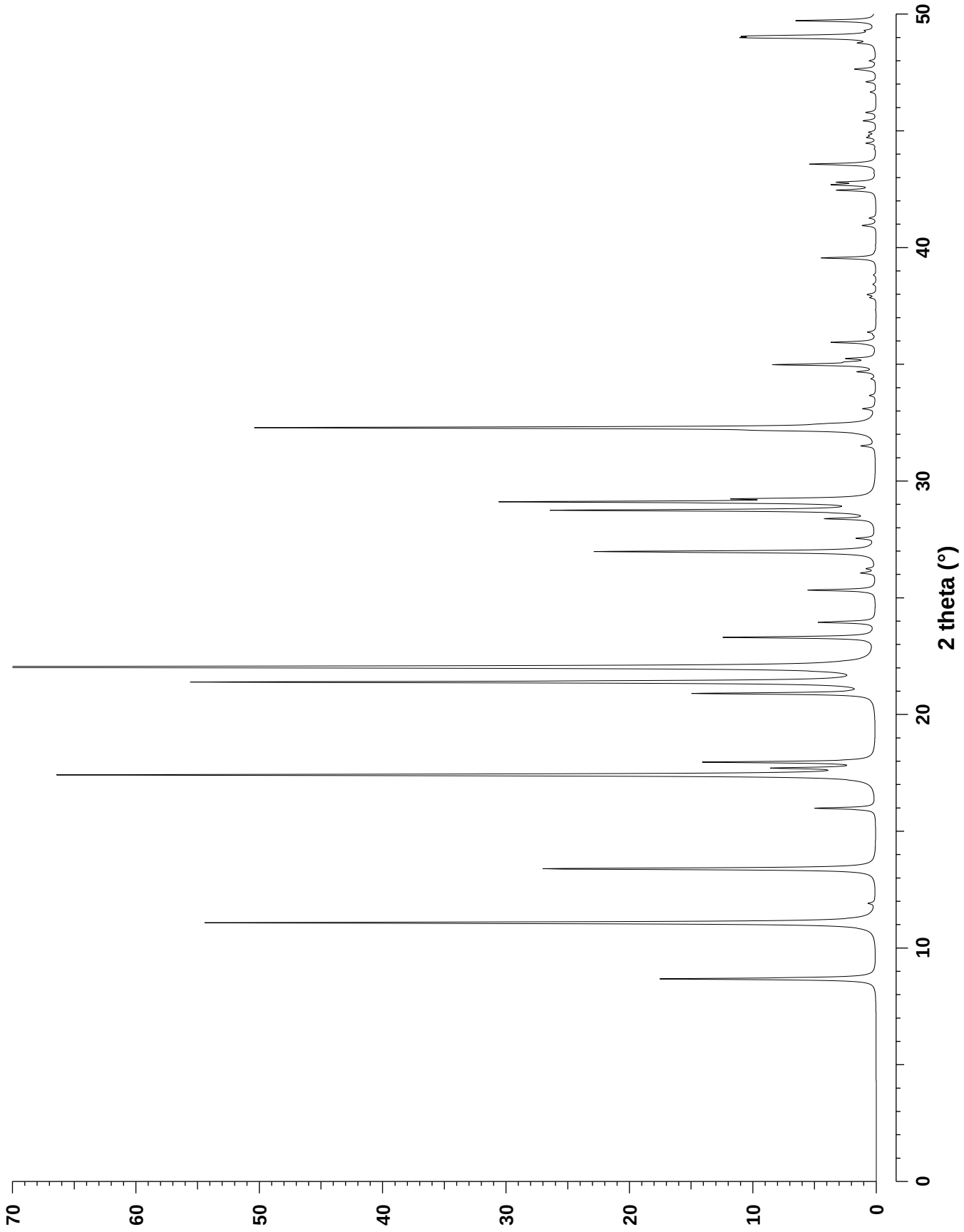
REFINED COMPOSITION: $|(C_{10}N)_6|\ [Si_{54}O_{108}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.2251$ Å $b = 13.2251$ Å $c = 22.2916$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.104$, $R_F = 0.060$

REFERENCE: L. B. McCusker,
Mat. Sci. Forum Vol. **133-136** 423–434 (1993).
And L. B. McCusker, Private communication (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	8.68	10.187	6	17.6	0	4	2	32.28	2.773	6	49.9	3	0	9	43.56	2.078	6	1.2
0	1	2	11.08	7.988	6	54.6	1	3	4	32.44	2.760	12	1.8	0	2	10	43.57	2.077	6	0.7
0	0	3	11.91	7.431	2	0.5	0	1	8	33.09	2.707	6	1.0	1	4	6	43.65	2.074	12	0.2
1	1	0	13.39	6.613	6	27.1	0	3	6	33.66	2.663	6	0.5	5	1	1	44.22	2.048	12	0.1
0	2	1	15.98	5.547	6	4.9	3	2	1	34.37	2.609	12	0.3	5	0	5	44.46	2.037	6	0.8
2	0	2	17.41	5.094	6	66.4	3	1	5	34.67	2.587	12	1.4	3	2	7	44.71	2.027	12	0.7
1	0	4	17.70	5.011	6	7.1	2	1	7	34.98	2.565	12	8.2	1	5	2	44.80	2.023	12	0.4
1	1	3	17.96	4.940	12	13.6	2	3	2	35.09	2.557	12	1.5	2	4	4	44.93	2.018	12	0.6
2	1	1	20.90	4.250	12	14.5	4	0	4	35.24	2.547	6	2.2	0	4	8	45.42	1.997	6	1.0
0	1	5	21.39	4.155	6	55.2	2	0	8	35.84	2.506	6	0.1	2	2	9	45.77	1.982	12	0.3
1	2	2	22.03	4.035	12	100.0	4	1	0	35.93	2.499	12	3.6	2	1	10	45.78	1.982	12	0.5
0	2	4	22.26	3.994	6	0.4	0	0	9	36.27	2.477	2	0.1	4	2	5	46.65	1.947	12	0.5
3	0	0	23.30	3.818	6	12.3	2	2	6	36.37	2.470	12	0.7	5	1	4	47.09	1.930	12	0.8
0	0	6	23.95	3.715	2	4.6	3	2	4	37.85	2.377	12	0.5	2	3	8	47.56	1.912	12	0.2
2	0	5	25.32	3.518	6	5.5	4	1	3	37.98	2.369	12	0.7	2	0	11	47.60	1.910	6	0.4
2	1	4	26.06	3.419	12	1.2	1	2	8	38.42	2.343	12	0.3	6	0	0	47.64	1.909	6	1.5
0	3	3	26.24	3.396	6	0.7	1	1	9	38.82	2.319	12	0.2	3	3	6	47.99	1.896	12	0.5
2	2	0	26.97	3.306	6	22.9	0	5	1	39.55	2.279	6	4.5	1	5	5	48.75	1.868	12	1.1
1	1	6	27.54	3.239	12	1.5	3	3	0	40.94	2.204	6	1.1	0	5	7	48.98	1.860	6	8.4
1	3	1	28.38	3.145	12	3.8	1	0	10	41.26	2.188	6	0.6	0	0	12	49.04	1.858	2	6.6
1	2	5	28.74	3.106	12	26.0	4	0	7	42.45	2.129	6	3.1	3	4	2	49.07	1.857	12	2.8
1	0	7	29.10	3.068	6	29.5	4	2	2	42.55	2.125	12	0.1	0	6	3	49.29	1.849	6	0.5
3	1	2	29.23	3.055	12	9.1	0	5	4	42.68	2.119	6	3.3	5	2	0	49.71	1.834	12	6.5
4	0	1	31.50	2.840	6	1.1	3	3	3	42.79	2.113	12	2.8							
0	2	7	32.16	2.783	6	4.7	0	3	9	43.56	2.078	6	3.5							

1-aminoadamantane NU-3 LEV



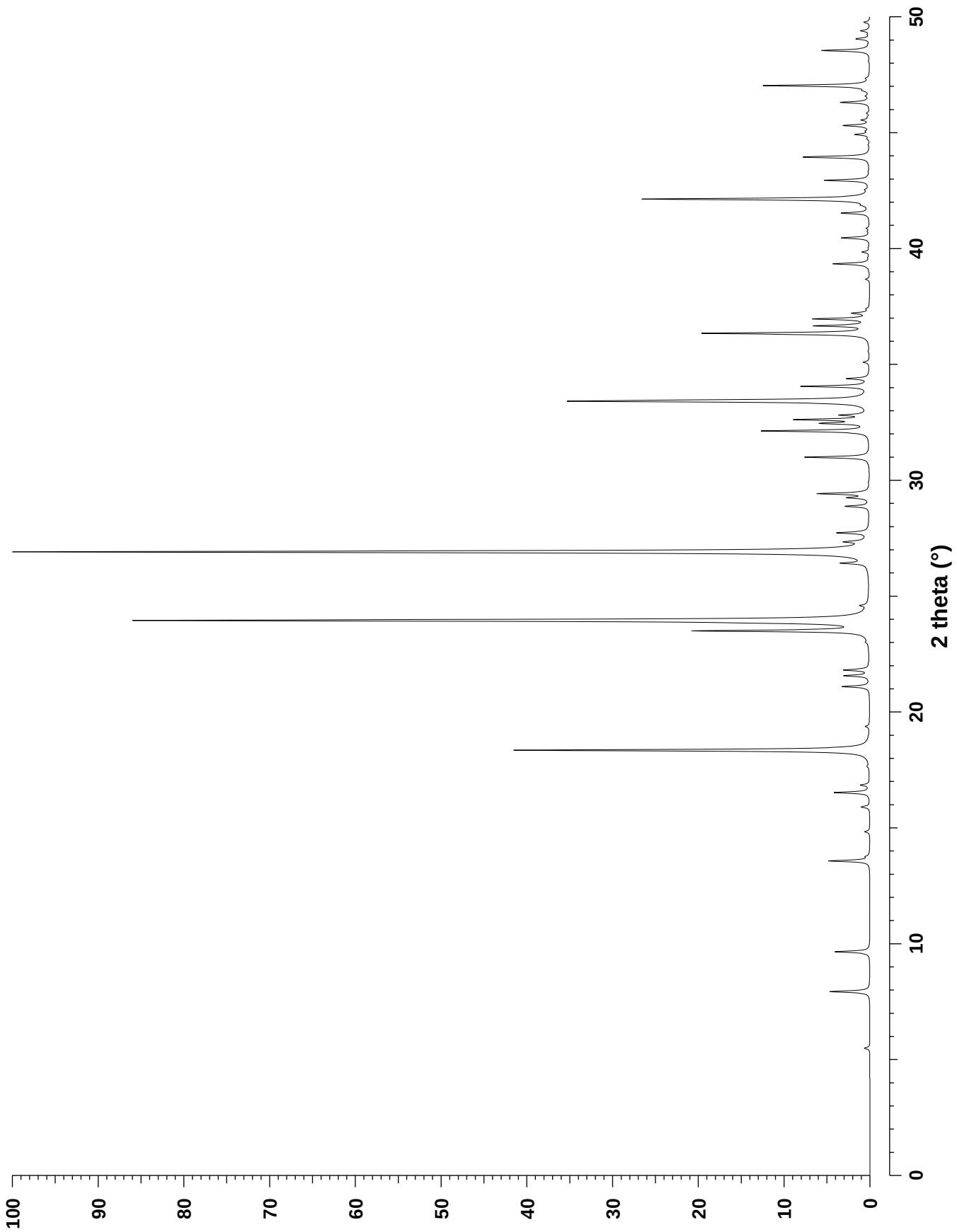
CHEMICAL COMPOSITION: $|Na_{9.96}(K,Ca)_{8.04}Ca_6(SO_4)_5Cl_{3.5}F_{0.5}|\ [Si_{18}Al_{18}O_{72}]$
Pitigliano, Tuscany, Italy

REFINED COMPOSITION: $|K_{13.788}Ca_6(SO_4)_5Cl_{3.5}F_{0.5}|\ [Si_{18}Al_{18}O_{72}]$

CRYSTAL DATA: $P\overline{6}$ (No. 174)
$a = 12.8701$ Å $b = 12.8701$ Å $c = 16.096$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_p = 0.0365$, $R_{wp} = 0.0829$

REFERENCE: P. Ballirano, S. Merlino and E. Bonaccorsi,
Canadian Mineralogist **34** 1021–1030 (1996).

h	k	l	2θ	d	M	I_{rel}
0	0	1	5.49	16.096	2	0.8
1	0	0	7.93	11.146	6	5.5
1	0	1	9.65	9.163	12	4.8
1	0	2	13.57	6.525	12	5.7
1	1	0	13.76	6.435	6	0.4
1	1	1	14.83	5.975	12	0.7
2	0	0	15.90	5.573	6	1.2
0	0	3	16.52	5.365	2	4.9
2	0	1	16.84	5.266	12	1.2
1	1	2	17.65	5.026	12	0.3
1	0	3	18.35	4.834	12	48.7
2	0	2	19.37	4.582	12	0.5
2	1	0	21.09	4.213	6	0.7
1	2	0	21.09	4.213	6	3.1
1	1	3	21.56	4.121	12	3.5
2	1	1	21.81	4.075	12	1.8
1	2	1	21.81	4.075	12	1.6
2	0	3	23.01	3.865	12	0.3
1	0	4	23.50	3.785	12	23.5
1	2	2	23.84	3.732	12	3.1
2	1	2	23.84	3.732	12	2.9
3	0	0	23.95	3.715	6	100.0
3	0	1	24.59	3.620	12	1.0
3	0	2	26.42	3.373	12	3.3
2	1	3	26.91	3.313	12	58.6
1	2	3	26.91	3.313	12	58.7
2	0	4	27.34	3.262	12	2.6
0	0	5	27.71	3.219	2	0.2
2	2	0	27.73	3.218	6	4.0
1	0	5	28.87	3.093	12	2.5
1	3	0	28.88	3.091	6	0.2
3	1	0	28.88	3.091	6	0.6
3	0	3	29.24	3.054	12	2.8
1	3	1	29.42	3.036	12	3.6
3	1	1	29.42	3.036	12	3.4
2	2	2	29.91	2.988	12	0.1
3	1	2	30.99	2.886	12	4.4
1	3	2	30.99	2.886	12	4.5
2	0	5	32.11	2.788	12	0.1
4	0	0	32.12	2.786	6	14.6
2	2	3	32.45	2.759	12	6.0
4	0	1	32.61	2.746	12	9.8
3	0	4	32.81	2.730	12	3.6
0	0	6	33.40	2.683	2	35.5
3	1	3	33.45	2.679	12	8.6
1	3	3	33.45	2.679	12	6.1
4	0	2	34.05	2.633	12	9.2
1	0	6	34.38	2.608	12	3.0
2	1	5	35.08	2.558	12	0.2
1	2	5	35.08	2.558	12	0.1
2	3	0	35.09	2.557	6	0.2
3	2	0	35.09	2.557	6	0.3
1	1	6	36.28	2.476	12	0.3
4	0	3	36.33	2.473	12	22.8
3	1	4	36.66	2.451	12	3.7
1	3	4	36.66	2.451	12	3.7
3	0	5	36.95	2.433	12	2.1
4	1	0	36.96	2.432	6	3.0
1	4	0	36.96	2.432	6	2.6
2	0	6	37.20	2.417	12	2.2
1	4	1	37.39	2.405	12	0.2
4	1	1	37.39	2.405	12	0.2
4	1	2	38.67	2.328	12	0.3
1	4	2	38.67	2.328	12	0.3
0	0	7	39.18	2.299	2	0.2
4	0	4	39.33	2.291	12	5.0
2	2	5	39.60	2.276	12	0.2
1	2	6	39.84	2.263	12	0.5
2	1	6	39.84	2.263	12	0.5
1	0	7	40.04	2.252	12	0.1
1	3	5	40.45	2.230	12	1.2
3	1	5	40.45	2.230	12	1.1
5	0	0	40.46	2.229	6	1.7
1	4	3	40.73	2.215	12	0.1
5	0	1	40.87	2.208	12	0.4
3	0	6	41.52	2.175	12	3.8
3	2	4	41.86	2.158	12	0.3
2	3	4	41.86	2.158	12	0.3
5	0	2	42.06	2.148	12	0.1
3	3	0	42.13	2.145	6	31.1
2	0	7	42.53	2.126	12	0.4
4	0	5	42.93	2.107	12	1.7
4	2	0	42.94	2.106	6	2.2
2	4	0	42.94	2.106	6	2.3
2	2	6	43.94	2.060	12	9.1
1	3	6	44.73	2.026	12	0.2
1	2	7	44.91	2.018	12	1.0
2	1	7	44.91	2.018	12	1.0
0	0	8	45.06	2.012	2	0.4
3	2	5	45.29	2.002	12	0.6
2	3	5	45.29	2.002	12	0.6
5	1	0	45.30	2.002	6	1.2
1	5	0	45.30	2.002	6	1.2
3	3	3	45.54	1.992	12	1.1
1	0	8	45.83	1.980	12	0.4
4	2	3	46.30	1.961	12	1.8
2	4	3	46.30	1.961	12	2.2
5	0	4	46.57	1.950	12	0.4
4	1	5	46.81	1.941	12	0.2
1	4	5	46.81	1.941	12	0.3
4	0	6	47.02	1.933	12	14.6
1	1	8	47.34	1.920	12	0.4
2	0	8	48.08	1.892	12	0.1
5	1	3	48.54	1.876	12	3.3
1	5	3	48.54	1.876	12	3.3
6	0	0	49.04	1.858	6	1.8
2	3	6	49.23	1.851	12	0.2
6	0	1	49.38	1.845	12	0.6
1	3	7	49.40	1.845	12	0.3
3	1	7	49.40	1.845	12	0.3
5	0	5	49.75	1.833	12	0.2
3	4	0	49.76	1.832	6	0.6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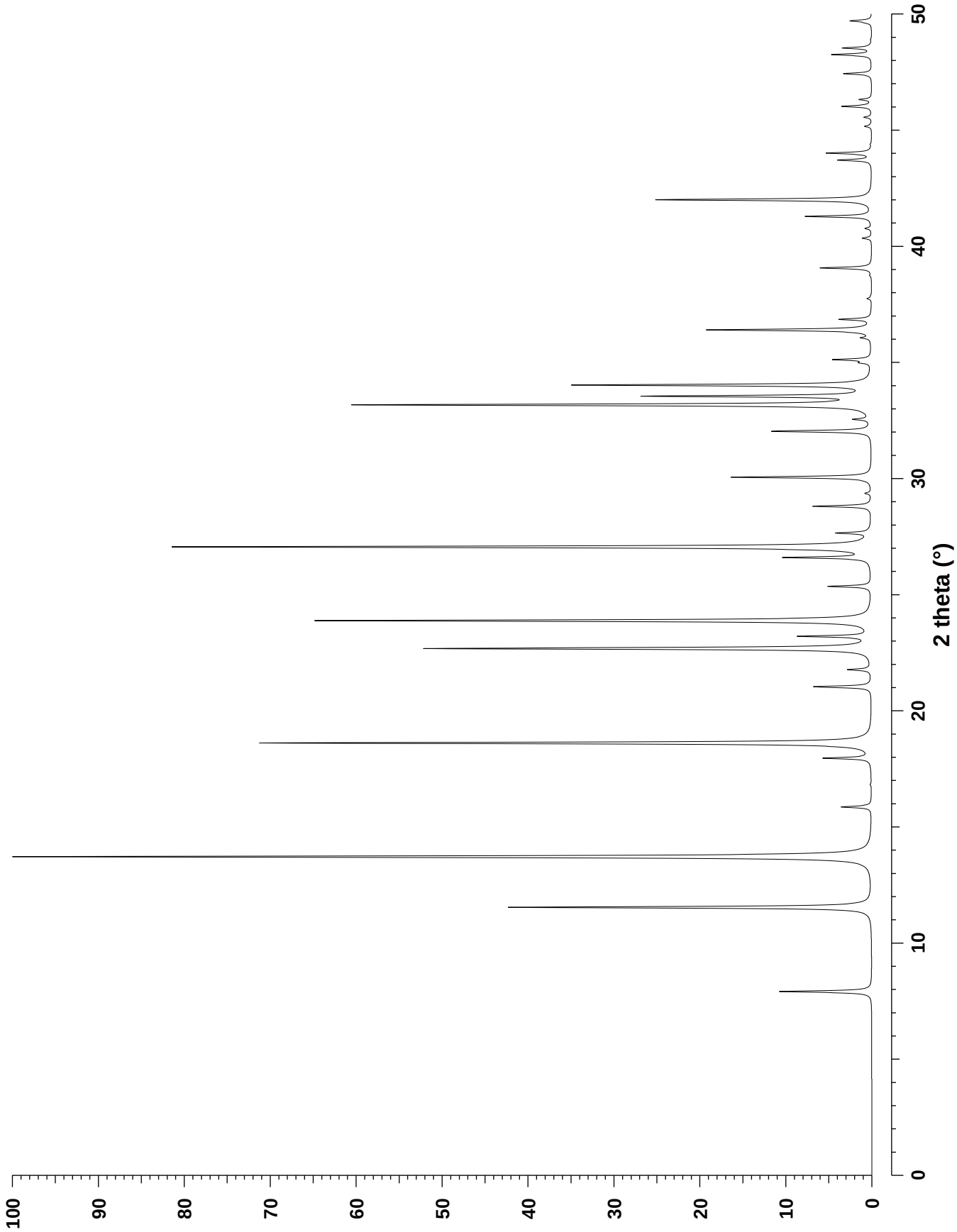
CHEMICAL COMPOSITION: $|Na_{12}(H_2O)_{18}|\ [Si_{12}Al_{12}O_{48}]$
Synthetic material

REFINED COMPOSITION: $|Na_{12.5}(H_2O)_{14.32}|\ [Si_{12}Al_{12}O_{48}]$

CRYSTAL DATA: $P6_3mc$ (No. 186)
$a = 12.906$ Å $b = 12.906$ Å $c = 10.541$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.154$, $R_F = 0.084$, $R_{exp} = 0.136$

REFERENCE: P. A. Schicker,
Ph.D. Thesis No. 8494, ETH Zurich (1988).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.91	11.177	6	10.8	2	2	2	32.54	2.752	12	1.9	3	3	0	42.00	2.151	6	12.8
1	0	1	11.54	7.669	12	42.3	2	1	3	33.16	2.701	24	13.7	1	0	5	43.69	2.072	12	0.3
1	1	0	13.72	6.453	6	100.0	4	0	1	33.17	2.701	12	47.3	3	2	3	43.70	2.071	24	2.9
2	0	0	15.86	5.588	6	3.5	3	1	2	33.54	2.672	24	25.9	4	2	1	43.71	2.071	24	0.7
0	0	2	16.82	5.270	2	0.1	0	0	4	34.02	2.635	2	34.6	5	0	2	44.00	2.058	12	5.3
2	0	1	17.96	4.937	12	5.4	1	0	4	34.98	2.565	12	0.9	2	2	4	44.38	2.041	12	0.1
1	0	2	18.61	4.767	12	71.2	3	2	0	34.99	2.564	12	0.2	3	1	4	45.16	2.008	24	0.8
2	1	0	21.03	4.224	12	6.7	3	0	3	35.11	2.556	12	4.4	3	3	2	45.55	1.992	12	0.9
1	1	2	21.77	4.082	12	2.7	3	2	1	36.05	2.492	24	1.1	2	0	5	46.01	1.973	12	0.3
2	1	1	22.68	3.921	24	52.1	4	0	2	36.39	2.469	12	19.2	5	1	1	46.02	1.972	24	3.3
2	0	2	23.20	3.834	12	8.2	1	1	4	36.84	2.440	12	2.1	4	2	2	46.31	1.961	24	1.4
3	0	0	23.88	3.726	6	64.7	4	1	0	36.85	2.439	12	1.7	4	0	4	47.42	1.917	12	3.3
3	0	1	25.35	3.513	12	5.0	2	0	4	37.74	2.384	12	0.5	2	1	5	48.24	1.886	24	4.5
1	0	3	26.59	3.352	12	9.8	3	1	3	38.74	2.325	24	0.2	5	0	3	48.25	1.886	12	0.1
2	1	2	27.05	3.296	24	81.4	3	2	2	39.06	2.306	24	6.0	5	1	2	48.53	1.876	24	3.4
2	2	0	27.65	3.226	6	3.9	2	1	4	40.34	2.236	24	1.0	3	2	4	49.60	1.838	24	0.2
3	1	0	28.80	3.100	12	6.8	5	0	0	40.35	2.235	6	0.1	4	3	0	49.61	1.837	12	0.3
3	0	2	29.36	3.042	12	0.7	4	1	2	40.76	2.213	24	0.7	3	0	5	49.69	1.835	12	1.1
2	0	3	30.04	2.975	12	0.9	4	0	3	41.28	2.187	12	6.7	6	0	1	49.70	1.834	12	1.4
3	1	1	30.05	2.974	24	15.5	5	0	1	41.28	2.187	12	1.0							
4	0	0	32.03	2.794	6	11.6	3	0	4	41.99	2.151	12	13.1							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LOV Lovdarite

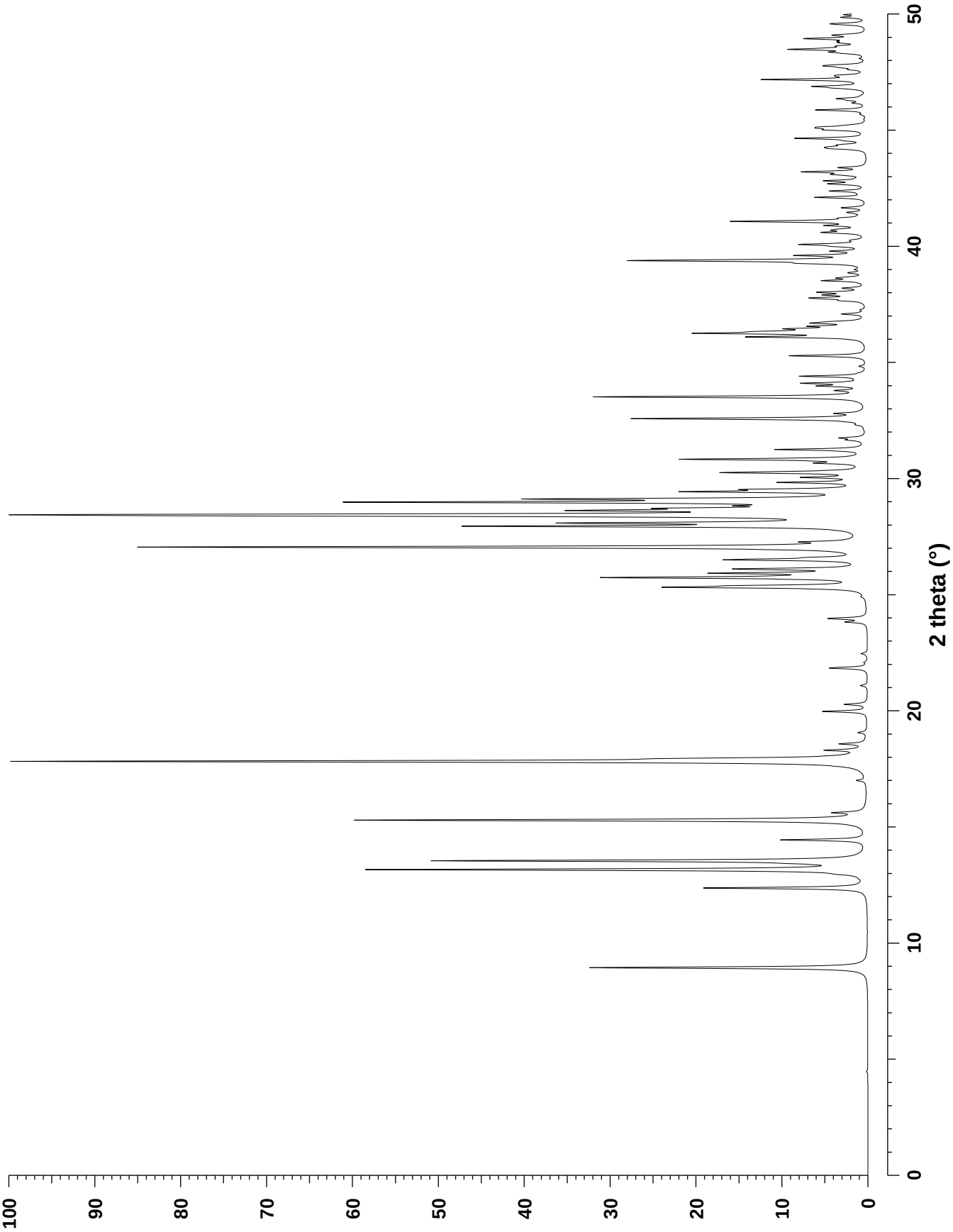
CHEMICAL COMPOSITION: $|Na_{12}K_4(H_2O)_{18}|\ [Si_{28}Be_8O_{72}]$
Mt. Karnasurt, Lovezero Pluton, Russia

REFINED COMPOSITION: $|Na_{12}K_4(H_2O)_{18}|\ [Si_{28}Be_8O_{72}]$

CRYSTAL DATA: $Pma2$ (No. 28)
$a = 39.576$ Å $b = 6.9308$ Å $c = 7.1526$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.09$

REFERENCE: S. Merlino,
Eur. J. Mineral. **2** 809–817 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
4	0	0	8.94	9.894	2	33.1	5	1	2	30.30	2.949	8	3.7	13	1	2	41.06	2.198	8	3.3
0	0	1	12.37	7.153	2	19.3	11	1	1	30.66	2.916	8	4.7	0	3	1	41.06	2.198	4	3.1
2	0	1	13.16	6.727	4	58.9	5	2	1	30.82	2.902	8	21.3	4	1	3	41.06	2.198	8	8.9
6	0	0	13.42	6.596	2	3.3	6	1	2	31.24	2.863	8	10.6	14	2	0	41.21	2.190	4	2.1
2	1	0	13.54	6.541	4	50.8	14	0	0	31.65	2.827	2	1.9	13	2	1	41.45	2.178	8	1.9
3	1	0	14.44	6.136	4	10.0	6	2	1	31.74	2.819	8	2.9	5	1	3	41.65	2.168	8	1.9
4	0	1	15.29	5.797	4	60.8	12	1	1	32.57	2.749	8	27.9	4	3	1	42.10	2.146	8	6.0
4	1	0	15.61	5.677	4	3.3	7	2	1	32.80	2.731	8	3.1	6	1	3	42.37	2.133	8	4.2
0	1	1	17.82	4.977	4	100.0	8	1	2	33.51	2.674	8	32.4	5	3	1	42.68	2.118	8	4.2
8	0	0	17.93	4.947	2	10.6	10	0	2	33.78	2.653	4	3.0	14	1	2	42.81	2.112	8	4.6
1	1	1	17.96	4.938	8	6.1	8	2	1	33.98	2.638	8	5.0	15	2	0	43.09	2.099	4	2.9
6	0	1	18.30	4.849	4	4.2	14	0	1	34.10	2.629	4	7.1	14	2	1	43.19	2.094	8	4.0
6	1	0	18.57	4.778	4	3.0	10	2	0	34.40	2.607	4	7.8	7	1	3	43.20	2.094	8	3.3
4	1	1	19.97	4.446	8	5.3	9	2	1	35.28	2.544	8	9.2	6	3	1	43.38	2.086	8	3.1
7	1	0	20.27	4.381	4	2.7	0	2	2	36.09	2.489	4	12.9	7	3	1	44.20	2.049	8	3.0
8	0	1	21.84	4.069	4	4.5	10	1	2	36.25	2.478	8	17.6	11	2	2	44.25	2.047	8	2.6
7	1	1	23.82	3.736	8	2.4	16	0	0	36.32	2.474	2	7.3	9	3	0	44.29	2.045	4	1.8
9	1	0	23.97	3.713	4	4.5	2	2	2	36.38	2.469	8	2.2	10	0	3	44.36	2.042	4	2.5
2	0	2	25.31	3.519	4	21.2	15	1	0	36.44	2.466	4	7.0	16	0	2	44.54	2.034	4	1.5
8	1	1	25.38	3.509	8	10.9	14	1	1	36.55	2.458	8	5.2	15	1	2	44.64	2.030	8	8.2
0	2	0	25.71	3.465	2	5.6	10	2	1	36.69	2.450	8	5.3	15	2	1	45.00	2.014	8	3.4
10	0	1	25.73	3.463	4	25.4	3	2	2	36.75	2.446	8	2.2	18	1	1	45.08	2.011	8	3.4
1	2	0	25.81	3.452	4	2.6	12	0	2	37.08	2.424	4	2.8	8	3	1	45.13	2.009	8	3.8
10	1	0	25.92	3.437	4	16.3	12	2	0	37.65	2.389	4	2.2	20	0	0	45.86	1.979	2	6.1
2	2	0	26.10	3.413	4	14.4	0	0	3	37.73	2.384	2	2.3	10	1	3	46.35	1.959	8	3.1
4	0	2	26.50	3.363	4	15.6	11	1	2	37.77	2.382	8	5.0	0	3	2	46.81	1.941	4	2.5
3	2	0	26.59	3.352	4	4.0	5	2	2	37.90	2.374	8	4.1	16	2	1	46.88	1.938	8	5.1
12	0	0	27.04	3.298	2	82.3	2	0	3	38.01	2.367	4	5.1	4	2	3	47.17	1.927	8	11.7
9	1	1	27.06	3.295	8	4.7	11	2	1	38.19	2.357	8	2.5	3	3	2	47.35	1.920	8	2.4
4	2	0	27.27	3.271	4	5.1	16	0	1	38.51	2.338	4	4.9	4	3	2	47.76	1.904	8	3.7
11	1	0	27.94	3.193	4	44.4	15	1	1	38.62	2.331	8	2.5	20	1	0	47.80	1.903	4	1.6
0	1	2	28.08	3.178	4	29.2	4	0	3	38.85	2.318	4	1.8	6	2	3	48.35	1.883	8	3.2
5	2	0	28.11	3.174	4	3.1	2	3	0	39.26	2.295	4	5.1	17	1	2	48.47	1.878	8	8.2
6	0	2	28.39	3.144	4	49.7	12	1	2	39.37	2.288	8	23.1	11	3	1	48.53	1.876	8	1.8
2	1	2	28.44	3.138	8	78.9	13	2	0	39.40	2.287	4	6.9	18	0	2	48.61	1.873	4	2.4
0	2	1	28.62	3.119	4	26.4	3	3	0	39.60	2.276	4	7.4	14	2	2	48.75	1.868	8	2.3
1	2	1	28.71	3.109	8	16.0	12	2	1	39.78	2.266	8	3.6	17	2	1	48.82	1.866	8	1.9
10	1	1	28.82	3.098	8	7.4	0	1	3	39.99	2.255	4	2.6	6	3	2	48.92	1.862	8	2.5
2	2	1	28.98	3.081	8	57.0	1	1	3	40.06	2.251	8	2.0	12	1	3	48.94	1.861	8	4.8
6	2	0	29.11	3.068	4	34.7	4	3	0	40.08	2.250	4	5.7	18	2	0	49.07	1.857	4	2.4
3	2	1	29.43	3.035	8	19.1	8	2	2	40.58	2.223	8	2.8	7	2	3	49.10	1.855	8	1.6
4	1	2	29.52	3.026	8	10.9	3	1	3	40.59	2.222	8	2.0	13	3	0	49.53	1.840	4	1.5
12	0	1	29.83	2.995	4	9.5	14	0	2	40.68	2.218	4	2.2	20	1	1	49.57	1.839	8	3.6
4	2	1	30.04	2.974	8	6.5	16	1	1	40.73	2.215	8	1.7	12	3	1	49.85	1.829	8	2.8
7	2	0	30.25	2.955	4	15.3	17	1	0	40.89	2.207	4	4.0	8	2	3	49.96	1.826	8	2.5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LTA Linde Type A, Hydrated

CHEMICAL COMPOSITION: $|Na_{96}(H_2O)_{216}|\ [Si_{96}Al_{96}O_{384}]$

REFINED COMPOSITION: $|Na_{64}(H_2O)_{326.71}|\ [Si_{96}Al_{96}O_{384}]$

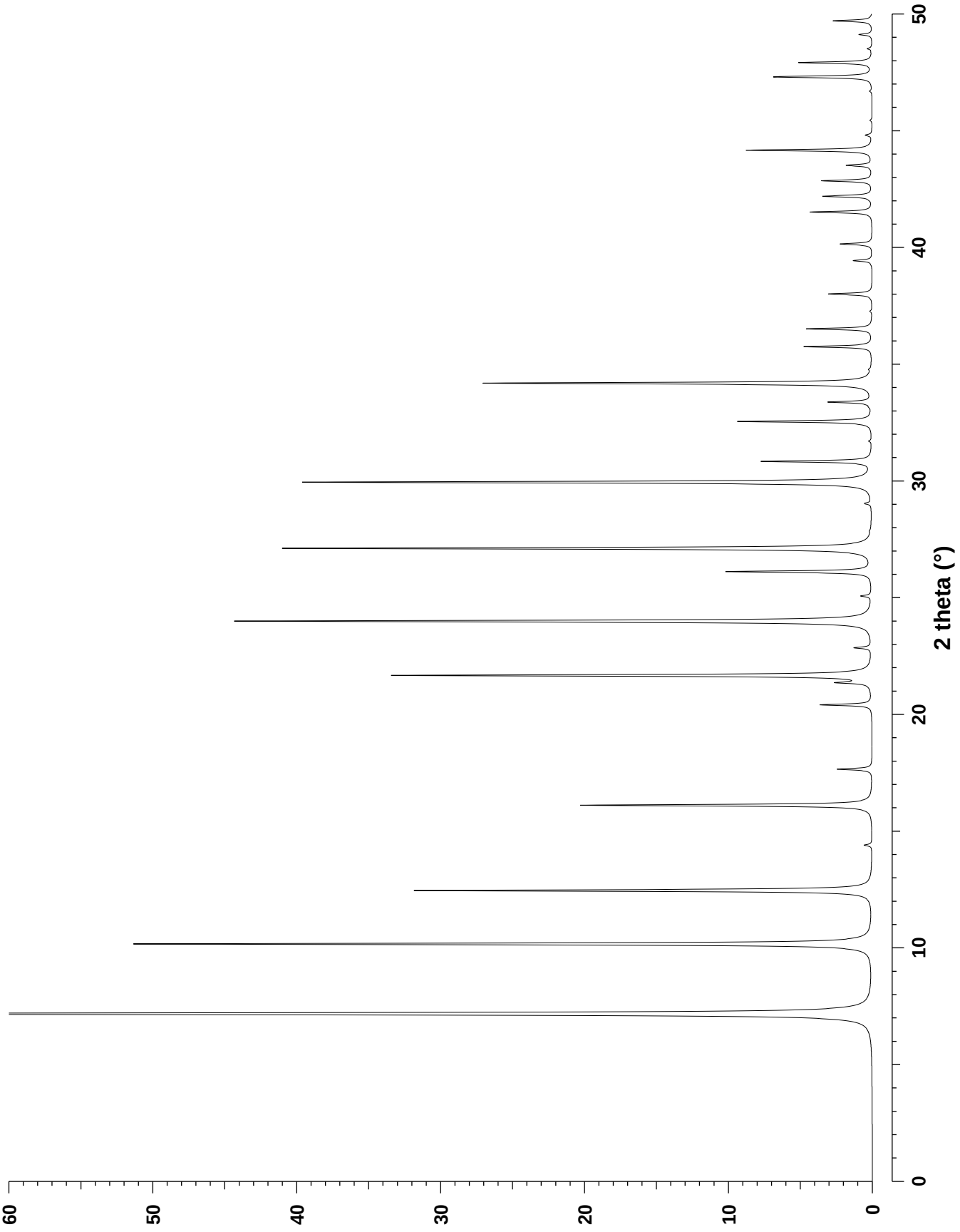
CRYSTAL DATA: $Fm\overline{3}c$ (No. 226)
$a = 24.61$ Å $b = 24.61$ Å $c = 24.61$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: V. Gramlich and W. M. Meier,
Z. Kristallogr. **133** 134–149 (1971).

h	k	l	2θ	d	M	I_{rel}
2	0	0	7.18	12.305	6	100.0
2	2	0	10.17	8.701	12	51.3
2	2	2	12.46	7.104	8	31.8
4	0	0	14.40	6.153	6	0.5
4	2	0	16.11	5.503	24	20.3
4	2	2	17.65	5.023	24	2.4
4	4	0	20.41	4.350	12	3.6
5	3	1	21.36	4.160	48	2.1
6	0	0	21.67	4.102	6	10.6
4	4	2	21.67	4.102	24	22.8
6	2	0	22.85	3.891	24	1.2
6	2	2	23.99	3.710	24	44.3
4	4	4	25.07	3.552	8	0.7
6	4	0	26.11	3.413	24	10.1
6	4	2	27.11	3.289	48	41.0
8	0	0	29.03	3.076	6	0.4
6	4	4	29.94	2.984	24	19.7
8	2	0	29.94	2.984	24	19.9
8	2	2	30.83	2.900	24	5.4
6	6	0	30.83	2.900	12	2.3
6	6	2	31.70	2.823	24	0.2
8	4	0	32.54	2.751	24	9.3
8	4	2	33.37	2.685	48	3.0
6	6	4	34.18	2.623	24	27.1
9	3	1	34.77	2.580	48	0.1
8	4	4	35.75	2.512	24	4.7
10	0	0	36.51	2.461	6	4.1
8	6	0	36.51	2.461	24	0.4
10	2	0	37.26	2.413	24	0.1
10	2	2	38.00	2.368	24	1.6
6	6	6	38.00	2.368	8	1.4
8	6	4	39.43	2.285	48	1.0
10	4	0	39.43	2.285	24	0.3
10	4	2	40.14	2.247	48	2.2
8	8	0	41.51	2.175	12	4.3
10	4	4	42.19	2.142	24	3.4
8	6	6	42.85	2.110	24	2.3
10	6	0	42.85	2.110	24	1.2
10	6	2	43.51	2.080	48	1.8
8	8	4	44.16	2.051	24	0.9
12	0	0	44.16	2.051	6	7.8
12	2	0	44.80	2.023	24	0.5
12	2	2	45.44	1.996	24	0.1
12	4	0	46.69	1.946	24	0.2
10	8	0	47.30	1.922	24	2.3
8	8	6	47.30	1.922	24	4.2
12	4	2	47.30	1.922	48	0.3
10	8	2	47.91	1.899	48	5.1
10	6	6	48.51	1.876	24	0.3
12	4	4	49.11	1.855	24	0.9
10	8	4	49.70	1.834	48	1.8
12	6	0	49.70	1.834	24	0.9

Linde Type A, Hydrated

LTA



LTA Linde Type A, Dehydrated

CHEMICAL COMPOSITION: $|Na_{91.7}|\ [Si_{96}Al_{96}O_{384}]$

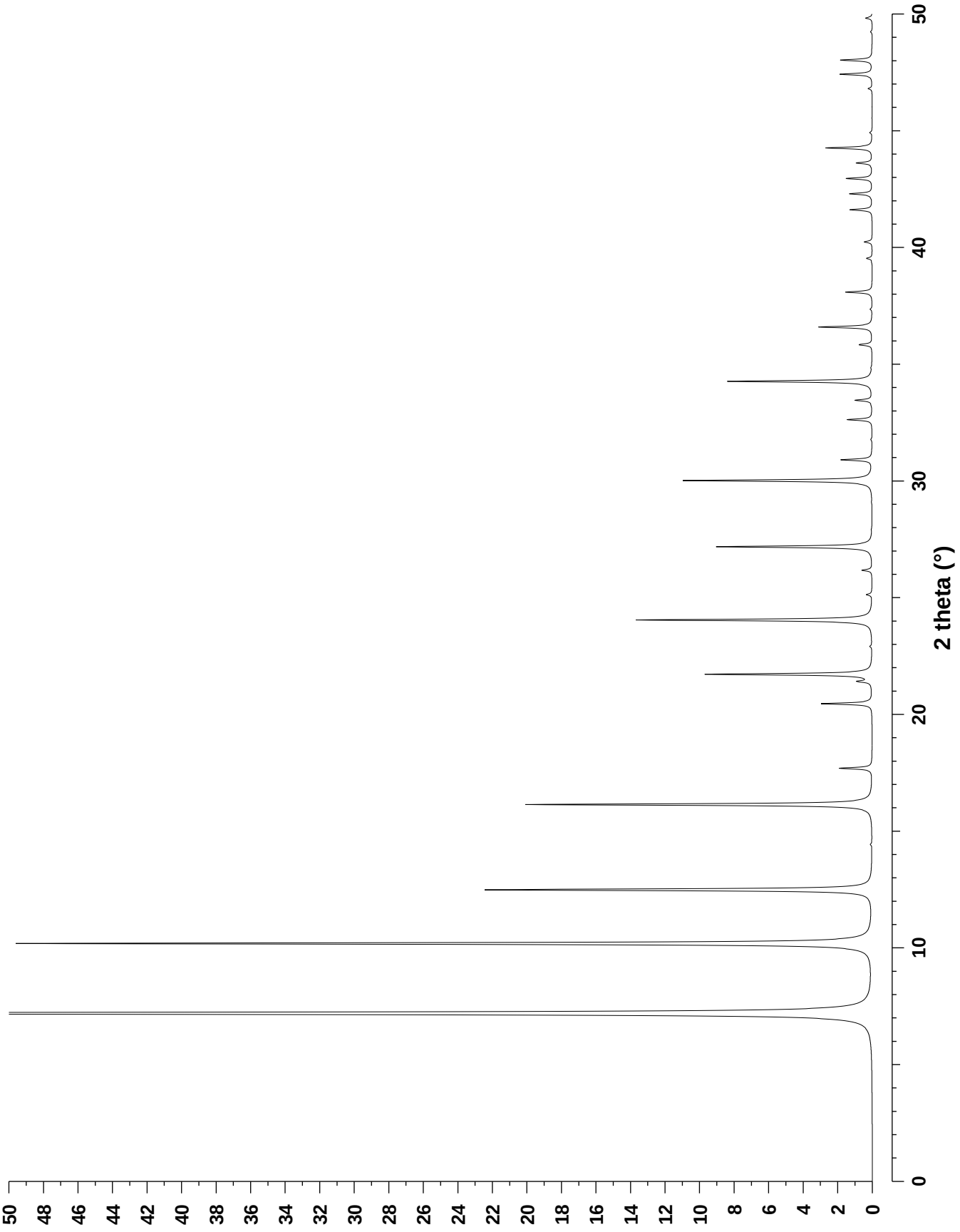
REFINED COMPOSITION: $|Na_{91.78}|\ [Si_{96}Al_{96}O_{384}]$

CRYSTAL DATA: $Fm\overline{3}c$ (No. 226)
$a = 24.555$ Å $b = 24.555$ Å $c = 24.555$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.023$

REFERENCE: J. J. Pluth and J. V. Smith,
J. Am. Chem. Soc. **102** 4704–4708 (1980).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	7.20	12.278	6	100.0	6	4	4	30.01	2.978	24	4.6	8	8	0	41.61	2.170	12	1.3
2	2	0	10.19	8.682	12	49.6	8	2	0	30.01	2.978	24	6.4	10	4	4	42.29	2.137	24	1.3
2	2	2	12.49	7.088	8	22.4	6	6	0	30.90	2.894	12	0.6	8	6	6	42.95	2.106	24	1.0
4	2	0	16.14	5.491	24	20.1	8	2	2	30.90	2.894	24	1.2	10	6	0	42.95	2.106	24	0.5
4	2	2	17.69	5.012	24	1.9	8	4	0	32.62	2.745	24	1.4	10	6	2	43.61	2.075	48	0.9
4	4	0	20.46	4.341	12	3.0	8	4	2	33.45	2.679	48	1.0	12	0	0	44.26	2.046	6	2.2
5	3	1	21.41	4.151	48	0.8	6	6	4	34.26	2.618	24	8.4	8	8	4	44.26	2.046	24	0.5
6	0	0	21.72	4.093	6	1.3	8	4	4	35.83	2.506	24	0.8	12	2	0	44.91	2.018	24	0.1
4	4	2	21.72	4.093	24	8.4	10	0	0	36.59	2.455	6	3.0	12	4	0	46.80	1.941	24	0.2
6	2	0	22.91	3.882	24	0.1	6	6	6	38.08	2.363	8	1.3	8	8	6	47.41	1.917	24	1.2
6	2	2	24.04	3.702	24	13.7	10	2	2	38.08	2.363	24	0.2	10	8	0	47.41	1.917	24	0.6
4	4	4	25.13	3.544	8	0.3	8	6	4	39.53	2.280	48	0.2	10	8	2	48.02	1.894	48	1.8
6	4	0	26.17	3.405	24	0.6	10	4	0	39.53	2.280	24	0.1	10	8	4	49.82	1.830	48	0.4
6	4	2	27.18	3.281	48	9.0	10	4	2	40.23	2.242	48	0.5							

Linde Type A, Dehydrated LTA



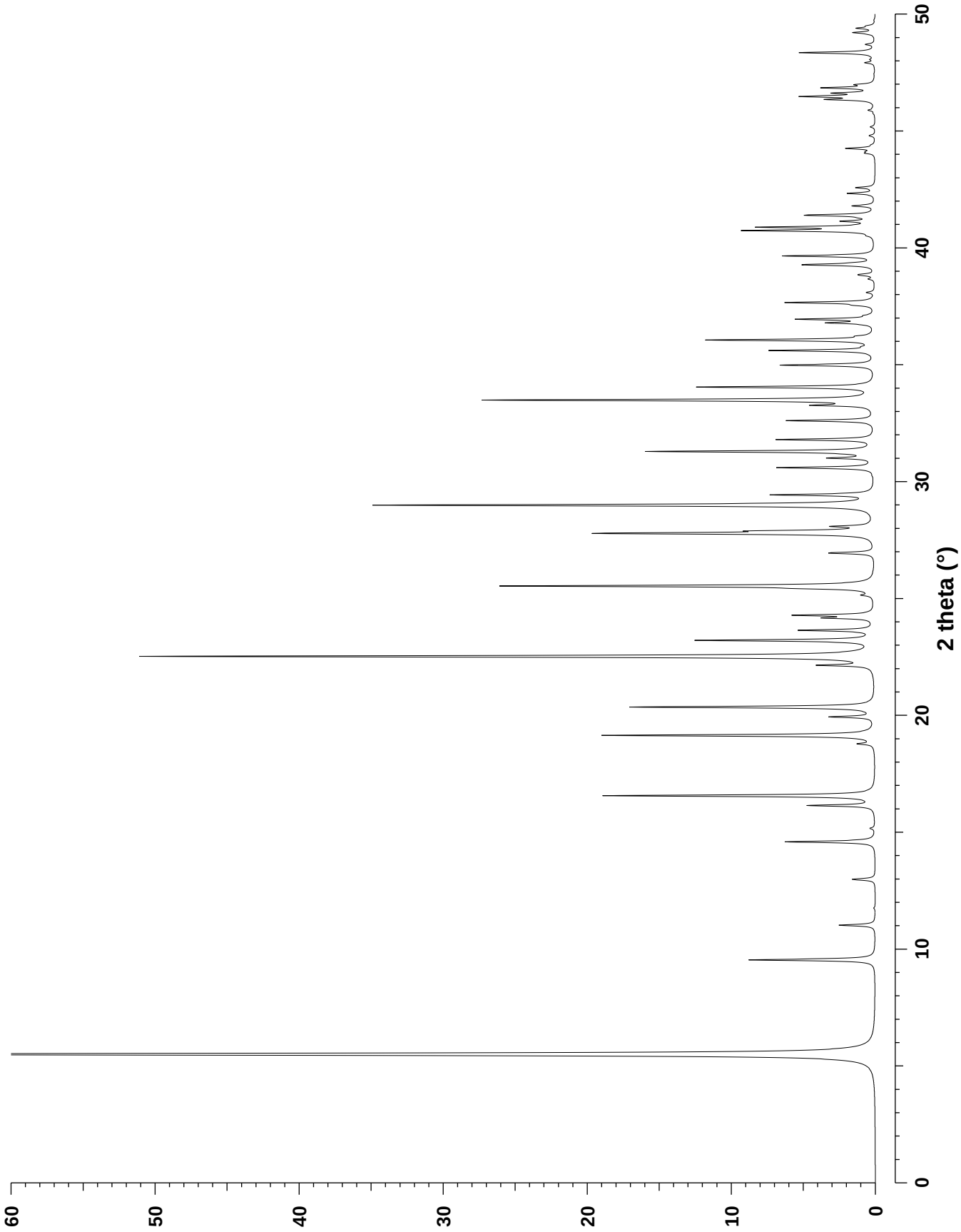
CHEMICAL COMPOSITION: $|K_{12}(H_2O)_{20}|\ [Si_{24}Al_{12}O_{72}]$
Murun Massif, Russia

REFINED COMPOSITION: $|K_{7.56}Tl_{3.8}(H_2O)_{22.46}|\ [Si_{24}Al_{12}O_{72}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 18.5432$ Å $b = 18.5432$ Å $c = 7.5310$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R_{wp} = 0.20$, $R_p = 0.17$

REFERENCE: G. Artioli and Å. Kvick,
Eur. J. Mineral. **2** 749–759 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.50	16.059	6	100.0	5	1	0	31.00	2.884	12	3.0	2	2	3	40.88	2.207	12	7.7
1	1	0	9.54	9.272	6	8.8	3	3	1	31.28	2.859	12	15.8	7	0	1	41.13	2.195	12	2.0
2	0	0	11.02	8.029	6	2.5	4	2	1	31.79	2.815	24	6.8	3	1	3	41.28	2.187	24	0.4
1	0	1	12.98	6.818	12	1.6	4	0	2	32.60	2.746	12	6.1	6	0	2	41.39	2.182	12	4.7
2	1	0	14.59	6.070	12	6.3	5	1	1	33.26	2.693	24	3.6	4	3	2	41.79	2.162	24	1.5
1	1	1	15.16	5.846	12	0.3	6	0	0	33.48	2.676	6	27.1	6	2	1	42.32	2.136	24	1.9
2	0	1	16.14	5.493	12	4.6	4	3	0	33.96	2.640	12	0.1	5	2	2	42.57	2.124	24	1.3
3	0	0	16.56	5.353	6	18.9	3	2	2	34.04	2.633	24	12.2	5	4	0	44.04	2.056	12	0.6
2	1	1	18.78	4.726	24	1.0	5	2	0	34.89	2.571	12	0.1	6	1	2	44.11	2.053	24	0.4
2	2	0	19.14	4.636	6	19.0	4	1	2	34.98	2.565	24	6.5	7	1	1	44.25	2.047	24	2.0
3	1	0	19.93	4.454	12	3.0	6	0	1	35.60	2.522	12	7.2	4	1	3	44.39	2.041	24	0.2
3	0	1	20.35	4.363	12	17.0	0	0	3	35.77	2.510	2	0.4	6	3	0	44.79	2.023	12	0.4
4	0	0	22.14	4.015	6	3.5	4	3	1	36.05	2.491	24	11.7	8	0	0	45.17	2.007	6	0.3
2	2	1	22.52	3.948	12	51.0	1	0	3	36.22	2.480	12	0.7	5	0	3	45.88	1.978	12	0.4
3	1	1	23.20	3.834	24	12.3	5	0	2	36.78	2.444	12	3.1	5	3	2	46.34	1.959	24	2.2
0	0	2	23.63	3.765	2	5.1	5	2	1	36.94	2.434	24	5.3	7	0	2	46.34	1.959	12	0.9
3	2	0	24.16	3.684	12	3.1	1	1	3	37.10	2.423	12	0.4	6	3	1	46.47	1.954	24	4.8
1	0	2	24.28	3.666	12	5.4	2	0	3	37.54	2.396	12	0.8	3	3	3	46.61	1.949	12	2.6
4	0	1	25.14	3.543	12	0.7	3	3	2	37.65	2.389	12	6.1	8	0	1	46.84	1.940	12	3.6
4	1	0	25.42	3.504	12	2.8	4	2	2	38.08	2.363	24	0.5	4	2	3	46.97	1.934	24	1.1
1	1	2	25.53	3.489	12	25.7	6	1	1	38.66	2.329	24	0.4	7	2	1	47.91	1.899	24	0.7
3	2	1	26.94	3.309	24	3.2	2	1	3	38.82	2.320	24	0.5	5	1	3	48.05	1.894	24	0.2
5	0	0	27.78	3.212	6	18.7	4	4	0	38.85	2.318	6	0.8	0	0	4	48.34	1.883	2	5.3
2	1	2	27.88	3.200	24	6.3	7	0	0	39.27	2.294	6	2.8	1	0	4	48.69	1.870	12	0.6
4	1	1	28.08	3.177	24	2.6	5	3	0	39.27	2.294	12	2.1	5	5	0	49.13	1.854	6	0.3
3	3	0	28.89	3.091	6	0.1	5	1	2	39.35	2.290	24	0.7	7	1	2	49.20	1.852	24	1.4
3	0	2	28.99	3.080	12	34.8	3	0	3	39.65	2.273	12	6.4	1	1	4	49.39	1.845	12	1.2
4	2	0	29.43	3.035	12	7.0	6	2	0	40.51	2.227	12	0.2	6	4	0	49.48	1.842	12	0.5
2	2	2	30.59	2.923	12	6.7	4	4	1	40.73	2.215	12	8.7							


0
10
20
30
40
50
2 theta (°)
60
50
40
30
20
10
0

LTL Linde Type L

CHEMICAL COMPOSITION: $|Na_3K_6(H_2O)_{21}|\ [Si_{27}Al_9O_{72}]$
Synthetic material

REFINED COMPOSITION: $|Na_5K_{4.7}(H_2O)_{20.8}|\ [Si_{27}Al_9O_{72}]$

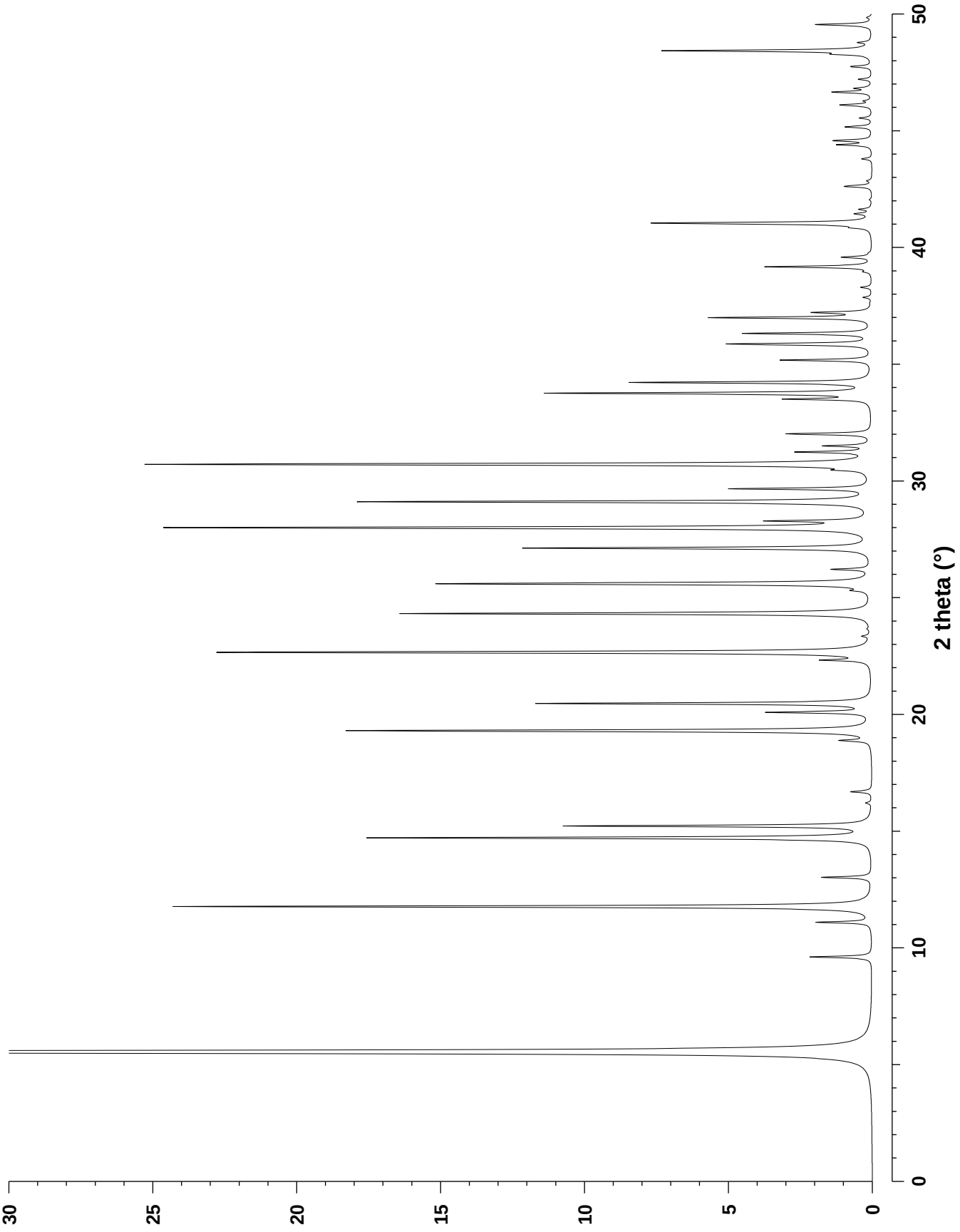
CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 18.40$ Å $b = 18.40$ Å $c = 7.52$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R_F = 0.13$

REFERENCE: R. M. Barrer and H. Villiger,
Z. Kristallogr. **128** 352–270 (1969).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.55	15.935	6	100.0	5	0	1	30.46	2.934	12	0.8	3	1	3	41.41	2.180	24	0.1
1	1	0	9.61	9.200	6	2.2	2	2	2	30.71	2.911	12	25.2	5	3	1	41.44	2.179	24	0.4
2	0	0	11.10	7.967	6	1.9	3	1	2	31.23	2.864	24	2.3	6	0	2	41.63	2.169	12	0.4
0	0	1	11.77	7.520	2	24.3	5	1	0	31.25	2.862	12	0.2	4	0	3	42.61	2.122	12	0.8
1	0	1	13.02	6.801	12	1.7	3	3	1	31.50	2.840	12	1.6	6	2	1	42.64	2.120	24	0.2
2	1	0	14.71	6.023	12	17.5	4	2	1	32.01	2.796	24	2.9	7	1	0	42.85	2.111	12	0.1
1	1	1	15.22	5.822	12	10.6	5	1	1	33.50	2.675	24	2.8	3	2	3	43.79	2.067	24	0.4
2	0	1	16.21	5.469	12	0.2	6	0	0	33.75	2.656	6	11.3	6	1	2	44.39	2.041	24	1.1
3	0	0	16.69	5.312	6	0.7	3	2	2	34.21	2.621	24	8.3	4	1	3	44.56	2.033	24	0.9
2	1	1	18.88	4.701	24	1.0	4	1	2	35.15	2.553	24	0.1	7	1	1	44.59	2.032	24	0.5
2	2	0	19.30	4.600	6	18.3	5	2	0	35.17	2.552	12	3.1	6	3	0	45.16	2.008	12	0.9
3	1	0	20.09	4.420	12	3.5	0	0	3	35.82	2.507	2	0.8	8	0	0	45.54	1.992	6	0.4
3	0	1	20.47	4.339	12	11.6	6	0	1	35.86	2.504	12	4.6	5	0	3	46.07	1.970	12	0.4
4	0	0	22.32	3.984	6	1.5	1	0	3	36.28	2.476	12	0.1	5	4	1	46.10	1.969	24	0.9
2	2	1	22.66	3.924	12	22.7	4	3	1	36.31	2.474	24	4.4	4	4	2	46.27	1.962	12	0.2
3	1	1	23.35	3.810	24	0.3	5	0	2	36.97	2.431	12	0.1	5	3	2	46.64	1.947	24	0.7
1	0	2	24.32	3.660	12	16.1	6	1	0	36.99	2.430	12	5.5	7	0	2	46.64	1.947	12	0.2
3	2	0	24.35	3.656	12	0.5	1	1	3	37.17	2.419	12	0.3	7	2	0	46.66	1.947	12	0.6
4	0	1	25.30	3.520	12	0.4	5	2	1	37.21	2.416	24	1.8	3	3	3	46.81	1.941	12	0.5
1	1	2	25.59	3.481	12	11.5	3	3	2	37.86	2.376	12	0.3	8	0	1	47.20	1.925	12	0.4
4	1	0	25.62	3.477	12	5.3	4	2	2	38.29	2.350	24	0.4	6	2	2	47.74	1.905	24	0.7
2	0	2	26.21	3.400	12	1.3	6	1	1	38.95	2.312	24	0.2	5	1	3	48.26	1.886	24	0.8
3	2	1	27.12	3.288	24	12.1	4	4	0	39.17	2.300	6	3.7	7	2	1	48.29	1.885	24	0.3
2	1	2	27.97	3.189	24	5.7	5	1	2	39.57	2.277	24	0.5	0	0	4	48.42	1.880	2	7.2
5	0	0	28.00	3.187	6	20.9	7	0	0	39.59	2.276	6	0.2	1	0	4	48.77	1.867	12	0.4
4	1	1	28.28	3.156	24	3.2	5	3	0	39.59	2.276	12	0.4	1	1	4	49.48	1.842	12	0.1
3	0	2	29.10	3.069	12	15.4	6	2	0	40.84	2.210	12	0.4	7	1	2	49.52	1.840	24	0.2
3	3	0	29.12	3.067	6	3.0	2	2	3	41.00	2.201	12	2.0	5	5	0	49.54	1.840	6	1.7
4	2	0	29.66	3.011	12	4.8	4	4	1	41.04	2.199	12	6.7	2	0	4	49.84	1.830	12	0.1

Linde Type L

LTL



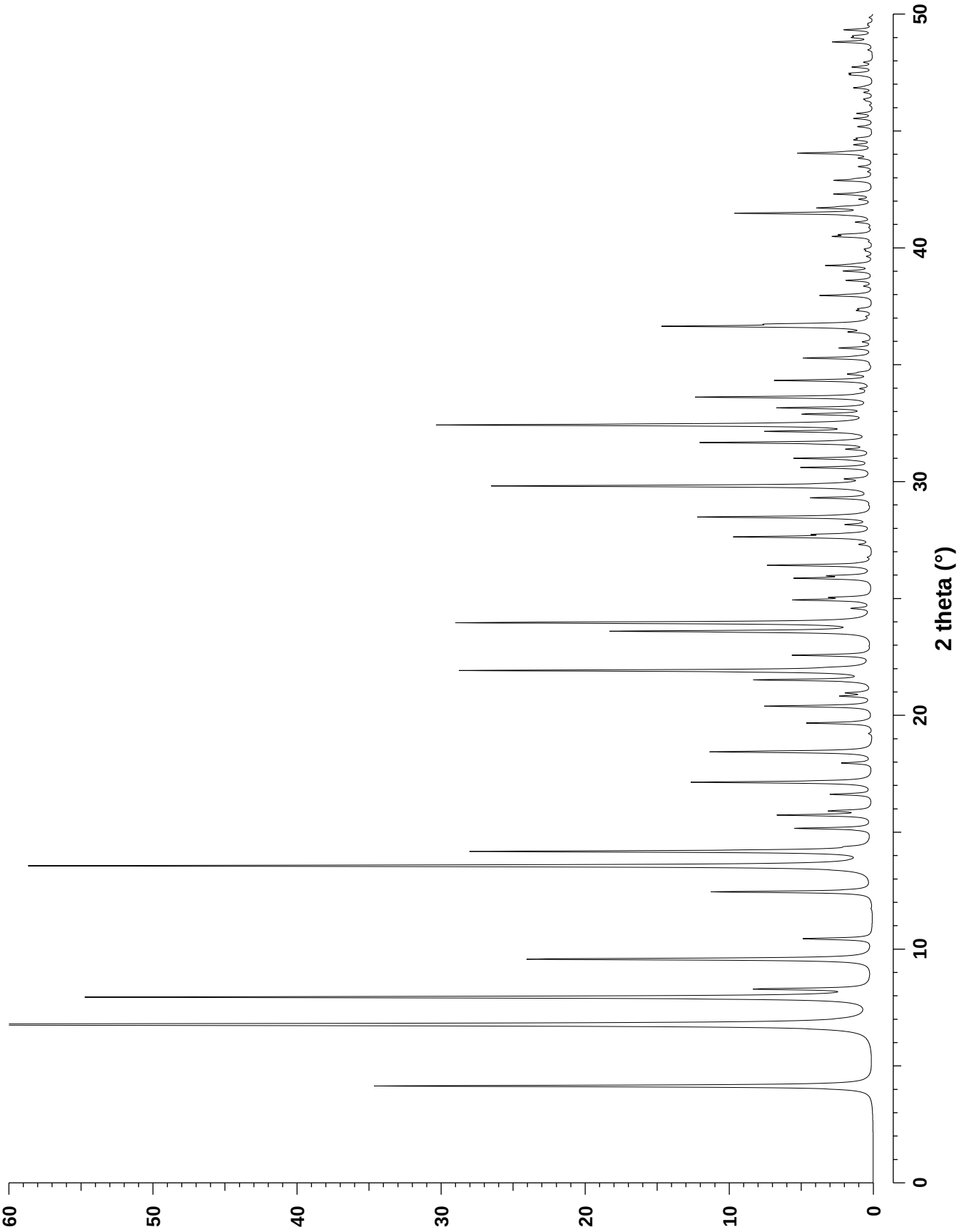
CHEMICAL COMPOSITION: $|Na_{384}(H_2O)_{394}|\ [Si_{384}Al_{384}O_{1536}]$

REFINED COMPOSITION: $|Na_{426.6}(H_2O)_{393.6}|\ [Si_{384}Al_{384}O_{1536}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre $(\overline{3})$
$a = 36.95$ Å $b = 36.95$ Å $c = 36.95$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.051$

REFERENCE: Y. F. Shepelev, Y. I. Smolin, I. K. Butikova and V. I. Tarasov, *Doklady Akad. Nauk SSSR* **272** 1133–1137 (1975).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	4.14	21.333	8	34.7	9	5	3	25.86	3.446	24	2.3	14	0	2	34.32	2.613	12	2.0
2	2	0	6.77	13.064	12	100.0	8	4	6	25.97	3.431	24	1.5	13	5	3	34.59	2.593	24	0.7
3	1	1	7.94	11.141	24	54.6	8	6	4	25.97	3.431	24	1.0	13	3	5	34.59	2.593	24	0.7
2	2	2	8.29	10.667	8	7.5	10	2	4	26.42	3.373	24	5.0	14	2	2	34.67	2.587	24	0.6
4	0	0	9.57	9.238	6	24.0	10	4	2	26.42	3.373	24	2.3	9	9	7	35.28	2.544	24	3.9
3	3	1	10.44	8.477	24	4.8	8	8	0	27.31	3.266	12	0.8	11	9	3	35.28	2.544	24	0.6
5	1	1	12.45	7.111	24	10.4	11	3	1	27.63	3.228	24	2.1	12	6	6	35.71	2.514	24	1.9
3	3	3	12.45	7.111	8	0.8	11	1	3	27.63	3.228	24	1.1	12	8	4	36.39	2.469	24	0.8
4	4	0	13.56	6.532	12	58.6	9	1	7	27.63	3.228	24	2.2	15	1	1	36.64	2.452	24	8.2
5	3	1	14.18	6.246	24	14.3	9	7	1	27.63	3.228	24	3.6	11	5	9	36.64	2.452	24	3.3
5	1	3	14.18	6.246	24	13.5	8	8	2	27.74	3.216	24	1.1	11	9	5	36.64	2.452	24	2.1
4	4	2	14.38	6.158	24	0.8	10	4	4	27.74	3.216	24	2.0	10	8	8	36.73	2.447	24	5.1
6	0	2	15.16	5.842	12	0.9	8	6	6	28.16	3.168	24	0.9	15	3	1	37.31	2.410	24	0.6
6	2	0	15.16	5.842	12	4.4	10	0	6	28.16	3.168	12	0.7	9	9	9	37.96	2.370	8	3.1
5	3	3	15.73	5.635	24	6.5	9	7	3	28.48	3.134	24	3.9	11	7	9	38.60	2.332	24	0.6
6	2	2	15.91	5.570	24	2.8	11	3	3	28.48	3.134	24	6.6	16	0	0	39.00	2.309	6	2.0
4	4	4	16.62	5.333	8	2.9	9	3	7	28.48	3.134	24	1.5	15	5	3	39.24	2.296	24	1.5
5	5	1	17.14	5.174	24	12.6	11	5	1	29.30	3.048	24	1.3	15	3	5	39.24	2.296	24	1.3
6	2	4	17.96	4.938	24	2.1	11	1	5	29.30	3.048	24	2.0	15	5	5	40.48	2.228	24	1.8
7	1	3	18.44	4.810	24	6.2	7	7	7	29.30	3.048	8	0.8	16	2	4	40.56	2.224	24	0.9
7	3	1	18.44	4.810	24	4.8	10	4	6	29.81	2.997	24	11.7	16	4	2	40.56	2.224	24	0.8
7	3	3	19.67	4.514	24	4.6	10	6	4	29.81	2.997	24	7.0	15	3	7	41.09	2.196	24	0.7
8	2	2	20.39	4.355	24	3.9	12	2	2	29.81	2.997	24	7.7	12	12	0	41.47	2.177	12	9.0
6	6	0	20.39	4.355	12	3.6	11	5	3	30.11	2.968	24	0.8	17	1	1	41.70	2.166	24	0.9
5	5	5	20.82	4.267	8	1.0	12	0	4	30.60	2.921	12	2.7	11	11	7	41.70	2.166	24	2.1
7	1	5	20.82	4.267	24	1.0	12	4	0	30.60	2.921	12	2.2	12	12	2	41.77	2.162	24	1.3
6	6	2	20.96	4.238	24	1.7	12	2	4	30.99	2.885	24	3.2	13	7	9	42.29	2.137	24	0.7
8	4	0	21.51	4.131	12	1.3	12	4	2	30.99	2.885	24	1.9	17	3	3	42.88	2.109	24	2.2
8	0	4	21.51	4.131	12	6.7	10	2	8	31.38	2.851	24	1.0	12	10	8	42.96	2.105	24	0.6
7	5	3	21.91	4.056	24	14.1	11	1	7	31.66	2.826	24	1.6	16	0	8	43.83	2.066	12	0.7
7	3	5	21.91	4.056	24	7.7	11	5	5	31.66	2.826	24	5.7	17	5	3	44.04	2.056	24	1.3
9	1	1	21.91	4.056	24	6.7	11	7	1	31.66	2.826	24	3.4	15	7	7	44.04	2.056	24	0.6
8	2	4	22.05	4.032	24	1.0	13	1	1	31.66	2.826	24	0.9	17	3	5	44.04	2.056	24	2.1
6	6	4	22.57	3.939	24	5.5	12	4	4	32.14	2.785	24	6.8	11	11	9	44.04	2.056	24	1.0
8	4	4	23.59	3.771	24	17.9	11	3	7	32.42	2.762	24	0.6	16	6	6	44.40	2.040	24	0.8
7	7	1	23.96	3.714	24	1.7	13	3	1	32.42	2.762	24	10.6	13	9	9	44.61	2.031	24	0.9
9	3	3	23.96	3.714	24	24.0	9	7	7	32.42	2.762	24	9.7	13	13	1	45.18	2.007	24	0.6
7	5	5	23.96	3.714	24	3.1	13	1	3	32.42	2.762	24	8.9	19	1	1	46.84	1.939	24	0.8
8	6	2	24.57	3.623	24	1.2	10	8	4	32.51	2.754	24	0.9	16	10	4	47.46	1.916	24	0.7
9	5	1	24.93	3.572	24	2.1	12	2	6	32.88	2.724	24	2.3	16	4	10	47.46	1.916	24	0.6
9	1	5	24.93	3.572	24	1.2	12	6	2	32.88	2.724	24	2.2	14	14	0	48.80	1.866	12	2.7
7	7	3	24.93	3.572	24	1.9	9	9	5	33.15	2.702	24	6.1	18	6	6	49.06	1.857	24	0.9
6	6	6	25.04	3.556	8	0.8	8	8	8	33.61	2.667	8	12.2	16	0	12	49.32	1.847	12	0.8
10	2	2	25.04	3.556	24	1.6	10	8	6	34.32	2.613	24	2.3	16	12	0	49.32	1.847	12	0.6
9	3	5	25.86	3.446	24	2.9	10	6	8	34.32	2.613	24	1.8	20	0	0	49.32	1.847	6	0.6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60

MAZ Mazzite

CHEMICAL COMPOSITION: $|Na_{0.8}K_{2.5}Ca_{1.4}Mg_{2.1}(H_2O)_{28}|\ [Si_{26.5}Al_{9.9}O_{72}]$
Mont Semiol, Loire, France

REFINED COMPOSITION: $|Na_{0.3}K_{2.52}Ca_{1.06}Mg_2(H_2O)_{31.48}|\ [Si_{26.28}Al_{9.72}O_{72}]$

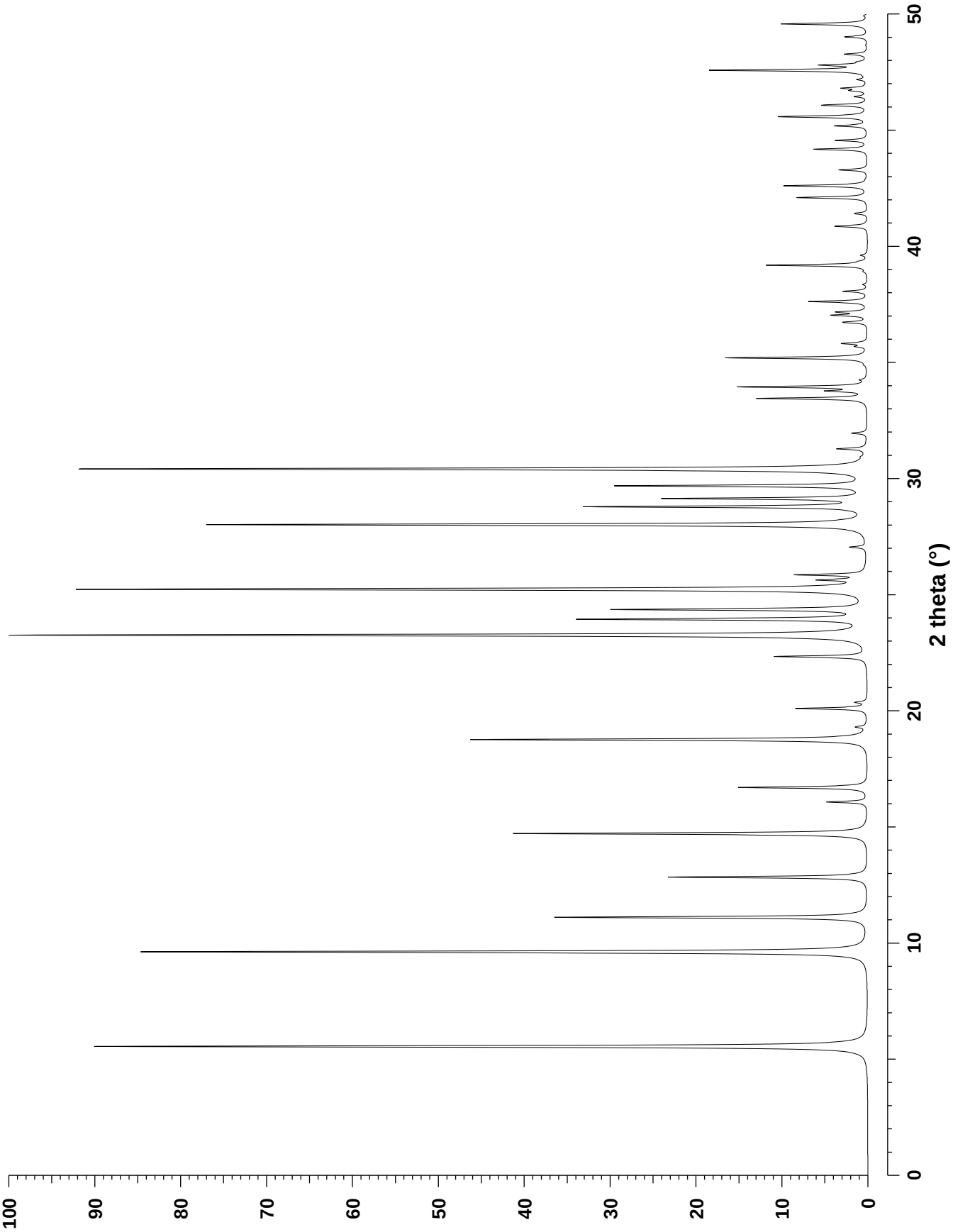
CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 18.392$ Å $b = 18.392$ Å $c = 7.646$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.05$

REFERENCE: E. Galli,
Rend. Soc. Ital. Mineral. Petrol. **31** 599–612 (1975).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.55	15.928	6	98.1	3	1	2	30.93	2.891	24	0.3	6	0	2	41.41	2.181	12	0.6
1	1	0	9.62	9.196	6	92.2	5	1	0	31.27	2.861	12	3.7	4	0	3	42.09	2.147	12	8.9
2	0	0	11.11	7.964	6	39.7	4	2	1	31.95	2.801	24	2.0	6	2	1	42.60	2.122	24	9.8
1	0	1	12.84	6.893	12	25.3	5	1	1	33.44	2.679	24	13.9	5	2	2	42.61	2.122	24	0.8
2	1	0	14.71	6.020	12	45.0	6	0	0	33.76	2.655	6	4.6	3	2	3	43.28	2.090	24	3.6
2	0	1	16.07	5.516	12	5.1	3	2	2	33.94	2.642	24	16.3	6	1	2	44.17	2.050	24	6.8
3	0	0	16.70	5.309	6	16.4	4	3	0	34.24	2.619	12	0.7	7	1	1	44.55	2.034	24	4.0
2	1	1	18.76	4.730	24	50.4	4	1	2	34.89	2.572	24	0.2	6	3	0	45.18	2.007	12	4.1
2	2	0	19.30	4.598	6	1.3	5	2	0	35.19	2.551	12	18.0	8	0	0	45.56	1.991	6	3.6
3	1	0	20.10	4.418	12	9.1	1	0	3	35.68	2.517	12	1.4	5	0	3	45.58	1.990	12	8.4
3	0	1	20.36	4.361	12	1.4	6	0	1	35.81	2.508	12	3.2	5	4	1	46.06	1.970	24	2.1
4	0	0	22.33	3.982	6	11.6	5	0	2	36.72	2.447	12	3.1	4	4	2	46.07	1.970	12	3.7
3	1	1	23.25	3.825	24	97.3	6	1	0	37.01	2.429	12	1.0	5	3	2	46.44	1.955	24	1.2
0	0	2	23.27	3.823	2	14.3	2	0	3	37.03	2.427	12	3.5	7	0	2	46.44	1.955	12	0.4
1	0	2	23.94	3.717	12	36.2	5	2	1	37.16	2.419	24	3.7	7	2	0	46.68	1.946	12	0.5
3	2	0	24.36	3.654	12	31.9	3	3	2	37.61	2.392	12	7.4	4	2	3	46.70	1.945	24	1.4
4	0	1	25.22	3.532	12	0.2	4	2	2	38.05	2.365	24	3.1	6	3	1	46.80	1.941	24	3.1
1	1	2	25.23	3.530	12	100.0	2	1	3	38.35	2.347	24	0.5	8	0	1	47.17	1.927	12	1.1
4	1	0	25.63	3.476	12	5.2	6	1	1	38.90	2.315	24	0.4	6	2	2	47.54	1.913	24	0.5
2	0	2	25.85	3.446	12	8.7	4	4	0	39.18	2.299	6	12.7	0	0	4	47.57	1.911	2	19.6
3	2	1	27.04	3.297	24	2.1	3	0	3	39.21	2.298	12	0.1	5	1	3	47.79	1.903	24	5.6
5	0	0	28.01	3.186	6	83.7	5	1	2	39.34	2.290	24	0.5	1	0	4	47.93	1.898	12	0.8
4	1	1	28.20	3.164	24	0.4	7	0	0	39.61	2.275	6	0.3	7	2	1	48.26	1.886	24	2.9
3	0	2	28.78	3.102	12	35.4	5	3	0	39.61	2.275	12	0.5	1	1	4	48.65	1.871	12	0.2
3	3	0	29.13	3.065	6	25.4	6	2	0	40.85	2.209	12	3.4	2	0	4	49.01	1.859	12	2.8
4	2	0	29.68	3.010	12	31.6	3	1	3	40.88	2.208	24	1.2	5	5	0	49.56	1.839	6	10.5
5	0	1	30.40	2.941	12	54.5	7	0	1	41.40	2.181	12	0.7	6	0	3	49.58	1.839	12	0.6
2	2	2	30.41	2.940	12	48.2	5	3	1	41.40	2.181	24	0.3	6	4	0	49.91	1.827	12	0.3

Mazzite

MAZ



MEI

ZSM-18, SiO_2 Framework

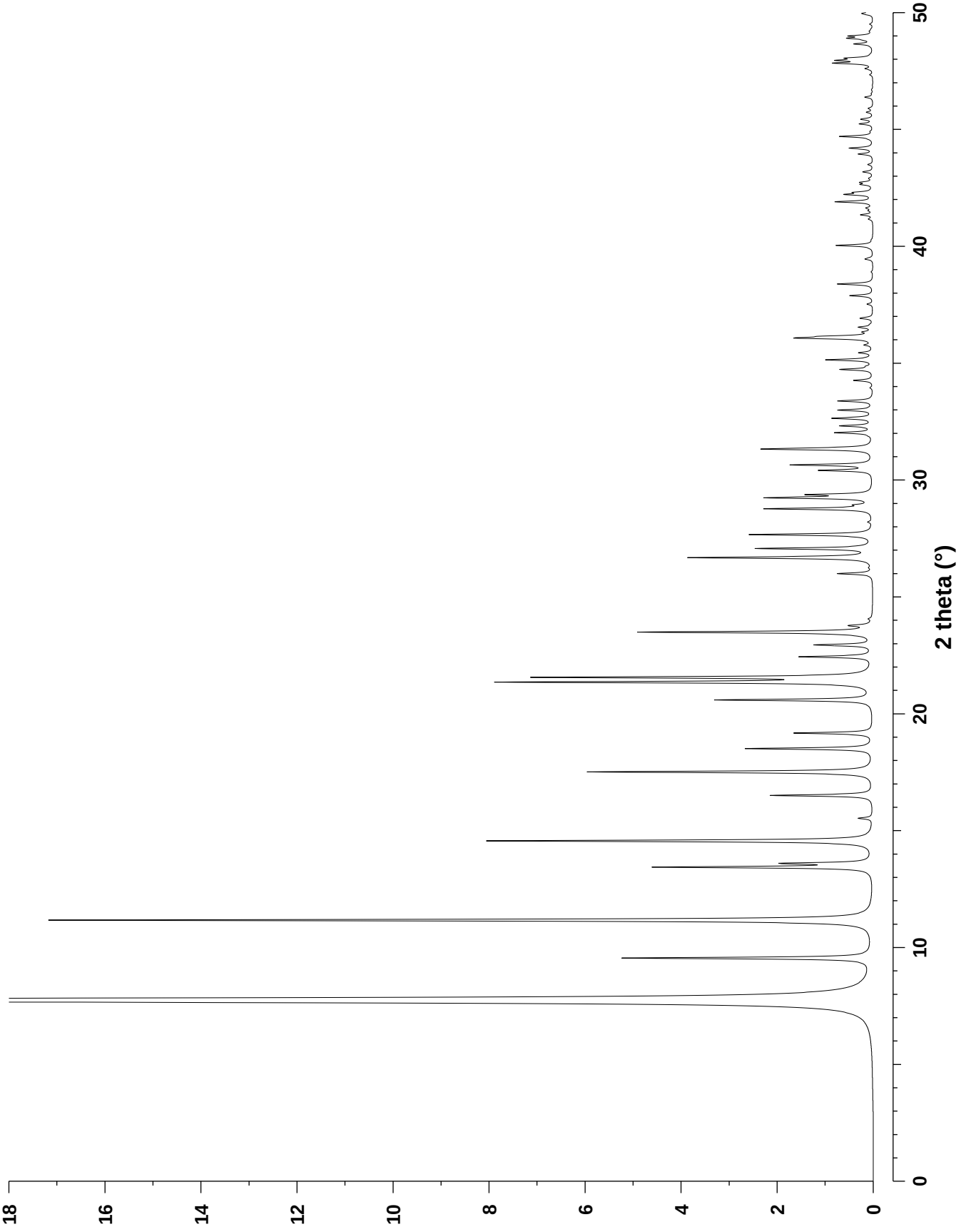
CHEMICAL COMPOSITION: $[Si_{34}O_{68}]$

REFINED COMPOSITION: $[Si_{34}O_{68}]$

CRYSTAL DATA: $P6_3/m$ (No. 176)
$a = 13.175$ Å $b = 13.175$ Å $c = 15.848$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
DLS refinement

REFERENCE: S. L. Lawton and W. J. Rohrbaugh,
Science **247** 1319–1322 (1990).

h	k	l	2θ	d	M	I_{rel}
1	0	0	7.75	11.410	6	100.0
1	0	1	9.55	9.260	12	5.2
0	0	2	11.17	7.924	2	17.2
1	1	0	13.44	6.587	6	4.5
1	0	2	13.60	6.508	12	1.7
1	1	1	14.56	6.083	12	8.0
2	0	0	15.53	5.705	6	0.3
2	0	1	16.51	5.368	12	2.1
1	1	2	17.51	5.066	12	5.9
1	0	3	18.51	4.794	12	2.6
2	0	2	19.17	4.630	12	1.6
2	1	0	20.59	4.313	6	2.8
1	2	0	20.59	4.313	6	0.5
1	2	1	21.35	4.161	12	7.5
1	1	3	21.56	4.121	12	6.9
0	0	4	22.44	3.962	2	1.5
2	0	3	22.94	3.876	12	1.2
3	0	0	23.39	3.803	6	0.1
1	2	2	23.49	3.788	12	4.8
1	0	4	23.77	3.743	12	0.4
3	0	2	25.99	3.429	12	0.7
1	2	3	26.68	3.341	12	3.6
2	1	3	26.68	3.341	12	0.2
2	2	0	27.07	3.294	6	2.4
2	2	1	27.66	3.225	12	2.6
3	1	1	28.77	3.103	12	2.2
3	0	3	28.93	3.087	12	0.3
1	0	5	29.24	3.054	12	2.2
2	2	2	29.37	3.041	12	1.2
1	3	2	30.41	2.939	12	0.2
3	1	2	30.41	2.939	12	0.9
1	2	4	30.64	2.918	12	1.7
1	1	5	31.32	2.856	12	2.0
4	0	0	31.36	2.852	6	0.7
2	2	3	32.02	2.795	12	0.8
2	0	5	32.31	2.771	12	0.7
3	0	4	32.64	2.744	12	0.8
1	3	3	32.99	2.715	12	0.6
3	1	3	32.99	2.715	12	0.1
4	0	2	33.38	2.684	12	0.7
2	3	0	34.26	2.618	6	0.3
2	3	1	34.73	2.583	12	0.4
3	2	1	34.73	2.583	12	0.3
2	1	5	35.14	2.554	12	0.7
1	2	5	35.14	2.554	12	0.3
2	2	4	35.44	2.533	12	0.3
4	0	3	35.77	2.510	12	0.1
4	1	0	36.07	2.490	6	0.2
1	4	0	36.07	2.490	6	1.2
2	3	2	36.14	2.486	12	0.3
3	2	2	36.14	2.486	12	0.5
3	1	4	36.33	2.473	12	0.2
1	4	1	36.53	2.460	12	0.2
4	1	1	36.53	2.460	12	0.1
3	0	5	36.92	2.435	12	0.3
2	0	6	37.52	2.397	12	0.1
4	1	2	37.88	2.375	12	0.3
1	4	2	37.88	2.375	12	0.2
3	2	3	38.38	2.345	12	0.3
2	3	3	38.38	2.345	12	0.5
2	2	5	39.45	2.284	12	0.1
1	2	6	40.03	2.252	12	0.4
1	4	3	40.03	2.252	12	0.3
3	2	4	41.34	2.184	12	0.1
2	3	4	41.34	2.184	12	0.1
3	0	6	41.63	2.169	12	0.1
2	4	0	41.90	2.156	6	0.4
4	2	0	41.90	2.156	6	0.3
1	1	7	42.21	2.141	12	0.5
4	2	1	42.30	2.137	12	0.3
4	0	5	42.64	2.120	12	0.2
3	3	2	42.73	2.116	12	0.2
5	0	3	43.18	2.095	12	0.2
2	2	6	43.94	2.061	12	0.3
5	1	0	44.19	2.049	6	0.3
1	5	0	44.19	2.049	6	0.2
1	3	6	44.69	2.028	12	0.3
3	3	3	44.69	2.028	12	0.4
1	2	7	45.23	2.005	12	0.2
2	4	3	45.43	1.996	12	0.1
5	1	2	45.73	1.984	12	0.1
1	4	5	46.37	1.958	12	0.2
6	0	0	47.83	1.902	6	0.8
1	1	8	47.95	1.897	12	0.6
4	2	4	48.04	1.894	12	0.3
2	4	4	48.04	1.894	12	0.1
2	0	8	48.65	1.871	12	0.4
4	3	1	48.89	1.863	12	0.5
3	2	6	48.99	1.859	12	0.1
2	3	6	48.99	1.859	12	0.3
4	3	2	49.96	1.825	12	0.1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MEL ZSM-11, Calcined

CHEMICAL COMPOSITION: $[Si_{96}O_{192}]$

REFINED COMPOSITION: $[Si_{96}O_{192}]$

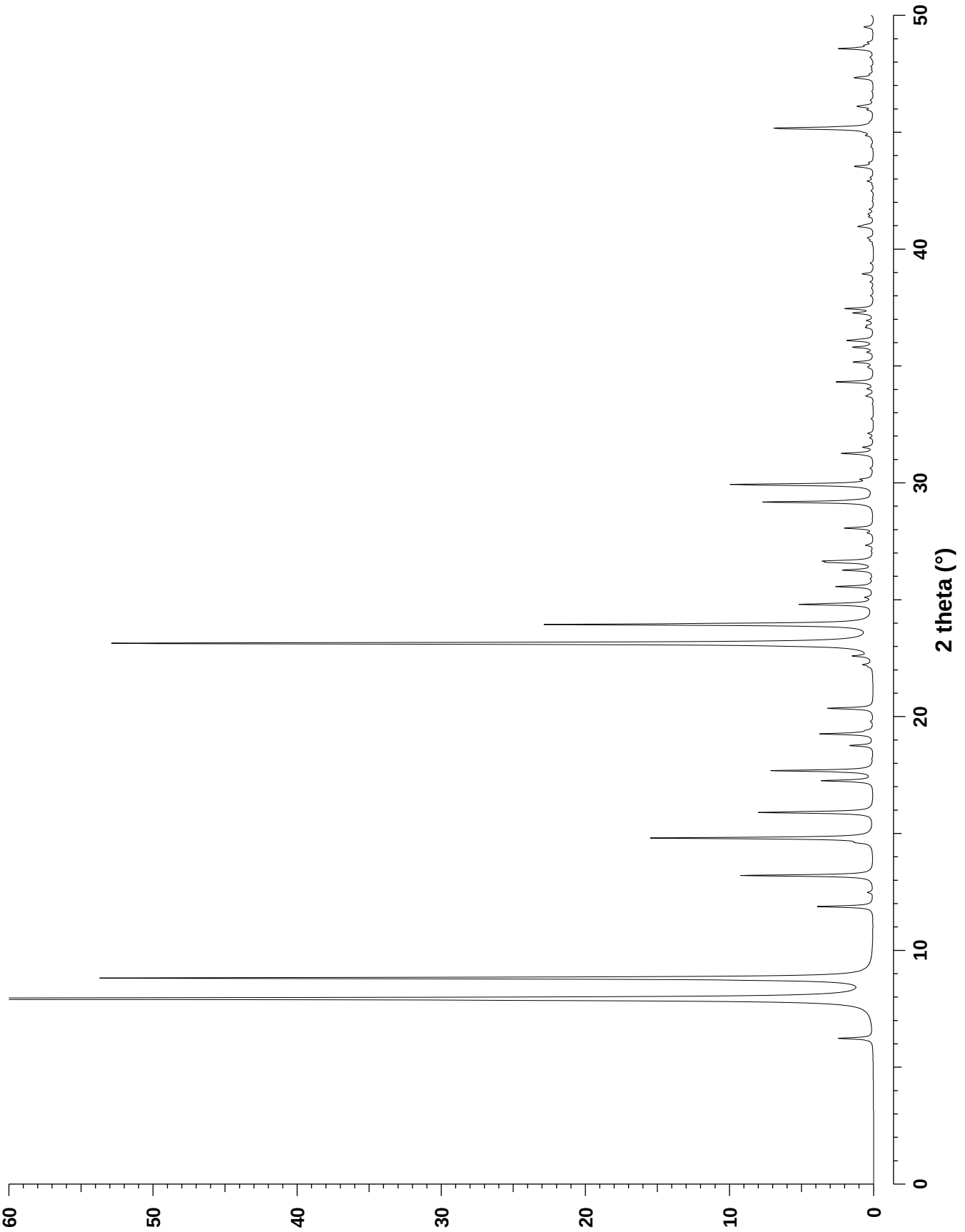
CRYSTAL DATA: $I\bar{4}m2$ (No. 119)
$a = 20.067$ Å $b = 20.067$ Å $c = 13.411$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_p = 0.13$

REFERENCE: C. A. Fyfe, H. Gies, G. T. Kokotailo, C. Pasztor, H. Strobl and D. E. Cox, *J. Am. Chem. Soc.* **111** 2470–2474 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.23	14.190	4	2.4	5	4	1	29.26	3.052	16	0.4	5	0	5	40.45	2.230	8	0.1
1	0	1	7.93	11.150	8	100.0	5	0	3	29.92	2.986	8	9.6	6	5	3	40.49	2.228	16	0.3
2	0	0	8.81	10.033	4	53.6	4	3	3	29.92	2.986	16	0.3	7	5	2	40.96	2.203	16	1.0
2	1	1	11.87	7.458	16	3.9	3	1	4	30.15	2.964	16	0.7	9	0	1	41.03	2.199	8	0.4
2	2	0	12.48	7.095	4	0.4	6	3	1	30.62	2.920	16	0.2	2	0	6	41.38	2.182	8	0.3
0	0	2	13.20	6.706	2	9.2	6	2	2	31.18	2.868	16	0.1	5	2	5	41.48	2.177	16	0.2
1	1	2	14.61	6.063	8	0.7	5	2	3	31.25	2.862	16	2.2	5	5	4	41.70	2.166	8	0.2
3	0	1	14.80	5.986	8	15.5	7	1	0	31.52	2.838	8	0.1	8	4	2	42.49	2.128	16	0.2
2	0	2	15.90	5.575	8	8.0	5	5	0	31.52	2.838	4	0.6	3	1	6	42.90	2.108	16	0.4
3	2	1	17.25	5.140	16	3.6	7	0	1	31.92	2.803	8	0.2	8	5	1	43.06	2.101	16	0.2
4	0	0	17.68	5.017	4	7.1	4	0	4	32.11	2.788	8	0.4	6	1	5	43.48	2.081	16	0.1
3	3	0	18.76	4.730	4	1.6	3	3	4	32.74	2.735	8	0.2	8	3	3	43.53	2.079	16	1.3
3	1	2	19.26	4.609	16	3.7	1	0	5	33.71	2.659	8	0.5	7	3	4	43.69	2.072	16	0.3
4	1	1	19.40	4.575	16	0.3	6	1	3	33.77	2.654	16	0.2	4	0	6	44.37	2.042	8	0.1
4	2	0	19.79	4.487	8	0.2	7	3	0	34.02	2.635	8	0.4	3	3	6	44.85	2.021	8	0.4
1	0	3	20.35	4.363	8	3.2	7	1	2	34.31	2.613	16	0.3	9	4	1	45.00	2.014	16	0.2
4	0	2	22.13	4.017	8	0.2	5	5	2	34.31	2.613	8	2.3	8	0	4	45.14	2.008	8	3.6
2	1	3	22.22	4.001	16	0.6	2	1	5	34.91	2.570	16	0.1	10	0	0	45.18	2.007	4	4.7
5	1	0	22.59	3.935	8	1.2	5	4	3	34.96	2.566	16	0.3	8	6	0	45.18	2.007	8	0.2
3	3	2	23.01	3.865	8	1.2	5	1	4	35.16	2.552	16	1.4	10	1	1	45.95	1.975	16	0.4
5	0	1	23.13	3.845	8	52.5	6	5	1	35.58	2.523	16	0.4	8	2	4	46.09	1.969	16	0.9
4	3	1	23.13	3.845	16	0.3	8	0	0	35.80	2.508	4	1.4	10	2	0	46.13	1.968	8	0.4
4	2	2	23.86	3.729	16	0.1	3	0	5	36.08	2.490	8	1.6	7	0	5	46.36	1.959	8	0.2
3	0	3	23.94	3.717	8	22.7	6	3	3	36.13	2.486	16	0.6	10	0	2	47.28	1.922	8	0.3
5	2	1	24.80	3.590	16	5.1	7	3	2	36.64	2.452	16	0.5	8	5	3	47.33	1.921	16	1.2
4	4	0	25.10	3.547	4	0.5	8	1	1	36.72	2.447	16	0.3	7	5	4	47.48	1.915	16	0.2
3	2	3	25.56	3.485	16	2.6	8	2	0	36.94	2.433	8	0.4	10	3	1	47.80	1.903	16	0.2
5	3	0	25.89	3.441	8	0.1	3	2	5	37.21	2.416	16	0.2	10	2	2	48.20	1.888	16	0.2
5	1	2	26.26	3.394	16	2.1	7	0	3	37.26	2.413	8	1.3	5	3	6	48.57	1.875	16	2.4
0	0	4	26.59	3.353	2	2.4	5	3	4	37.45	2.402	16	1.9	8	7	1	48.71	1.869	16	0.5
6	0	0	26.65	3.345	4	2.7	6	0	4	38.00	2.368	8	0.2	8	4	4	48.84	1.865	16	0.3
1	1	4	27.33	3.263	8	0.5	7	5	0	38.59	2.333	8	0.2	3	0	7	49.49	1.842	8	0.7
6	1	1	27.85	3.203	16	0.4	8	3	1	38.93	2.313	16	0.8	8	1	5	49.99	1.824	16	0.2
2	0	4	28.06	3.180	8	2.0	8	2	2	39.39	2.288	16	0.2							
5	3	2	29.17	3.062	16	7.6	0	0	6	40.35	2.235	2	0.2							

ZSM-11, Calcined

MEL



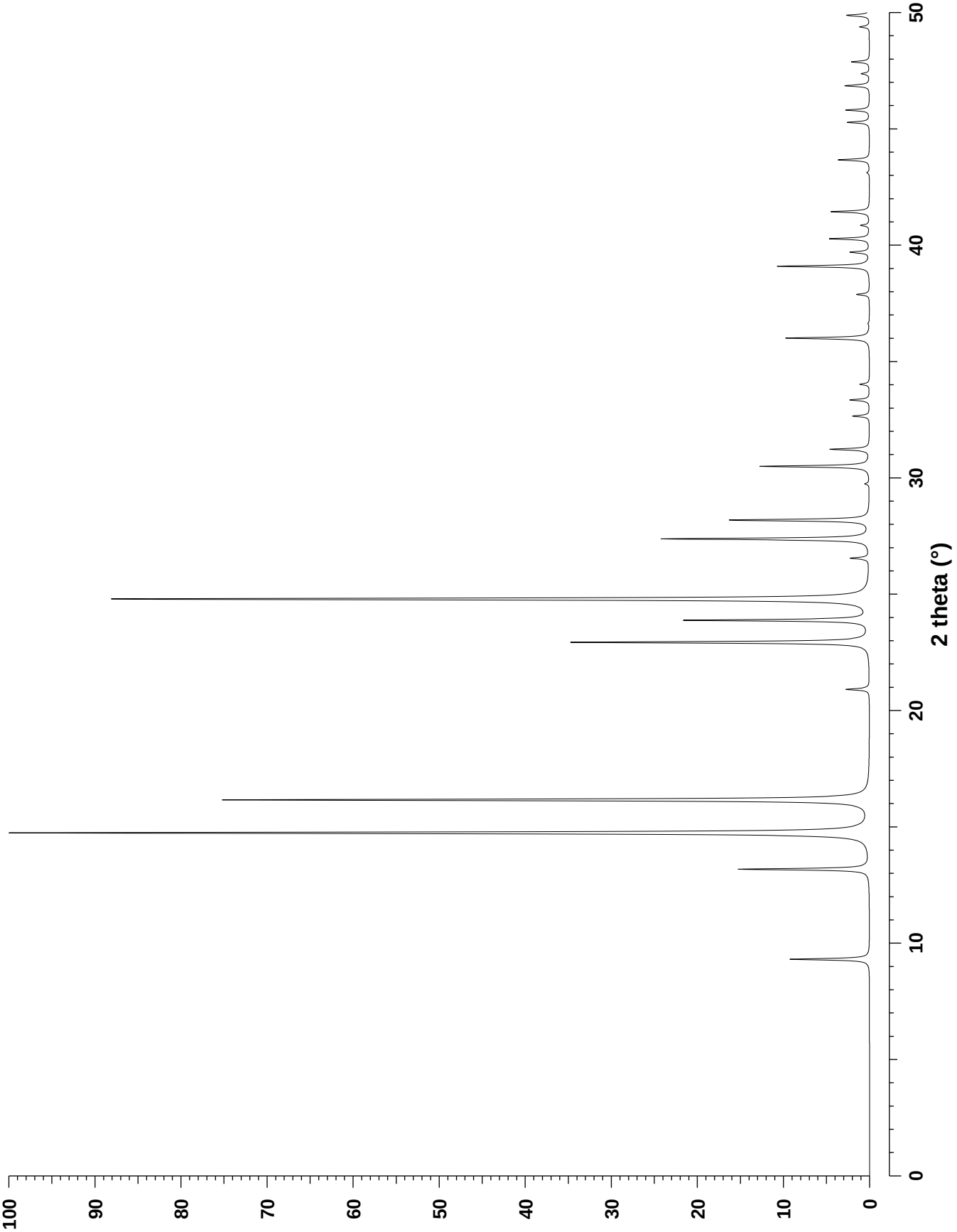
CHEMICAL COMPOSITION: $|(CH_4, N_2)_2(CO_2, N_2)_6|\ [Si_{46}O_{92}]$
Mt. Hamilton, California, U.S.A.

REFINED COMPOSITION: $|C_8|\ [Si_{46}O_{92}]$

CRYSTAL DATA: $Pm\overline{3}n$ (No. 223)
$a = 13.436$ Å $b = 13.436$ Å $c = 13.436$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: H. Gies,
Z. Kristallogr. **164** 247–257 (1983).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.31	9.501	12	9.3	4	2	2	32.65	2.743	24	2.0	5	4	0	43.11	2.098	24	0.3
2	0	0	13.18	6.718	6	15.2	4	3	0	33.34	2.687	24	2.3	5	4	1	43.66	2.073	48	3.7
2	1	0	14.74	6.009	24	100.0	5	1	0	34.02	2.635	24	1.1	6	3	0	45.27	2.003	24	0.3
2	1	1	16.16	5.485	24	75.2	5	2	0	36.00	2.495	24	0.2	5	4	2	45.27	2.003	48	2.2
3	1	0	20.91	4.249	24	2.7	4	3	2	36.00	2.495	48	9.6	6	3	1	45.80	1.981	48	2.8
2	2	2	22.93	3.879	8	34.7	5	2	1	36.63	2.453	48	0.2	4	4	4	46.85	1.939	8	2.9
3	2	0	23.88	3.726	24	21.4	4	4	0	37.88	2.375	12	1.5	6	3	2	47.36	1.919	48	1.0
3	2	1	24.79	3.591	48	88.1	5	3	0	39.09	2.304	24	7.6	7	1	0	47.87	1.900	24	0.2
4	0	0	26.54	3.359	6	2.2	4	3	3	39.09	2.304	24	3.1	5	5	0	47.87	1.900	12	1.9
4	1	0	27.37	3.259	24	24.2	5	3	1	39.69	2.271	48	2.2	7	2	0	49.38	1.846	24	0.8
4	1	1	28.18	3.167	24	1.0	4	4	2	40.27	2.239	24	1.0	6	4	1	49.38	1.846	48	0.3
3	3	0	28.18	3.167	12	15.3	6	0	0	40.27	2.239	6	3.7	5	5	2	49.87	1.828	24	0.1
4	2	0	29.74	3.004	24	0.5	6	1	0	40.85	2.209	24	1.0	7	2	1	49.87	1.828	48	0.3
4	2	1	30.49	2.932	48	12.7	6	1	1	41.43	2.180	24	0.2	6	3	3	49.87	1.828	24	2.3
3	3	2	31.22	2.865	24	4.6	5	3	2	41.43	2.180	48	4.3							


100
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50
2 theta (°)

MER Merlinoite

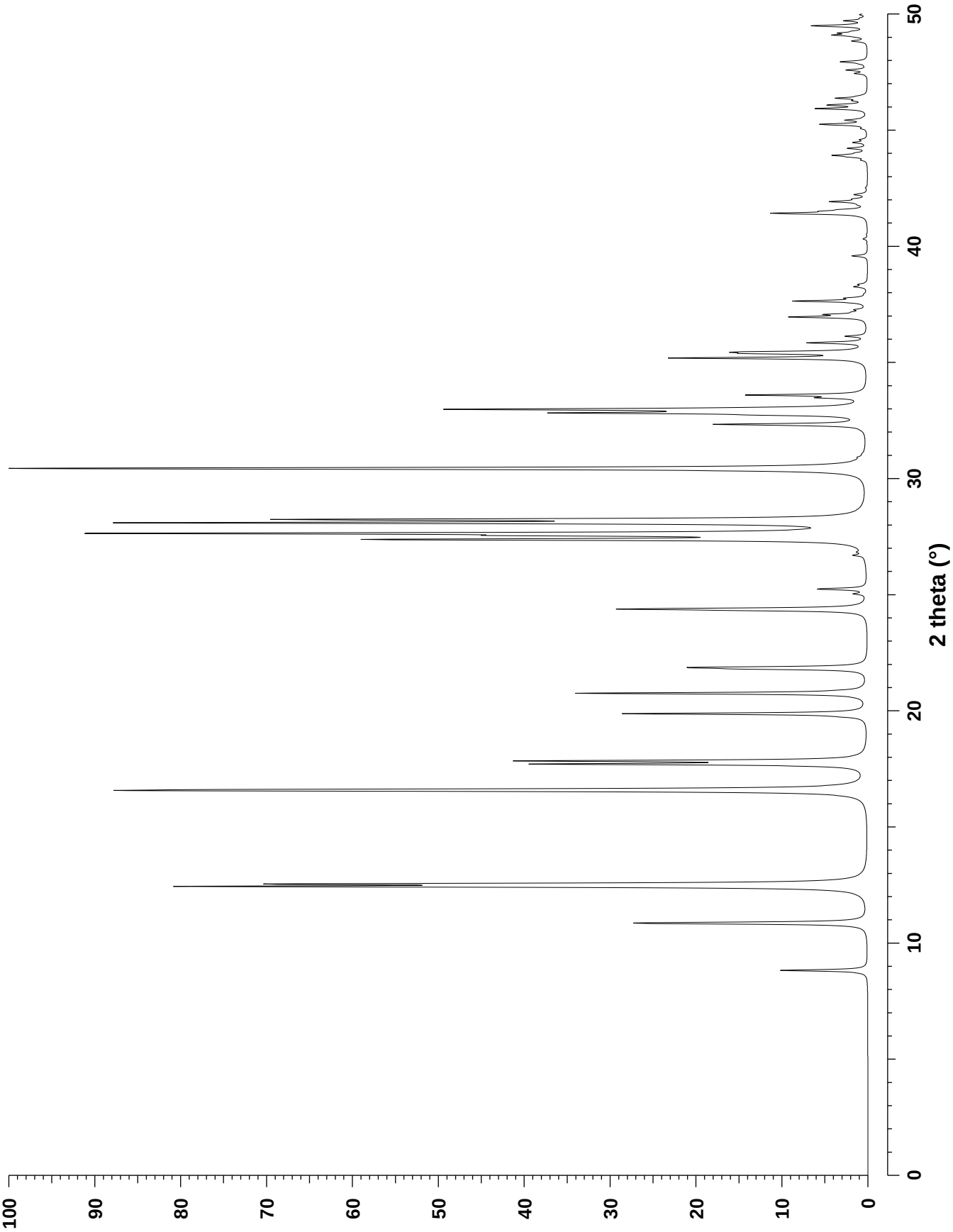
CHEMICAL COMPOSITION: $|Na_{0.55}K_{4.21}Ca_{1.49}Ba_{0.43}(H_2O)_{22.74}|\ [Si_{22.69}Al_{9.31}O_{64}]$
Cupaello, Italy

REFINED COMPOSITION: $|Na_{0.68}K_{5.28}Ca_{1.844}Ba_{0.444}(H_2O)_{19.44}|\ [Si_{22.72}Al_{9.28}O_{64}]$

CRYSTAL DATA: *Immm* (No. 71)
$a = 14.116$ Å $b = 14.229$ Å $c = 9.946$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.09$

REFERENCE: E. Galli, G. Gottardi and D. Pongiluppi,
Neues Jahrb. Miner. Monatsh. **1** 1–9 (1979).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.82	10.021	4	12.4	4	3	1	32.89	2.723	8	6.5	2	5	3	43.84	2.065	8	1.8
0	1	1	10.85	8.152	4	26.1	0	3	3	32.96	2.717	4	26.1	6	3	1	43.91	2.062	8	4.4
1	0	1	10.88	8.131	4	10.7	5	0	1	32.98	2.716	4	32.3	5	2	3	44.01	2.058	8	1.1
0	2	0	12.44	7.114	2	88.3	3	0	3	33.05	2.710	4	4.7	2	6	2	44.21	2.048	8	2.7
2	0	0	12.54	7.058	2	73.5	2	4	2	33.47	2.677	8	5.3	0	4	4	44.45	2.038	4	0.7
1	2	1	16.56	5.354	8	80.9	4	2	2	33.59	2.668	8	16.4	6	2	2	44.46	2.038	8	1.3
2	1	1	16.61	5.336	8	61.2	2	5	1	35.18	2.551	8	27.4	4	0	4	44.58	2.033	4	0.9
2	2	0	17.70	5.011	4	44.3	5	2	1	35.38	2.537	8	12.1	1	7	0	45.06	2.012	4	0.6
0	0	2	17.84	4.973	2	46.8	2	3	3	35.40	2.536	8	0.3	5	5	0	45.24	2.004	4	6.6
1	3	0	19.75	4.496	4	1.4	3	2	3	35.44	2.533	8	14.8	7	1	0	45.42	1.997	4	2.8
3	1	0	19.87	4.467	4	34.5	4	4	0	35.84	2.505	4	8.2	3	3	4	45.47	1.995	8	0.3
1	1	2	19.93	4.455	8	0.2	0	0	4	36.12	2.487	2	2.9	0	7	1	45.55	1.992	4	0.2
0	3	1	20.75	4.281	4	41.2	3	5	0	36.91	2.435	4	0.7	7	0	1	45.92	1.976	4	7.1
3	0	1	20.88	4.253	4	1.1	1	5	2	36.95	2.433	8	10.2	0	1	5	46.07	1.970	4	4.2
0	2	2	21.80	4.076	4	12.4	5	3	0	37.06	2.426	4	4.9	1	0	5	46.08	1.970	4	0.9
2	0	2	21.86	4.065	4	21.7	5	1	2	37.16	2.419	8	1.0	4	6	0	46.11	1.968	4	0.3
2	3	1	24.32	3.660	8	10.5	1	1	4	37.26	2.413	8	1.3	6	4	0	46.26	1.962	4	1.5
3	2	1	24.38	3.651	8	32.4	1	4	3	37.63	2.390	8	10.4	2	4	4	46.37	1.958	8	4.2
0	4	0	25.03	3.557	2	1.6	4	1	3	37.76	2.382	8	2.5	4	2	4	46.46	1.954	8	0.9
2	2	2	25.23	3.530	8	0.9	0	6	0	37.94	2.372	2	0.2	2	7	1	47.43	1.917	8	1.7
4	0	0	25.24	3.529	2	6.1	6	0	0	38.25	2.353	2	1.8	1	6	3	47.58	1.911	8	2.9
3	3	0	26.69	3.340	4	1.5	0	2	4	38.35	2.347	4	1.0	7	2	1	47.76	1.904	8	0.1
3	1	2	26.83	3.323	8	0.6	2	0	4	38.38	2.345	4	0.2	6	1	3	47.84	1.901	8	0.6
1	4	1	27.37	3.259	8	67.2	1	6	1	39.58	2.277	8	2.2	1	2	5	47.92	1.898	8	1.6
4	1	1	27.54	3.239	8	33.6	4	4	2	40.31	2.237	8	0.6	2	1	5	47.94	1.898	8	2.4
0	1	3	27.63	3.229	4	48.4	2	2	4	40.50	2.227	8	0.1	3	7	0	48.80	1.866	4	0.3
1	0	3	27.64	3.228	4	57.7	3	5	2	41.28	2.187	8	0.2	1	7	2	48.83	1.865	8	1.9
2	4	0	28.09	3.177	4	100.0	5	3	2	41.41	2.180	8	12.9	5	5	2	49.00	1.859	8	0.7
4	2	0	28.23	3.161	4	76.4	1	3	4	41.50	2.176	8	4.2	1	5	4	49.08	1.856	8	4.2
1	2	3	30.41	2.939	8	63.1	3	1	4	41.57	2.173	8	2.5	7	1	2	49.17	1.853	8	3.2
2	1	3	30.44	2.936	8	75.5	4	5	1	41.77	2.162	8	0.6	5	1	4	49.25	1.850	8	1.2
0	4	2	30.91	2.893	4	0.5	0	5	3	41.83	2.159	4	0.3	4	5	3	49.48	1.842	8	7.7
4	0	2	31.07	2.878	4	0.2	3	4	3	41.91	2.156	8	4.8	5	4	3	49.55	1.840	8	0.4
1	5	0	32.08	2.790	4	0.1	4	3	3	41.96	2.153	8	0.5	0	3	5	49.70	1.834	4	3.0
3	3	2	32.28	2.773	8	3.6	5	0	3	42.03	2.149	4	1.5	3	0	5	49.76	1.832	4	0.1
5	1	0	32.33	2.769	4	19.8	0	6	2	42.22	2.141	4	1.8	4	6	2	49.82	1.830	8	0.7
0	5	1	32.73	2.736	4	8.4	6	0	2	42.51	2.127	4	0.2	6	4	2	49.96	1.825	8	1.0
3	4	1	32.82	2.729	8	38.2	3	6	1	43.70	2.071	8	0.7							


0
10
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50
2 theta (°)
100
90
80
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60
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40
30
20
10
0

MER Barium Chloroaluminosilicate

CHEMICAL COMPOSITION: $|Ba_4(H_2O)_{12}(BaCl_2)_4|\ [Si_{21.33}Al_{10.67}O_{64}]$

REFINED COMPOSITION: $|(Ba_3Cl_2O)_4|\ [Si_{21.34}Al_{10.66}O_{64}]$

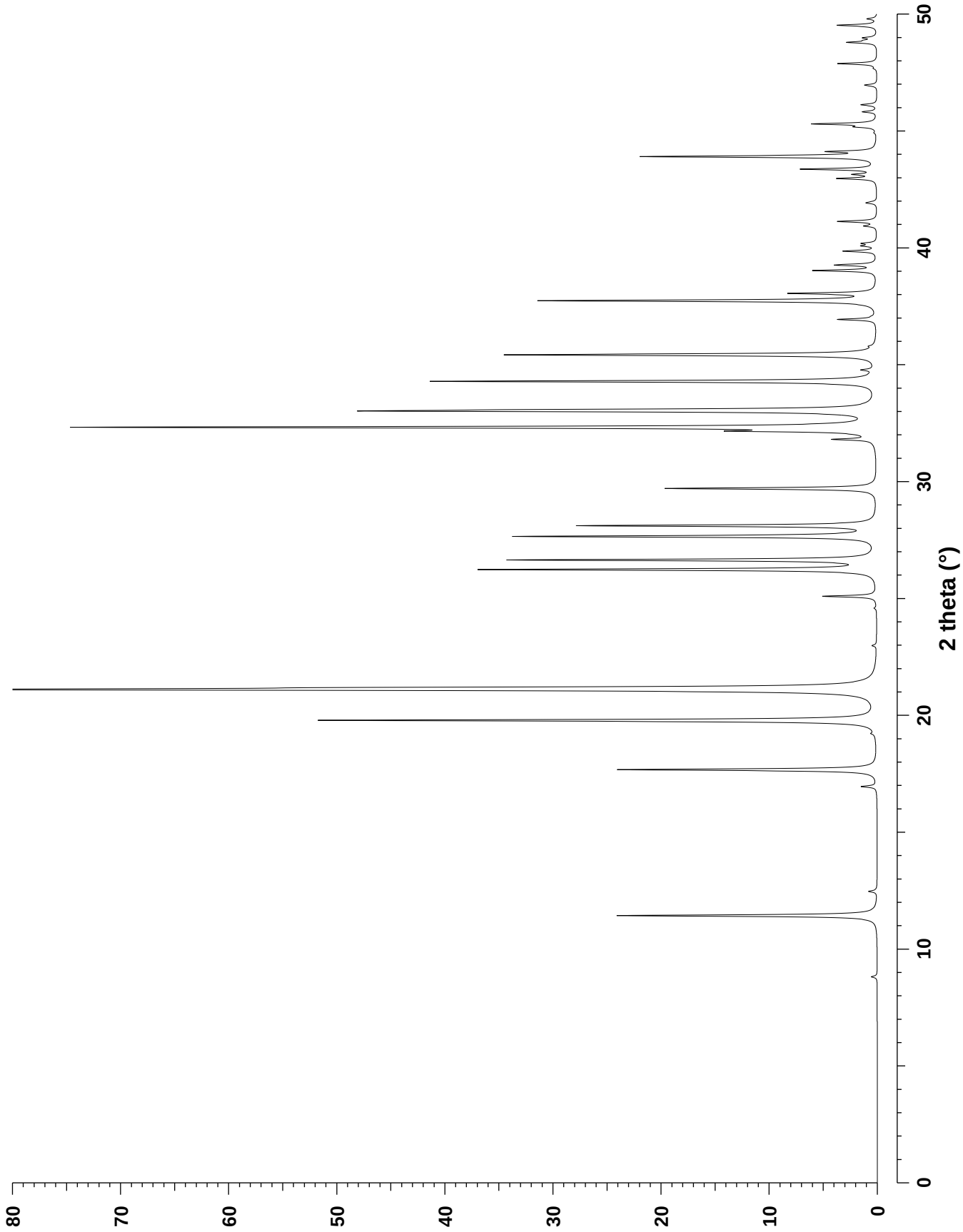
CRYSTAL DATA: $I\,4/m\,mm$ (No. 139)
$a = 14.194$ Å $b = 14.194$ Å $c = 9.234$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.14$

REFERENCE: L. P. Solov'eva, S. V. Borisov and V. V. Bakakin, *Sov. Phys. – Crystallogr.* **16** 1035–1038 (1972).

h	k	l	2θ	d	M	$I_{\rm rel}$
1	1	0	8.81	10.037	4	0.6
1	0	1	11.43	7.740	8	25.9
2	0	0	12.47	7.097	4	0.8
2	1	1	16.95	5.231	16	1.5
2	2	0	17.67	5.018	4	25.8
0	0	2	19.22	4.617	2	0.3
3	1	0	19.78	4.489	8	55.4
3	0	1	21.10	4.211	8	100.0
1	1	2	21.18	4.194	8	36.2
2	0	2	22.98	3.870	8	0.4
3	2	1	24.58	3.621	16	0.2
4	0	0	25.09	3.549	4	5.3
2	2	2	26.23	3.398	8	39.3
3	3	0	26.64	3.346	4	36.3
4	1	1	27.65	3.226	16	35.5
3	1	2	27.72	3.218	16	1.8
4	2	0	28.11	3.174	8	29.6
1	0	3	29.70	3.008	8	21.0
4	0	2	31.80	2.814	8	3.9
5	1	0	32.15	2.784	8	10.9
2	1	3	32.32	2.770	16	79.3
4	3	1	33.01	2.713	16	36.4
5	0	1	33.01	2.713	8	7.7
3	3	2	33.07	2.709	8	23.3
4	2	2	34.28	2.615	16	44.2
3	0	3	34.77	2.580	8	1.2
5	2	1	35.42	2.535	16	37.0
4	4	0	35.79	2.509	4	0.4
5	3	0	36.93	2.434	8	3.8
3	2	3	37.07	2.425	16	0.2
5	1	2	37.73	2.384	16	33.6
6	0	0	38.04	2.366	4	8.3
0	0	4	39.02	2.309	2	6.3
4	1	3	39.26	2.295	16	4.1
6	1	1	39.85	2.262	16	3.3
1	1	4	40.08	2.250	8	1.4
6	2	0	40.18	2.244	8	1.4
4	4	2	40.93	2.205	8	1.2
2	0	4	41.12	2.195	8	3.9
5	4	1	41.91	2.155	16	1.0
5	3	2	41.96	2.153	16	0.3
6	0	2	42.96	2.105	8	3.8
2	2	4	43.13	2.097	8	2.1
5	0	3	43.36	2.087	8	3.3
4	3	3	43.36	2.087	16	4.1
6	3	1	43.90	2.062	16	23.4
3	1	4	44.11	2.053	16	4.4
6	2	2	44.91	2.018	16	0.2
7	1	0	45.17	2.007	8	1.7
5	2	3	45.29	2.002	16	6.3
7	0	1	45.81	1.981	8	1.4
6	4	0	46.11	1.968	8	1.6
4	0	4	46.95	1.935	8	1.2
7	2	1	47.67	1.908	16	0.3
3	3	4	47.87	1.900	8	3.9
4	2	4	48.78	1.867	16	2.9
7	3	0	48.87	1.864	8	0.8
6	1	3	48.98	1.860	16	1.3
5	5	2	49.51	1.841	8	3.8
7	1	2	49.51	1.841	16	0.2
1	0	5	49.79	1.831	8	1.0

Barium Chloroaluminosilicate

MER



MFI Tetrapropylammonium ZSM-5

CHEMICAL COMPOSITION: $|((C_3H_7)_4NOH)_4|\ [Si_{95.7}Al_{0.3}O_{192}]$
$(C_3H_7)_4NOH$ = tetrapropylammonium hydroxide

REFINED COMPOSITION: $|(C_{12}N)_4|\ [Si_{96}O_{192}]$

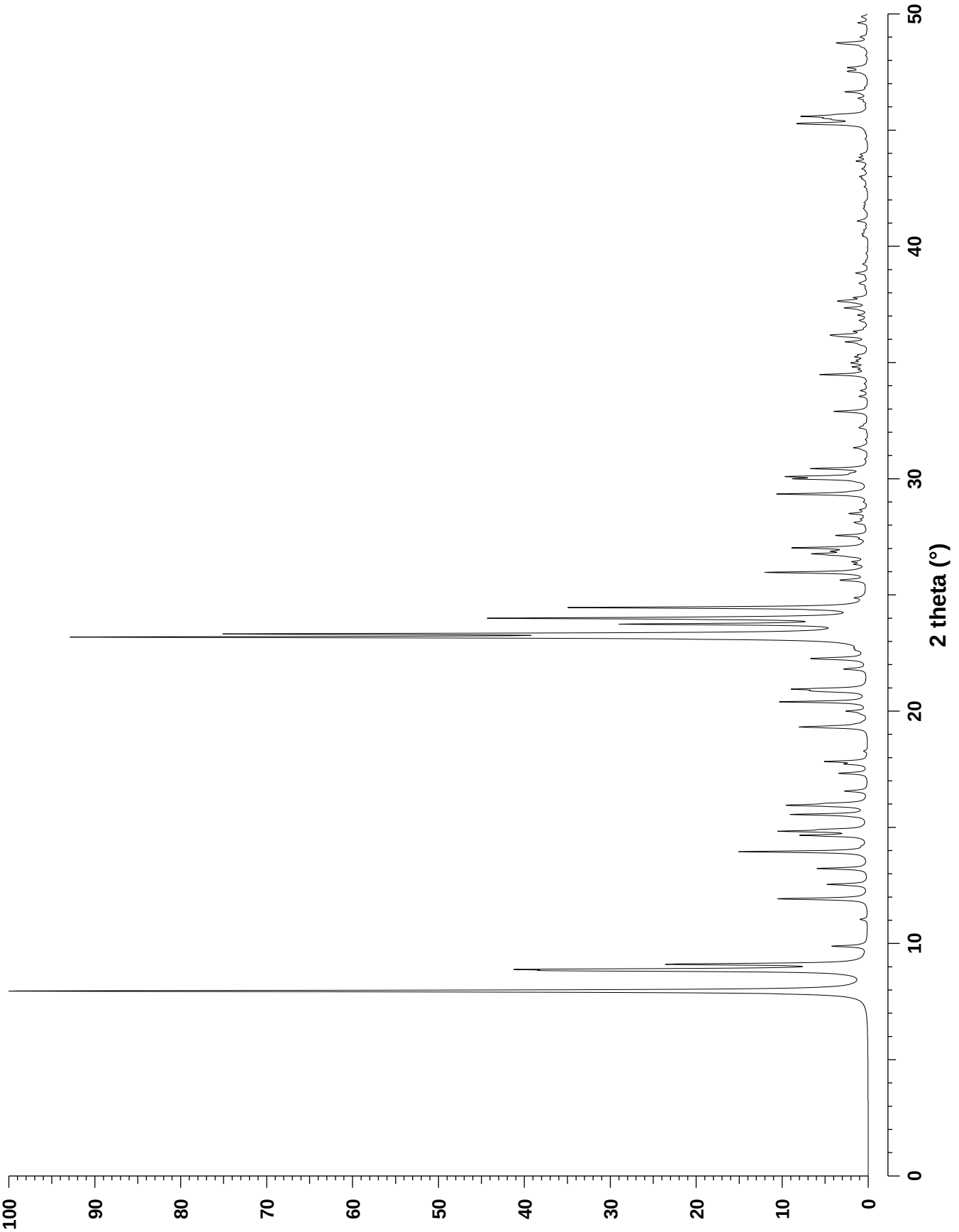
CRYSTAL DATA: *Pnma* (No. 62)
$a = 20.022$ Å $b = 19.899$ Å $c = 13.383$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: H. van Koningsveld, H. van Bekkum and J. C. Jansen, *Acta Cryst.* **B43** 127–132 (1987).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	7.95	11.126	4	68.4	0	5	1	23.32	3.815	4	78.7	6	5	0	35.09	2.557	4	1.0
0	1	1	7.96	11.105	4	50.3	1	5	1	23.74	3.747	8	31.0	5	1	4	35.24	2.546	8	1.4
2	0	0	8.83	10.011	2	31.3	3	0	3	23.99	3.709	4	47.7	1	5	4	35.33	2.540	8	1.0
0	2	0	8.89	9.950	2	36.8	0	3	3	24.04	3.702	4	4.0	5	6	1	35.79	2.509	8	0.5
1	1	1	9.11	9.711	8	25.4	2	5	0	24.06	3.698	4	1.8	8	0	0	35.88	2.503	2	2.6
2	1	0	9.89	8.943	4	4.7	1	3	3	24.45	3.640	8	39.7	0	8	0	36.11	2.487	2	1.9
2	0	1	11.04	8.016	4	1.0	5	2	1	24.87	3.579	8	1.2	3	0	5	36.16	2.484	4	1.9
2	1	1	11.90	7.436	8	2.8	3	2	3	25.63	3.475	8	3.0	0	3	5	36.19	2.482	4	2.1
1	2	1	11.93	7.417	8	10.4	2	3	3	25.66	3.472	8	0.6	2	5	4	36.20	2.481	8	1.0
2	2	0	12.54	7.057	4	5.4	4	3	2	25.97	3.430	8	13.6	3	6	3	36.34	2.472	8	0.6
0	0	2	13.23	6.692	2	6.8	5	1	2	26.32	3.386	8	1.3	4	7	0	36.34	2.472	4	0.9
1	0	2	13.95	6.346	4	17.4	1	5	2	26.43	3.372	8	1.6	8	1	1	36.81	2.442	8	0.9
1	1	2	14.65	6.046	8	8.6	0	0	4	26.64	3.346	2	1.2	8	2	0	37.04	2.427	4	1.0
3	0	1	14.83	5.973	4	10.9	6	0	0	26.71	3.337	2	2.7	2	8	0	37.25	2.414	4	0.5
0	3	1	14.91	5.943	4	4.1	4	0	3	26.77	3.330	4	5.9	7	0	3	37.35	2.408	4	2.7
3	1	1	15.49	5.720	8	0.8	0	6	0	26.88	3.316	2	2.9	5	3	4	37.56	2.394	8	0.8
1	3	1	15.55	5.697	8	10.0	1	0	4	27.02	3.300	4	9.6	3	5	4	37.62	2.391	8	2.3
2	0	2	15.93	5.563	4	6.2	1	1	4	27.40	3.256	8	0.7	6	5	2	37.66	2.389	8	2.1
0	2	2	15.96	5.553	4	5.6	6	0	1	27.55	3.238	4	0.7	1	7	3	37.79	2.380	8	1.6
2	3	0	16.03	5.529	4	3.5	3	3	3	27.55	3.237	8	1.6	8	0	2	38.40	2.344	4	0.9
2	1	2	16.55	5.358	8	1.8	2	5	2	27.56	3.237	8	2.1	4	7	2	38.84	2.319	8	1.6
1	2	2	16.57	5.351	8	1.5	1	6	1	28.07	3.178	8	0.7	0	0	6	40.44	2.230	2	0.6
3	2	1	17.32	5.121	8	3.5	2	0	4	28.12	3.173	4	1.3	4	8	1	41.08	2.197	8	1.3
2	3	1	17.35	5.110	8	0.5	4	2	3	28.26	3.158	8	0.7	3	5	5	42.91	2.107	8	0.6
4	0	0	17.72	5.005	2	2.6	1	2	4	28.50	3.132	8	2.4	3	1	6	43.00	2.104	8	0.8
0	4	0	17.83	4.975	2	5.6	4	5	0	28.66	3.115	4	0.9	6	0	5	43.33	2.088	4	0.5
3	1	2	19.31	4.598	8	8.4	3	5	2	29.34	3.044	8	11.9	8	3	3	43.66	2.073	8	1.5
1	3	2	19.36	4.586	8	2.1	5	4	1	29.40	3.038	8	0.8	8	0	4	45.25	2.004	4	5.7
4	1	1	19.45	4.563	8	0.8	4	5	1	29.44	3.034	8	0.6	10	0	0	45.29	2.002	2	5.8
4	2	0	19.86	4.472	4	0.5	6	3	0	29.97	2.981	4	1.2	0	8	4	45.44	1.996	4	2.6
3	3	1	20.00	4.438	8	2.6	5	0	3	29.99	2.980	4	7.4	4	8	3	45.51	1.993	8	3.2
1	0	3	20.40	4.354	4	4.7	3	4	3	30.05	2.973	8	1.1	0	10	0	45.59	1.990	2	7.5
0	1	3	20.40	4.353	4	7.1	0	5	3	30.09	2.970	4	9.1	1	8	4	45.67	1.986	8	2.4
2	3	2	20.84	4.262	8	3.2	3	1	4	30.22	2.958	8	0.9	1	10	1	46.35	1.959	8	0.6
1	1	3	20.88	4.254	8	3.9	1	5	3	30.43	2.938	8	7.3	2	8	4	46.38	1.958	8	0.7
4	2	1	20.95	4.241	8	8.9	5	2	3	31.33	2.855	8	1.8	4	3	6	46.64	1.948	8	2.9
2	0	3	21.81	4.075	4	3.0	4	0	4	32.18	2.782	4	0.5	8	5	3	47.51	1.914	8	1.6
4	3	0	22.25	3.995	4	5.6	0	4	4	32.24	2.776	4	0.6	3	8	4	47.54	1.912	8	1.2
0	4	2	22.27	3.992	4	0.7	6	3	2	32.89	2.723	8	4.5	0	10	2	47.68	1.907	4	0.6
1	2	3	22.29	3.989	8	1.8	6	0	3	33.54	2.672	4	1.1	9	3	3	47.69	1.907	8	1.9
4	1	2	22.63	3.929	8	0.7	1	0	5	33.78	2.653	4	0.5	5	3	6	48.70	1.870	8	1.8
1	4	2	22.71	3.915	8	0.5	5	5	2	34.48	2.601	8	6.4	3	5	6	48.75	1.868	8	3.4
3	3	2	23.11	3.849	8	4.0	2	0	5	34.69	2.586	4	0.9	3	0	7	49.60	1.838	4	0.7
5	0	1	23.18	3.836	4	100.0	7	3	1	34.81	2.577	8	1.8	0	3	7	49.62	1.837	4	0.7
4	3	1	23.23	3.829	8	0.8	4	3	4	34.98	2.565	8	1.7	8	0	5	49.88	1.828	4	0.6

Tetrapropylammonium ZSM-5

MFI



MFI ZSM-5, Calcined

CHEMICAL COMPOSITION: $|H_{0.32}|\ [Si_{95.68}Al_{0.32}O_{192}]$

REFINED COMPOSITION: $[Si_{96}O_{192}]$

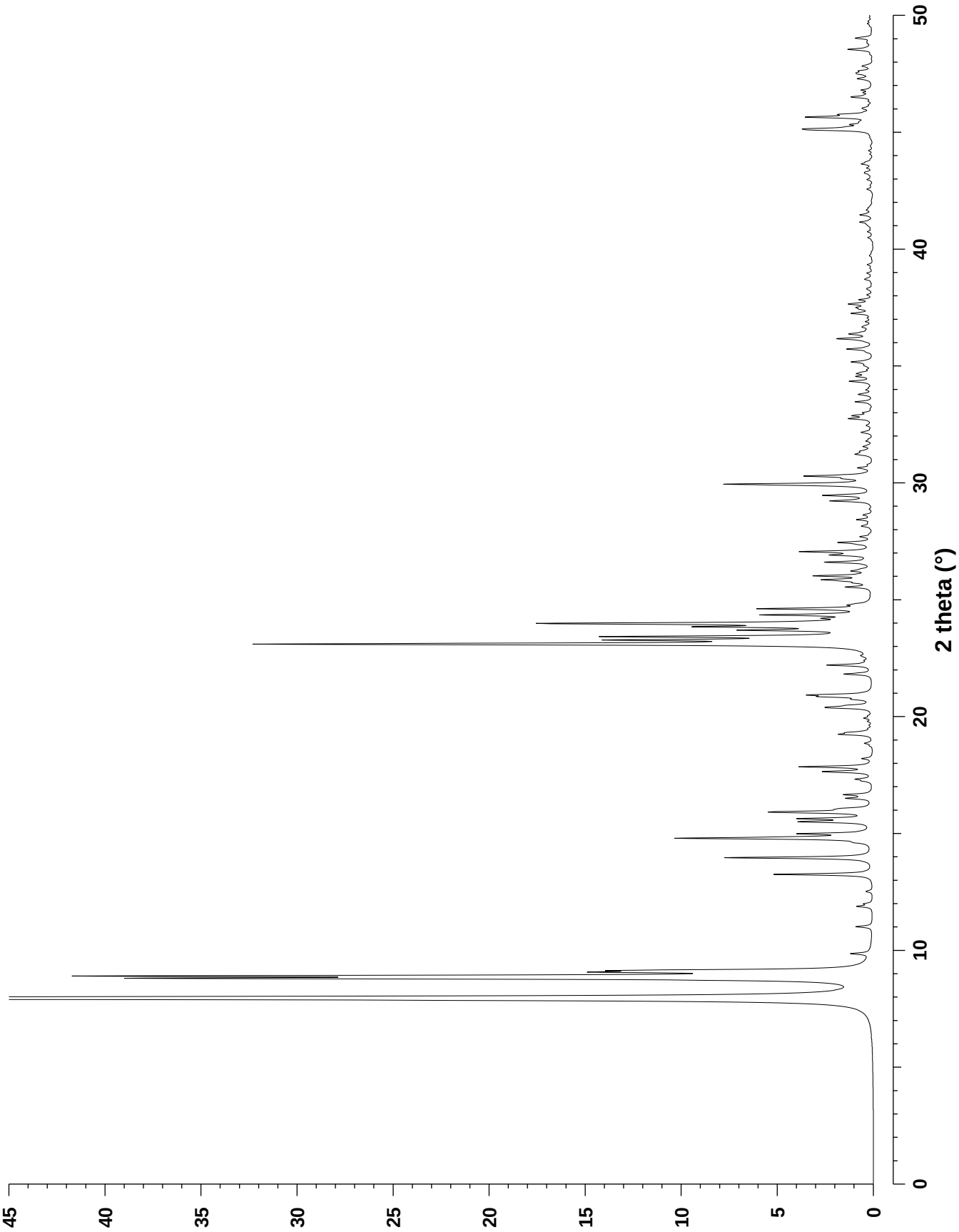
CRYSTAL DATA: $P1\,2_1/n\,1$ (No. 14) unique axis **b**, cell choice 2
$a = 19.879$ Å $b = 20.107$ Å $c = 13.369$ Å
$\alpha = 90°$ $\beta = 90.67°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.045$

REFERENCE: H. van Koningsveld, J. C. Jansen and H. van Bekkum, *Zeolites* **10** 235–242 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
-1	0	1	7.93	11.153	2	37.1	-5	0	1	23.27	3.823	2	16.1	5	4	2	31.78	2.816	4	0.4
0	1	1	7.94	11.132	4	100.0	5	0	1	23.42	3.798	2	18.2	-7	0	1	32.15	2.784	2	0.7
1	0	1	8.01	11.033	2	31.9	-5	1	1	23.69	3.756	4	8.1	-3	6	2	32.74	2.735	4	1.6
0	2	0	8.80	10.054	2	47.8	5	1	1	23.84	3.732	4	10.4	3	6	2	32.87	2.724	4	1.2
2	0	0	8.90	9.939	2	51.6	-3	0	3	23.93	3.718	2	1.4	3	3	4	32.99	2.715	4	0.4
-1	1	1	9.07	9.753	4	13.9	0	3	3	23.98	3.711	4	23.0	0	6	3	33.46	2.678	4	1.3
1	1	1	9.14	9.673	4	14.1	5	2	0	24.07	3.697	4	0.9	-1	0	5	33.77	2.654	2	0.9
1	2	0	9.86	8.971	4	1.4	3	0	3	24.20	3.678	2	2.1	0	7	2	33.97	2.639	4	0.4
0	2	1	11.01	8.035	4	1.2	-3	1	3	24.35	3.656	4	7.6	-5	5	2	34.34	2.612	4	1.6
-2	1	1	11.88	7.450	4	1.1	3	1	3	24.61	3.618	4	8.2	5	5	2	34.55	2.596	4	1.1
2	1	1	11.99	7.378	4	0.6	-2	5	1	24.77	3.595	4	1.0	-3	7	1	34.66	2.588	4	0.9
2	2	0	12.52	7.068	4	0.5	2	5	1	24.82	3.587	4	0.5	-5	1	4	35.16	2.552	4	0.6
0	0	2	13.25	6.684	2	7.3	-2	3	3	25.54	3.488	4	1.5	-1	5	4	35.17	2.552	4	0.9
0	1	2	13.96	6.343	4	11.0	-3	2	3	25.54	3.487	4	0.4	0	8	0	35.72	2.513	2	1.6
-1	1	2	14.61	6.062	4	0.7	2	3	3	25.71	3.465	4	0.9	8	0	0	36.15	2.485	2	1.1
0	3	1	14.79	5.991	4	13.7	3	2	3	25.79	3.454	4	1.0	0	3	5	36.17	2.483	4	1.4
-3	0	1	14.85	5.964	2	2.7	-3	4	2	25.85	3.446	4	3.1	7	4	0	36.34	2.472	4	0.7
3	0	1	14.99	5.909	2	4.9	3	4	2	26.02	3.425	4	4.1	-3	1	5	36.36	2.471	4	0.6
-3	1	1	15.50	5.718	4	5.0	-1	5	2	26.22	3.399	4	1.2	3	0	5	36.38	2.469	2	0.4
3	1	1	15.63	5.669	4	5.0	-5	1	2	26.32	3.385	4	0.4	2	8	0	36.89	2.437	4	0.4
-2	0	2	15.89	5.577	2	2.0	5	1	2	26.59	3.352	4	0.7	0	7	3	37.24	2.414	4	1.3
0	2	2	15.92	5.566	4	6.1	0	6	0	26.60	3.351	2	2.8	-5	3	4	37.44	2.402	4	0.5
3	2	0	16.02	5.532	4	1.3	6	0	0	26.91	3.313	2	2.7	-5	6	2	37.50	2.399	4	0.8
2	0	2	16.07	5.517	2	1.4	0	1	4	27.05	3.297	4	5.1	-7	1	3	37.63	2.390	4	0.9
-2	1	2	16.50	5.374	4	1.5	-1	1	4	27.37	3.258	4	0.6	3	5	4	37.65	2.389	4	0.7
2	1	2	16.66	5.320	4	2.0	0	6	1	27.44	3.251	4	1.1	5	3	4	37.83	2.378	4	0.9
-2	3	1	17.24	5.143	4	0.6	-5	2	2	27.44	3.250	4	0.8	-7	4	2	38.70	2.327	4	0.4
2	3	1	17.32	5.119	4	1.1	5	2	2	27.70	3.220	4	0.7	8	4	1	41.15	2.193	4	0.4
0	4	0	17.64	5.027	2	3.6	0	2	4	28.14	3.171	4	0.6	0	7	4	41.45	2.178	4	0.7
4	0	0	17.85	4.969	2	5.4	-2	1	4	28.42	3.140	4	1.1	0	10	0	45.09	2.011	2	3.2
1	4	0	18.20	4.873	4	0.7	2	1	4	28.62	3.118	4	0.4	0	8	4	45.14	2.009	4	3.4
0	4	1	18.86	4.705	4	0.6	-5	3	2	29.22	3.057	4	3.0	-8	0	4	45.22	2.005	2	0.9
-1	3	2	19.24	4.613	4	2.2	5	3	2	29.46	3.032	4	3.3	-8	4	3	45.32	2.001	4	1.1
1	3	2	19.31	4.596	4	1.5	3	6	0	29.88	2.990	4	0.7	10	0	0	45.64	1.988	2	4.6
-1	0	3	20.37	4.359	2	2.2	0	5	3	29.93	2.985	4	6.6	8	4	3	45.73	1.984	4	0.8
0	1	3	20.41	4.350	4	1.9	-5	0	3	29.94	2.984	2	4.0	8	0	4	45.76	1.983	2	1.4
1	0	3	20.48	4.337	2	1.3	-1	3	4	30.17	2.962	4	0.8	-3	4	6	46.50	1.953	4	1.4
-3	2	2	20.74	4.282	4	0.8	1	6	2	30.19	2.960	4	0.4	8	2	4	46.69	1.945	4	0.5
-2	4	1	20.85	4.259	4	2.6	-5	1	3	30.28	2.952	4	2.6	3	4	6	46.80	1.941	4	0.8
2	4	1	20.92	4.246	4	3.4	5	0	3	30.30	2.949	2	1.9	-5	8	3	47.28	1.922	4	0.8
3	2	2	20.94	4.242	4	0.7	5	1	3	30.64	2.918	4	0.9	-3	9	3	47.48	1.915	4	0.6
0	2	3	21.82	4.074	4	2.1	-2	5	3	31.21	2.865	4	1.0	5	8	3	47.53	1.913	4	0.6
3	4	0	22.20	4.005	4	2.8	-5	2	3	31.27	2.861	4	0.4	3	9	3	47.62	1.909	4	0.8
0	5	1	23.10	3.851	4	44.7	2	5	3	31.35	2.853	4	0.6	-5	3	6	48.54	1.875	4	1.4
3	3	2	23.19	3.836	4	1.0	-5	4	2	31.55	2.836	4	0.6	5	3	6	49.02	1.858	4	1.0

ZSM-5, Calcined

MFI



MFS ZSM-57, SiO_2 Framework

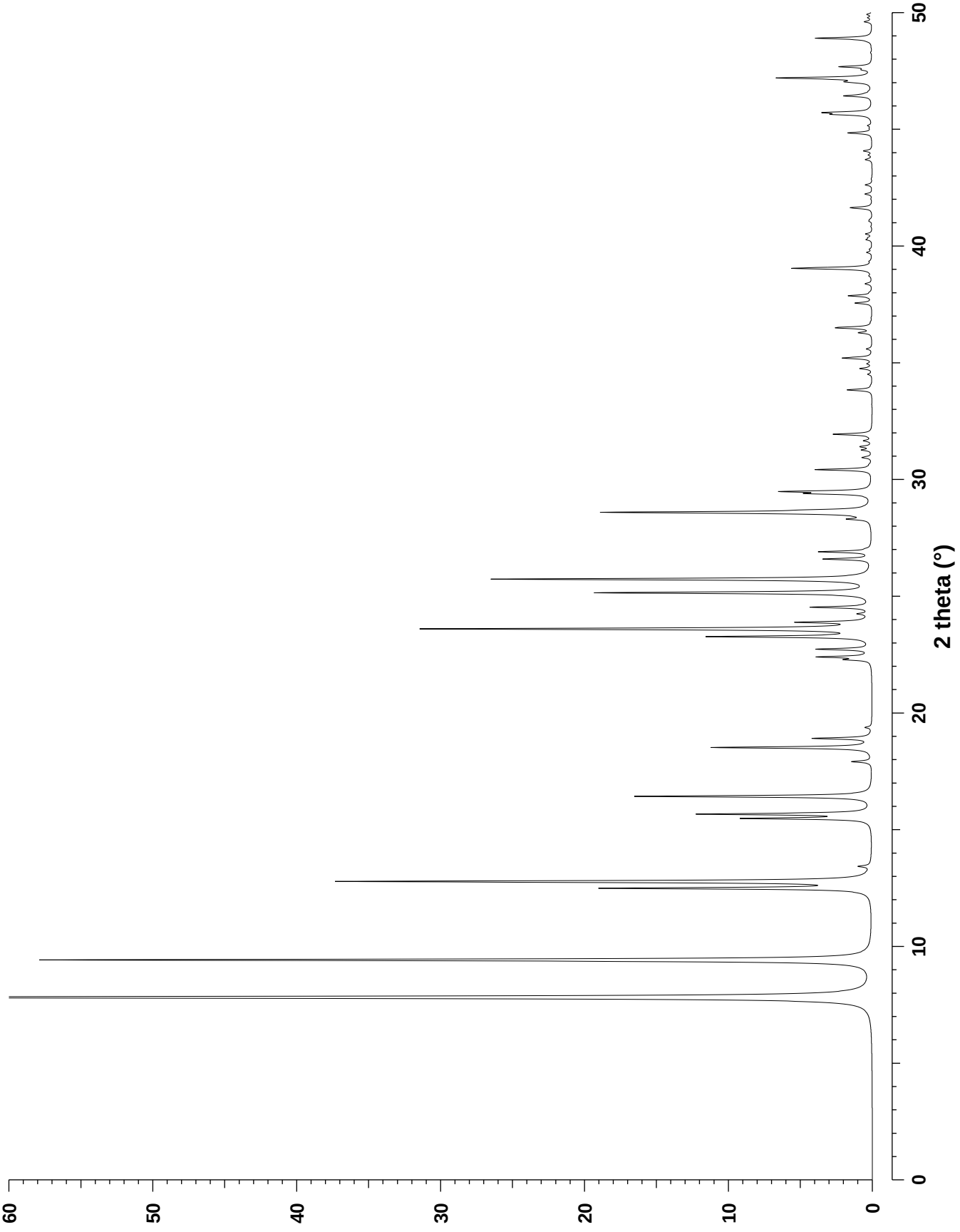
CHEMICAL COMPOSITION: $[Si_{36}O_{72}]$

REFINED COMPOSITION: $[Si_{36}O_{72}]$

CRYSTAL DATA: $Imm2$ (No. 44)
$a = 7.4510$ Å $b = 14.1711$ Å $c = 18.767$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
DLS refinement.

REFERENCE: J. L. Schlenker, J. B. Higgins and E. W. Valyocsik, *Zeolites* **10** 293–296 (1990).

h	k	l	2θ	d	M	I_{rel}
0	1	1	7.82	11.309	4	100.0
0	0	2	9.42	9.384	2	57.8
0	2	0	12.49	7.086	2	18.3
1	0	1	12.78	6.925	4	37.0
1	1	0	13.43	6.595	4	0.8
0	1	3	15.48	5.723	4	8.7
0	2	2	15.67	5.655	4	11.8
1	1	2	16.43	5.396	8	16.5
1	2	1	17.91	4.953	8	1.4
1	0	3	18.52	4.791	4	11.2
0	0	4	18.91	4.692	2	4.1
0	3	1	19.38	4.581	4	0.5
1	3	0	22.28	3.990	4	1.6
1	2	3	22.40	3.969	8	3.6
0	2	4	22.73	3.912	4	3.8
1	1	4	23.27	3.823	8	11.1
0	3	3	23.60	3.770	4	31.2
2	0	0	23.88	3.726	2	4.7
1	3	2	24.24	3.671	8	0.8
0	1	5	24.53	3.628	4	4.1
0	4	0	25.14	3.543	2	17.5
2	1	1	25.17	3.538	8	2.6
2	0	2	25.73	3.463	4	26.4
1	0	5	26.59	3.352	4	3.3
0	4	2	26.90	3.314	4	3.6
2	2	0	27.04	3.297	4	0.2
1	4	1	28.30	3.154	8	1.4
0	0	6	28.54	3.128	2	2.3
2	1	3	28.59	3.122	8	17.6
2	2	2	28.69	3.111	8	2.5
1	3	4	29.39	3.039	8	3.8
1	2	5	29.48	3.030	8	5.9
0	3	5	30.42	2.939	4	3.9
2	3	1	30.94	2.890	8	0.7
0	2	6	31.26	2.861	4	0.7
1	4	3	31.40	2.849	8	0.8
0	4	4	31.65	2.827	4	0.3
1	1	6	31.66	2.826	8	0.3
0	5	1	31.93	2.802	4	2.7
2	3	3	33.83	2.650	8	1.0
1	5	0	33.84	2.649	4	0.8
2	1	5	34.50	2.599	8	0.3
0	5	3	34.75	2.582	4	0.8
2	4	0	34.95	2.567	4	0.3
1	5	2	35.20	2.549	8	2.1
1	0	7	35.59	2.523	4	0.4
2	4	2	36.28	2.476	8	0.9
3	0	1	36.49	2.462	4	1.3
1	3	6	36.50	2.462	8	1.4
2	0	6	37.55	2.395	4	1.2
1	2	7	37.86	2.377	8	1.6
0	0	8	38.37	2.346	2	0.3
0	4	6	38.39	2.345	4	0.2
3	2	1	38.71	2.326	8	0.2
2	3	5	39.04	2.307	8	3.9
1	5	4	39.05	2.307	8	1.7
0	6	2	39.34	2.290	4	0.1
2	2	6	39.72	2.269	8	0.4
0	5	5	39.86	2.262	4	0.2
2	5	1	40.27	2.240	8	0.4
1	6	1	40.35	2.235	8	0.2
0	2	8	40.51	2.227	4	0.4
3	3	0	41.06	2.198	4	0.2
3	2	3	41.13	2.195	8	0.2
3	1	4	41.63	2.169	8	1.5
3	3	2	42.22	2.140	8	0.5
2	5	3	42.61	2.122	8	0.5
3	0	5	43.70	2.071	4	0.5
0	1	9	43.89	2.063	4	0.2
1	4	7	44.07	2.055	8	0.6
1	3	8	44.82	2.022	8	0.2
1	5	6	44.84	2.021	8	1.5
0	7	1	45.04	2.013	4	0.1
1	0	9	45.15	2.008	4	0.3
3	2	5	45.63	1.988	8	2.2
2	0	8	45.70	1.985	4	1.6
2	4	6	45.72	1.984	8	1.7
0	4	8	46.42	1.956	4	1.9
1	7	0	46.48	1.954	4	0.3
2	6	2	46.54	1.951	8	0.2
0	5	7	46.63	1.948	4	0.1
3	4	3	46.98	1.934	8	0.3
2	5	5	47.00	1.933	8	0.2
1	2	9	47.03	1.932	8	1.2
1	6	5	47.07	1.931	8	0.2
3	1	6	47.16	1.927	8	1.2
0	7	3	47.19	1.926	4	5.8
1	7	2	47.54	1.913	8	0.4
0	3	9	47.67	1.908	4	2.2
3	5	0	48.75	1.868	4	0.1
4	0	0	48.89	1.863	2	3.9
4	1	1	49.60	1.838	8	0.5
3	5	2	49.77	1.832	8	0.3
4	0	2	49.91	1.827	4	0.4


0
10
20
30
40
50
2 theta (°)
60
50
40
30
20
10
0

MON Montesommaite

CHEMICAL COMPOSITION: $|Na_{0.1}K_{4.3}(H_2O)_5|\ [Si_{11.3}Al_{4.7}O_{32}]$
Pollena, Mt. Somma-Vesuvius, Italy

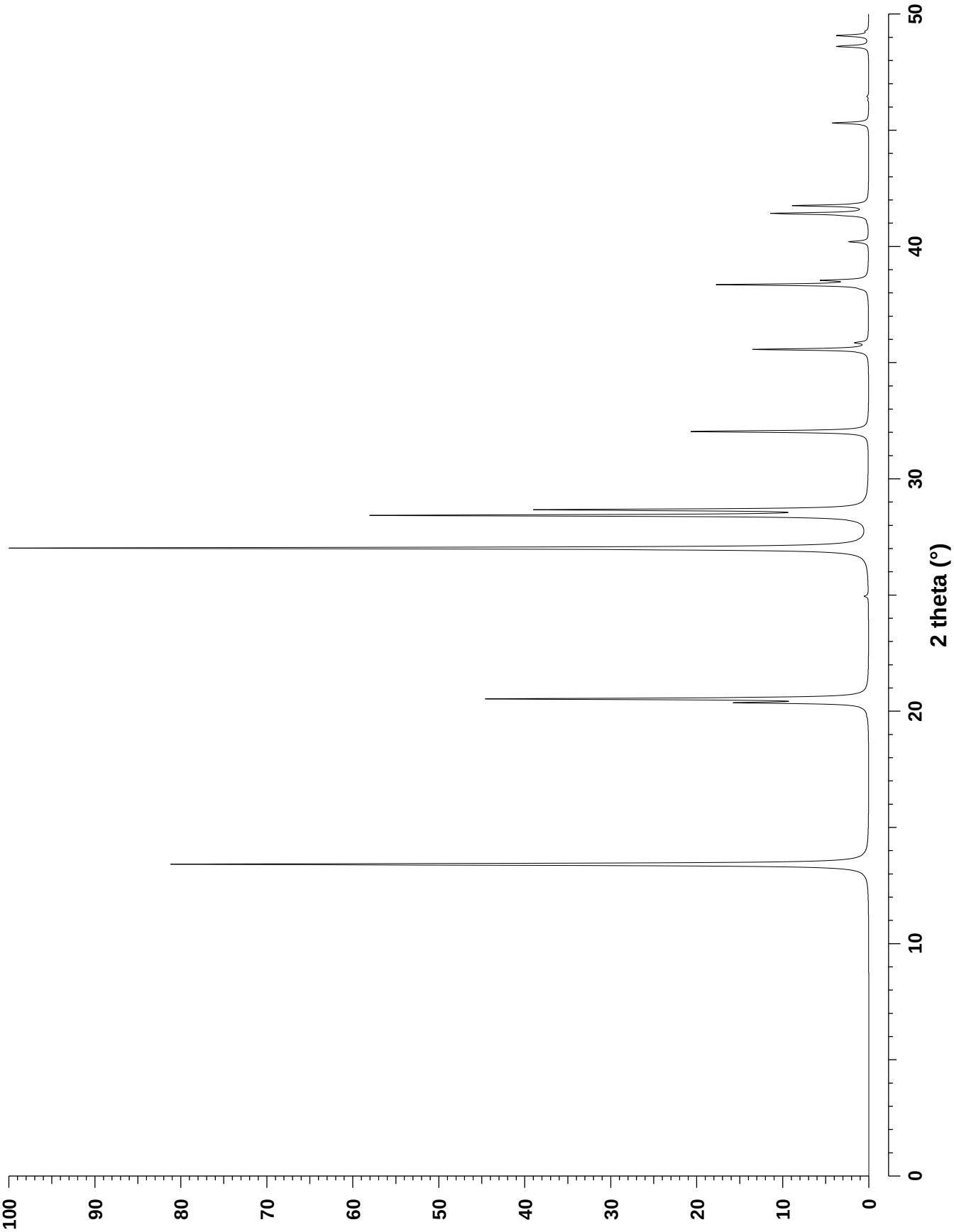
REFINED COMPOSITION: $|K_{4.24}(H_2O)_4|\ [Si_{11.3}Al_{4.7}O_{32}]$

CRYSTAL DATA: $I\,4_1/a\,md$ (No. 141) origin at centre $(\,2/m\,)$
$a = 7.141$ Å $b = 7.141$ Å $c = 17.307$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray powder refinement of idealized substructure, $R = 0.10$

REFERENCE: R. C. Rouse, P. J. Dunn, J. D. Grice, J. L. Schlenker and J. B. Higgins, *American Mineralogist* **75** 1415–1420 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	13.41	6.601	8	81.3	2	2	0	35.56	2.525	4	13.5	0	0	8	41.75	2.163	2	8.8
1	1	2	20.36	4.361	8	13.5	1	1	6	35.85	2.505	8	1.4	3	1	4	45.30	2.002	16	4.3
0	0	4	20.53	4.327	2	43.9	3	0	1	38.16	2.358	8	0.3	3	0	5	46.29	1.961	8	0.1
2	0	0	24.94	3.570	4	0.5	2	1	5	38.35	2.347	16	17.5	2	1	7	46.45	1.955	16	0.2
2	0	2	27.01	3.301	8	100.0	1	0	7	38.53	2.336	8	4.8	3	2	3	48.60	1.873	16	3.8
2	1	1	28.42	3.141	16	57.0	2	0	6	40.19	2.244	8	2.3	1	0	9	49.06	1.857	8	3.7
1	0	5	28.66	3.115	8	37.4	3	1	2	41.32	2.185	16	1.2	2	0	8	49.25	1.850	8	0.3
2	1	3	32.03	2.794	16	20.7	2	2	4	41.41	2.181	8	11.1							

Montesommaite MON



MOR Mordenite

CHEMICAL COMPOSITION: $|Na_8(H_2O)_{24}|\ [Si_{40}Al_8O_{96}]$
Challis, Idaho, U.S.A.

REFINED COMPOSITION: $|Na_8(H_2O)_{25}|\ [Si_{40}Al_8O_{96}]$

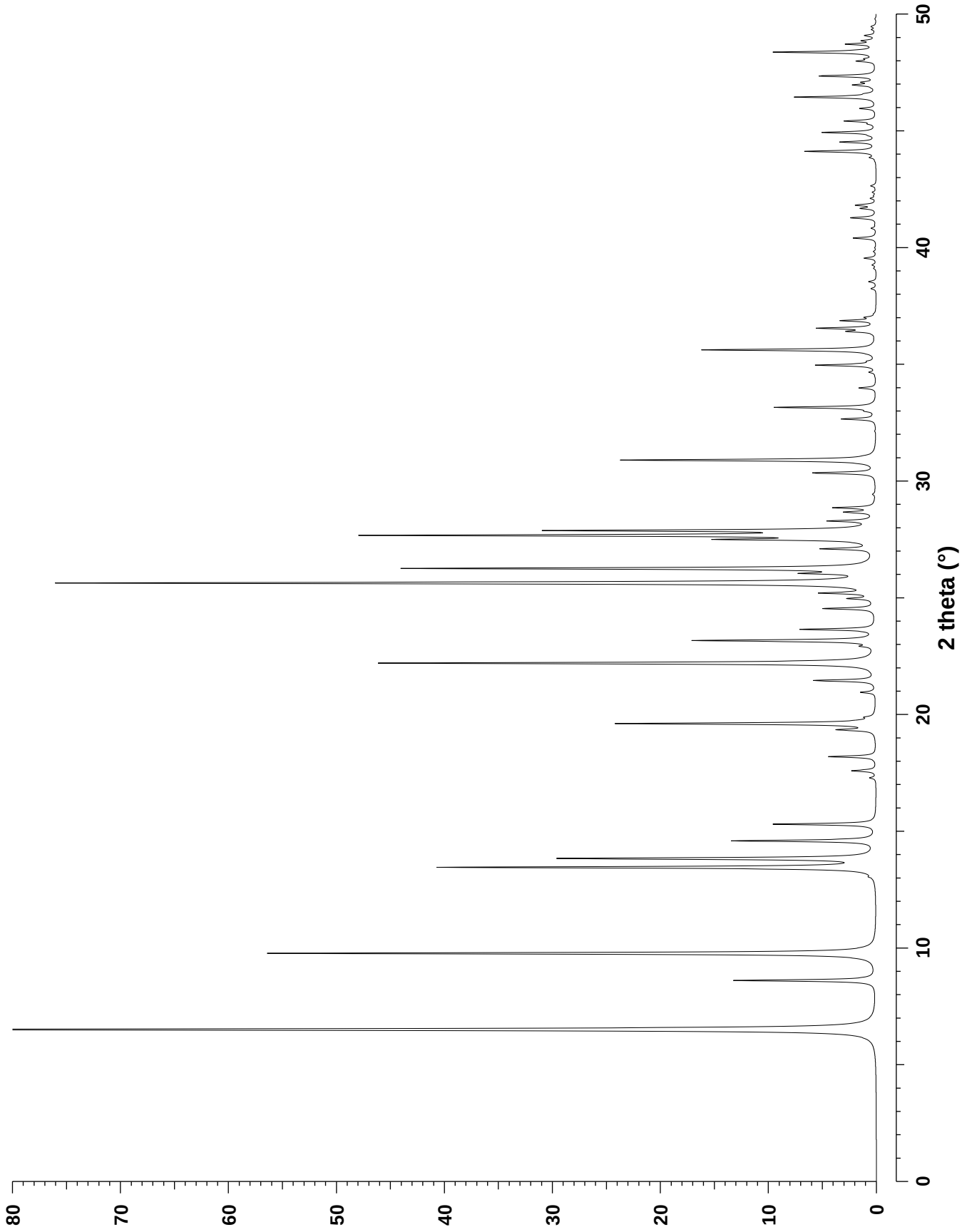
CRYSTAL DATA: *Cmcm* (No. 63)
$a = 18.11$ Å $b = 20.53$ Å $c = 7.528$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: V. Gramlich,
PhD dissertation, ETH, Zurich, (1971).
And V. Gramlich, Private communication.

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.51	13.581	4	100.0	5	3	1	30.34	2.946	8	0.3	3	7	2	41.81	2.160	8	1.8
0	2	0	8.61	10.265	2	13.1	2	6	1	30.34	2.946	8	5.5	4	2	3	42.10	2.146	8	0.5
2	0	0	9.77	9.055	2	56.4	6	2	0	30.88	2.896	4	2.0	6	4	2	42.22	2.140	8	0.2
2	2	0	13.04	6.791	4	0.3	4	0	2	30.89	2.894	4	12.9	3	9	0	42.36	2.134	4	0.3
1	1	1	13.45	6.584	8	40.4	3	3	2	30.89	2.894	8	8.8	0	8	2	42.64	2.120	4	0.5
1	3	0	13.83	6.402	4	29.1	2	4	2	31.08	2.878	8	0.2	2	8	2	43.85	2.064	8	0.5
0	2	1	14.59	6.071	4	13.3	1	5	2	32.65	2.743	8	3.2	0	10	0	44.11	2.053	2	5.3
3	1	0	15.30	5.791	4	9.5	5	5	0	32.98	2.716	4	0.6	3	9	1	44.11	2.053	8	0.8
0	4	0	17.28	5.133	2	0.6	6	2	1	33.15	2.703	8	2.8	5	1	3	44.13	2.052	8	0.6
2	2	1	17.59	5.042	8	2.3	1	7	1	33.15	2.702	8	6.6	7	3	2	44.51	2.036	8	3.3
1	3	1	18.19	4.877	8	4.4	3	7	0	33.98	2.638	4	1.6	0	6	3	44.79	2.024	4	0.3
3	1	1	19.34	4.590	8	3.2	5	1	2	34.65	2.589	8	0.6	4	4	3	44.92	2.018	8	4.9
4	0	0	19.61	4.528	2	1.4	7	1	0	34.95	2.567	4	0.2	9	1	0	45.28	2.003	4	0.5
3	3	0	19.61	4.527	4	22.7	0	8	0	34.96	2.566	2	5.4	8	4	1	45.41	1.997	8	2.9
2	4	0	19.88	4.465	4	0.6	5	5	1	35.12	2.555	8	0.5	5	3	3	45.95	1.975	8	0.8
0	4	1	20.95	4.241	4	1.4	4	4	2	35.61	2.521	8	0.6	2	6	3	45.95	1.975	8	0.7
4	2	0	21.45	4.142	4	5.7	3	5	2	35.61	2.521	8	15.5	6	8	0	46.44	1.955	4	7.5
1	5	0	22.20	4.004	4	46.1	2	8	0	36.39	2.469	4	1.3	5	7	2	46.58	1.950	8	0.6
3	3	1	22.92	3.880	8	1.0	1	1	3	36.41	2.468	8	1.2	9	1	1	46.95	1.935	8	1.8
2	4	1	23.16	3.840	8	16.9	6	4	1	36.54	2.459	8	5.3	2	10	1	46.96	1.935	8	0.2
0	0	2	23.64	3.764	2	6.9	5	3	2	36.86	2.439	8	1.2	9	3	0	47.07	1.930	4	0.9
4	2	1	24.53	3.629	8	4.5	2	6	2	36.86	2.438	8	1.8	5	9	0	47.08	1.930	4	0.2
1	1	2	24.54	3.627	8	0.3	0	2	3	36.87	2.438	4	0.2	4	8	2	47.34	1.920	8	5.2
5	1	0	24.96	3.567	4	2.3	7	1	1	37.00	2.429	8	0.4	6	2	3	47.97	1.896	8	0.6
1	5	1	25.19	3.535	8	0.3	0	8	1	37.01	2.429	4	0.5	1	7	3	47.98	1.896	8	1.1
0	2	2	25.20	3.534	4	4.3	7	3	0	37.15	2.420	4	0.1	7	5	2	48.08	1.892	8	0.7
2	0	2	25.63	3.476	4	75.7	6	0	2	38.22	2.355	4	0.1	0	0	4	48.36	1.882	2	9.4
0	6	0	26.04	3.422	2	5.0	2	2	3	38.24	2.354	8	0.4	7	7	1	48.45	1.879	8	0.5
3	5	0	26.25	3.395	4	43.5	1	3	3	38.53	2.336	8	0.7	4	10	0	48.70	1.870	4	0.1
2	2	2	27.09	3.292	8	4.7	7	3	1	39.10	2.304	8	0.2	5	9	1	48.70	1.870	8	2.5
1	3	2	27.49	3.245	8	12.6	6	2	2	39.25	2.295	8	0.4	1	1	4	48.85	1.864	8	1.2
5	1	1	27.67	3.223	8	46.1	5	7	0	39.54	2.279	4	1.1	1	11	0	49.07	1.857	4	0.5
5	3	0	27.87	3.201	4	28.8	8	0	0	39.82	2.264	2	0.1	3	9	2	49.07	1.856	8	0.5
2	6	0	27.87	3.201	4	0.1	0	4	3	39.99	2.254	4	0.1	4	6	3	49.33	1.847	8	0.4
3	1	2	28.28	3.156	8	4.0	4	8	0	40.40	2.233	4	2.2	5	5	3	49.45	1.843	8	0.1
0	6	1	28.66	3.115	4	2.7	8	2	0	40.82	2.211	4	0.4	2	0	4	49.46	1.843	4	0.3
4	4	1	28.85	3.095	8	3.3	7	5	0	41.24	2.189	4	0.3	8	6	1	49.79	1.831	8	0.1
3	5	1	28.85	3.095	8	0.5	2	4	3	41.27	2.188	8	2.2							
0	4	2	29.43	3.035	4	0.2	6	6	1	41.67	2.168	8	1.4							

Mordenite

MOR



MOR Maricopaite

CHEMICAL COMPOSITION: $|Pb_7Ca_2(H_2O)_{28}|\ [Si_{36}Al_{12}(O,OH)_{100}]$
Moon Anchor Mine, Tonopah, AZ, U.S.A.

REFINED COMPOSITION: $|Pb_{10.68}(H_2O)_{26.5}O_4|\ [Si_{36.38}Al_{11.02}O_{100}]$

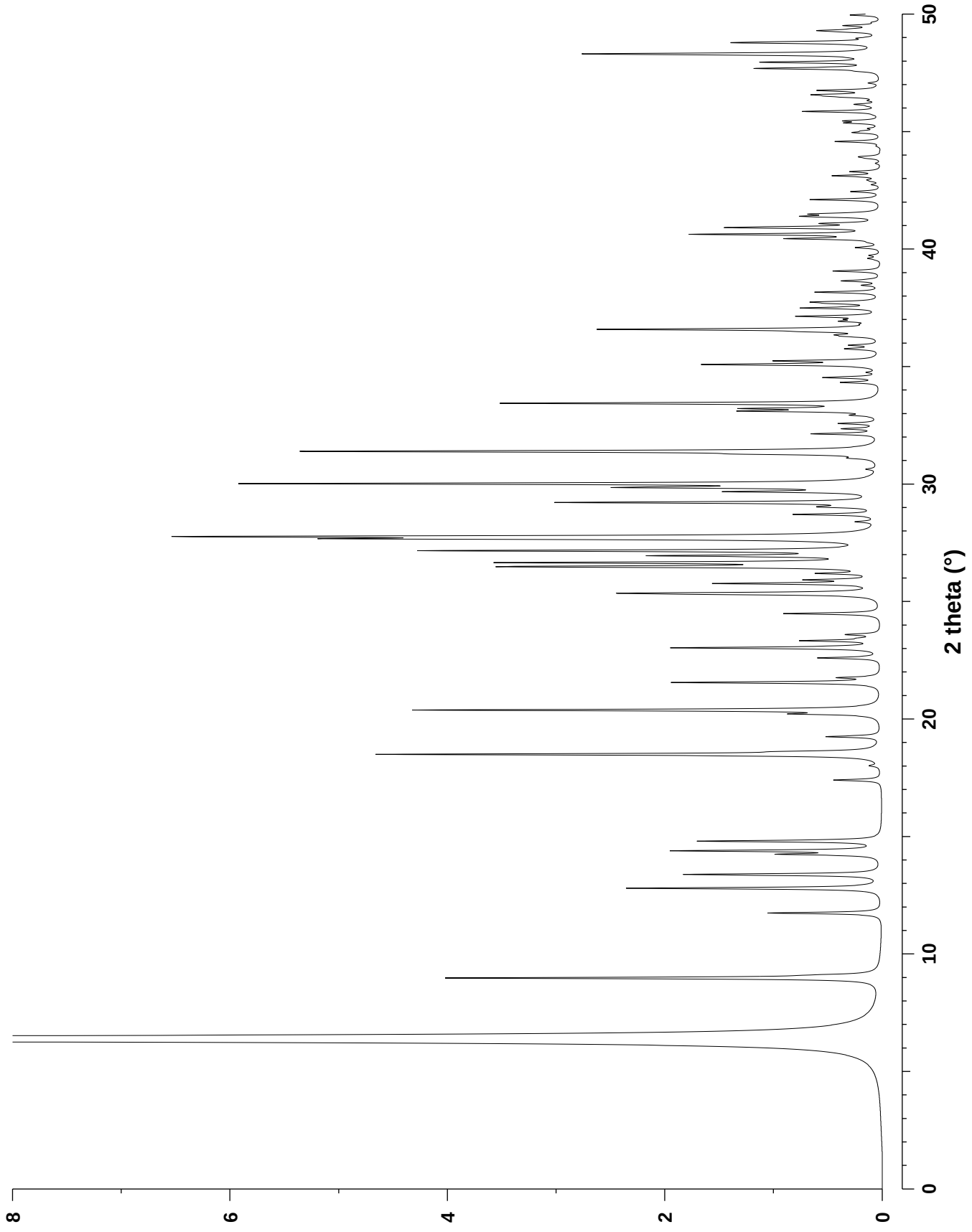
CRYSTAL DATA: $Cm2m$ (No. 38) **bca** setting
$a = 19.432$ Å $b = 19.702$ Å $c = 7.538$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.051$

REFERENCE: R. C. Rouse and D. R. Peacor,
American Mineralogist **79** 175–184 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.39	13.835	4	100.0	6	0	1	30.03	2.976	4	0.2	6	4	2	41.06	2.198	8	0.2
0	2	0	8.98	9.851	2	4.0	2	6	1	31.10	2.876	8	0.2	4	8	0	41.09	2.197	4	0.3
2	0	0	9.10	9.716	2	0.3	2	4	2	31.27	2.861	8	0.8	5	7	1	41.38	2.182	8	0.6
0	0	1	11.74	7.538	2	1.0	4	2	2	31.38	2.850	8	3.6	8	4	0	41.45	2.179	4	0.1
2	2	0	12.80	6.917	4	2.3	6	2	1	31.40	2.849	8	2.0	4	2	3	41.48	2.177	8	0.4
1	1	1	13.38	6.619	8	1.8	1	7	0	32.13	2.786	4	0.6	1	9	0	41.51	2.175	4	0.2
1	3	0	14.24	6.222	4	0.9	5	5	0	32.35	2.767	4	0.3	9	1	0	42.10	2.146	4	0.7
3	1	0	14.39	6.153	4	1.9	7	1	0	32.57	2.749	4	0.4	3	7	2	42.44	2.130	8	0.3
0	2	1	14.80	5.986	4	1.7	4	6	0	32.92	2.720	4	0.2	5	1	3	43.11	2.098	8	0.4
2	2	1	17.40	5.097	8	0.4	6	4	0	33.10	2.706	4	1.1	1	9	1	43.29	2.090	8	0.3
1	3	1	18.49	4.798	8	4.6	1	5	2	33.21	2.697	8	1.1	0	8	2	43.92	2.062	4	0.2
3	1	1	18.61	4.767	8	0.6	5	1	2	33.43	2.680	8	3.5	4	4	3	44.57	2.033	8	0.4
3	3	0	19.25	4.612	4	0.5	1	7	1	34.32	2.613	8	0.3	2	8	2	44.95	2.017	8	0.2
2	4	0	20.21	4.393	4	0.6	5	5	1	34.53	2.598	8	0.5	3	5	3	45.02	2.014	8	0.1
4	2	0	20.38	4.357	4	4.3	4	6	1	35.07	2.559	8	0.9	8	2	2	45.36	1.999	8	0.3
0	4	1	21.55	4.123	4	1.9	7	3	0	35.09	2.557	4	0.8	0	6	3	45.45	1.995	4	0.3
4	0	1	21.76	4.083	4	0.3	4	4	2	35.22	2.548	8	0.1	9	3	1	45.85	1.979	8	0.7
3	3	1	22.60	3.934	8	0.6	6	4	1	35.24	2.547	8	0.8	6	6	2	46.15	1.967	8	0.2
1	5	0	23.03	3.862	4	1.9	0	0	3	35.73	2.513	2	0.1	2	6	3	46.46	1.955	8	0.1
5	1	0	23.33	3.813	4	0.7	3	5	2	35.76	2.511	8	0.2	8	6	0	46.50	1.953	4	0.3
2	4	1	23.44	3.796	8	0.1	5	3	2	35.90	2.502	8	0.3	5	7	2	46.56	1.951	8	0.5
4	2	1	23.58	3.772	8	0.2	0	6	2	36.28	2.476	4	0.2	7	5	2	46.72	1.944	8	0.1
0	0	2	23.60	3.769	2	0.1	1	1	3	36.34	2.472	8	0.3	10	0	0	46.75	1.943	2	0.5
1	1	2	24.48	3.636	8	0.9	0	8	0	36.48	2.463	2	0.4	2	10	0	47.06	1.931	4	0.1
0	2	2	25.30	3.520	4	1.0	6	0	2	36.58	2.456	4	2.5	7	7	1	47.56	1.912	8	0.1
2	0	2	25.35	3.514	4	2.0	0	2	3	36.92	2.435	4	0.3	5	9	0	47.68	1.907	4	1.0
4	4	0	25.76	3.459	4	1.5	8	0	0	37.01	2.429	2	0.2	10	2	0	47.70	1.906	4	0.1
1	5	1	25.92	3.437	8	0.6	7	3	1	37.13	2.421	8	0.7	4	8	2	47.93	1.898	8	0.3
5	1	1	26.19	3.402	8	0.5	2	6	2	37.49	2.399	8	0.7	6	8	1	47.95	1.897	8	0.8
3	5	0	26.48	3.366	4	3.3	2	8	0	37.68	2.387	4	0.3	8	4	2	48.25	1.886	8	0.4
5	3	0	26.65	3.345	4	3.3	6	2	2	37.74	2.383	8	0.5	0	0	4	48.29	1.885	2	1.6
2	2	2	26.94	3.310	8	1.9	8	2	0	38.16	2.358	4	0.6	1	9	2	48.31	1.884	8	1.1
0	6	0	27.16	3.284	2	4.1	0	8	1	38.45	2.341	4	0.2	1	1	4	48.77	1.867	8	1.1
1	3	2	27.67	3.224	8	4.2	1	3	3	38.64	2.330	8	0.3	1	7	3	48.81	1.866	8	0.4
3	1	2	27.76	3.214	8	5.8	6	6	0	39.06	2.306	4	0.4	5	5	3	48.97	1.860	8	0.1
4	4	1	28.39	3.144	8	0.2	2	8	1	39.60	2.276	8	0.1	0	2	4	49.23	1.851	4	0.2
2	6	0	28.70	3.111	4	0.8	8	2	1	40.06	2.251	8	0.2	5	9	1	49.28	1.849	8	0.2
6	2	0	29.02	3.077	4	0.4	5	5	2	40.44	2.230	8	0.8	10	2	1	49.30	1.848	8	0.3
5	3	1	29.21	3.057	8	2.9	7	1	2	40.62	2.221	8	1.7	4	6	3	49.37	1.846	8	0.1
0	6	1	29.67	3.010	4	1.3	3	3	3	40.90	2.206	8	0.2	6	4	3	49.50	1.841	8	0.3
0	4	2	29.85	2.993	4	2.1	4	6	2	40.91	2.206	8	0.9	4	10	0	49.95	1.826	4	0.3
4	0	2	30.01	2.978	4	5.6	6	6	1	40.93	2.205	8	0.3							

Maricopaite

MOR



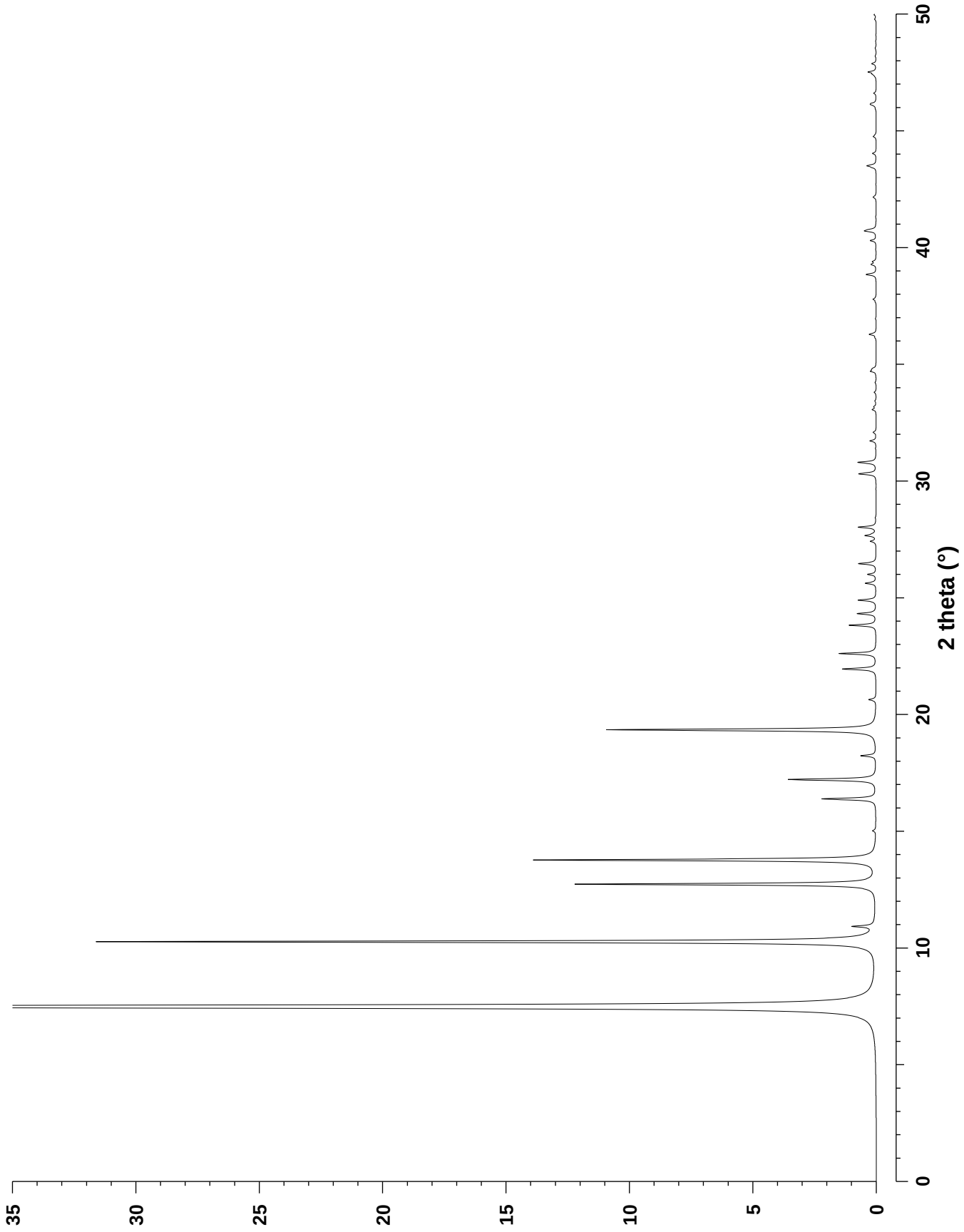
CHEMICAL COMPOSITION: $|(C_{12}H_{24}O_6)_{36}|\ [Si_{33.48}Al_{2.52}O_{78}]$
$C_{12}H_{24}O_6$ = 1,4,7,10,13,16-hexaoxacyclooctadecane (18-crown-6 ether)

REFINED COMPOSITION: $|K_{9.38}C_{12}H_{48}|\ [Si_{36}O_{78}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) rhombohedral setting
$a = 11.841$ Å $b = 11.841$ Å $c = 11.841$ Å
$\alpha = 93.29°$ $\beta = 93.29°$ $\gamma = 93.29°$
X-ray Rietveld refinement, $R_p = 0.0533$, $R_{wp} = 0.0704$

REFERENCE: D. F. Shantz, A. Burton and R. F. Lobo,
Microporous and Mesoporous Materials **31** 61–73 (1999).

h	k	l	2θ	d	M	I_{rel}
1	0	0	7.49	11.800	6	100.0
1	0	-1	10.27	8.610	6	31.6
1	1	0	10.92	8.101	6	0.8
1	1	-1	12.73	6.955	6	12.2
1	1	1	13.77	6.432	2	13.9
2	0	0	15.02	5.900	6	0.1
2	0	-1	16.38	5.410	12	2.2
2	1	0	17.21	5.153	12	3.6
2	1	-1	18.23	4.867	12	0.6
2	1	1	19.34	4.590	6	10.9
2	0	-2	20.63	4.305	6	0.3
2	2	0	21.94	4.050	6	1.3
2	1	-2	21.98	4.044	12	0.2
3	0	0	22.61	3.933	6	1.1
2	2	-1	22.61	3.933	6	0.4
2	2	1	23.82	3.736	6	1.1
3	-1	-1	24.32	3.660	6	0.8
3	1	-1	24.89	3.578	12	0.7
2	2	-2	25.62	3.478	6	0.4
3	1	1	26.00	3.427	6	0.3
3	0	-2	26.46	3.369	12	0.7
3	-1	-2	27.41	3.254	12	0.2
3	1	-2	27.66	3.224	12	0.4
3	2	0	28.02	3.184	12	0.7
4	0	0	30.30	2.950	6	0.5
2	2	-3	30.32	2.948	6	0.2
3	2	-2	30.79	2.904	12	0.7
4	1	0	31.71	2.822	12	0.3
4	1	-1	32.07	2.791	12	0.1
3	2	2	33.05	2.711	6	0.2
3	3	1	34.69	2.586	6	0.2
3	2	-3	34.76	2.581	12	0.1
4	2	0	34.82	2.576	12	0.1
4	2	1	36.28	2.476	12	0.3
3	3	2	37.78	2.381	6	0.1
5	-1	-1	38.84	2.318	6	0.2
3	3	-3	38.84	2.318	6	0.2
4	3	0	39.28	2.294	12	0.1
5	0	-2	40.29	2.239	12	0.2
4	3	1	40.69	2.218	12	0.2
5	1	1	40.71	2.217	6	0.2
5	-1	-2	40.76	2.213	12	0.2
3	3	3	42.15	2.144	2	0.1
5	2	1	43.43	2.084	12	0.1
4	3	2	43.50	2.080	12	0.3
4	3	-3	44.02	2.057	12	0.2
4	4	0	44.75	2.025	6	0.1
4	4	1	46.11	1.969	6	0.2
6	0	0	46.16	1.967	6	0.2
6	1	-1	47.42	1.917	12	0.1
4	3	3	47.51	1.914	6	0.3
6	0	-2	47.86	1.901	12	0.1


0
10
20
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40
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2 theta (°)
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25
20
15
10
5
0

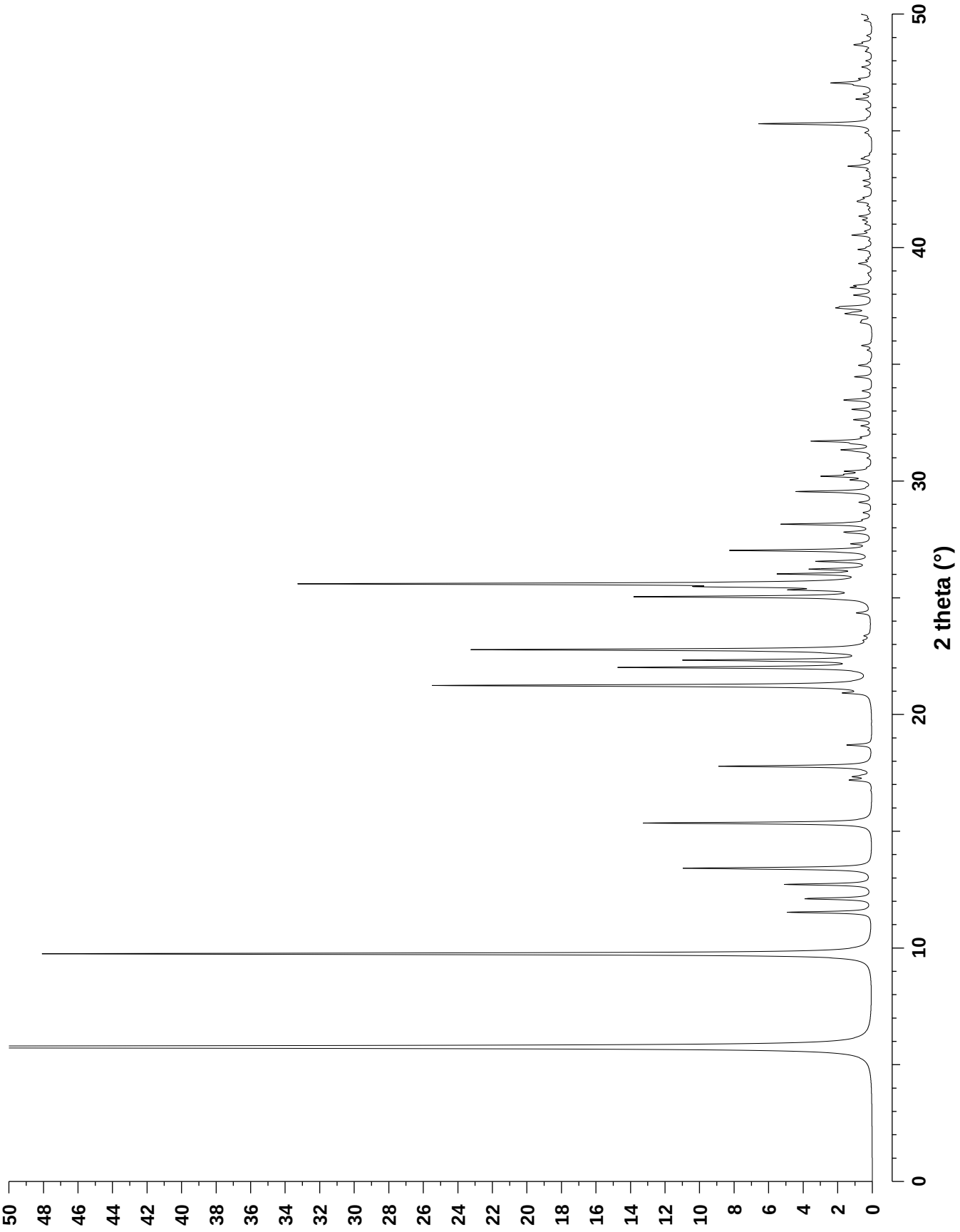
CHEMICAL COMPOSITION: $[Si_{44}O_{88}]$

REFINED COMPOSITION: $[Si_{44}O_{88}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.5000$ Å $b = 30.7096$ Å $c = 7.3133$ Å
$\alpha = 90.0°$ $\beta = 91.7113°$ $\gamma = 90.0°$
X-ray synchrotron Rietveld refinement, $R_p = 0.0729$, $R_{wp} = 0.0916$, $R_b = 0.0302$

REFERENCE: P. A. Barrett, M.-J. Diaz-Cabanas and M. A. Camblor,
Chemistry of Materials **11** 2919–2927 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	5.76	15.355	2	100.0	-3	1	1	30.58	2.923	4	0.2	4	0	1	40.29	2.238	2	0.2
1	1	0	9.75	9.072	4	48.1	-2	2	2	30.98	2.887	4	0.2	-3	9	1	40.53	2.226	4	1.2
0	4	0	11.53	7.677	2	4.9	3	1	1	31.26	2.861	4	0.5	-1	5	3	40.69	2.217	4	0.4
0	0	1	12.11	7.310	2	3.8	2	0	2	31.33	2.855	2	1.6	3	5	2	41.00	2.201	4	0.3
1	3	0	12.72	6.962	4	5.0	0	10	1	31.60	2.831	4	0.7	-1	13	1	41.18	2.192	4	0.4
0	2	1	13.41	6.600	4	10.9	-3	3	1	31.70	2.823	4	3.4	-4	4	1	41.34	2.184	4	0.7
-1	1	1	15.35	5.773	4	13.3	2	2	2	31.88	2.807	4	0.5	-1	11	2	41.63	2.169	4	0.2
1	5	0	17.19	5.157	4	1.2	-2	8	1	32.18	2.782	4	0.2	-2	12	1	41.79	2.161	4	0.2
0	6	0	17.33	5.118	2	0.9	3	3	1	32.36	2.767	4	0.6	4	6	0	41.95	2.154	4	0.5
-1	3	1	17.40	5.097	4	0.3	2	8	1	32.61	2.746	4	0.1	1	11	2	41.99	2.152	4	0.4
1	3	1	17.78	4.987	4	8.9	-2	4	2	32.62	2.745	4	0.9	4	4	1	42.05	2.149	4	0.3
2	0	0	18.69	4.748	2	1.5	-1	7	2	33.06	2.710	4	1.2	2	12	1	42.14	2.144	4	0.4
-1	5	1	20.92	4.247	4	1.3	1	11	0	33.45	2.678	4	1.1	2	2	3	42.62	2.121	4	0.5
0	6	1	21.19	4.193	4	2.4	2	4	2	33.48	2.676	4	0.4	-2	4	3	42.86	2.110	4	0.5
1	5	1	21.24	4.182	4	24.5	1	7	2	33.48	2.676	4	0.3	-1	7	3	43.29	2.090	4	0.3
2	4	0	22.01	4.038	4	13.6	-3	5	1	33.83	2.649	4	0.2	-4	6	1	43.48	2.081	4	1.4
-2	0	1	22.02	4.037	2	0.9	0	8	2	33.86	2.647	4	0.4	1	7	3	43.80	2.067	4	0.6
1	7	0	22.32	3.983	4	10.5	3	5	1	34.46	2.603	4	1.0	2	4	3	43.88	2.063	4	0.3
2	0	1	22.63	3.929	2	0.7	3	7	0	34.95	2.567	4	0.8	-4	0	2	44.90	2.019	2	0.3
-2	2	1	22.77	3.904	4	23.0	0	12	0	35.06	2.559	2	0.1	-2	6	3	44.94	2.017	4	0.1
0	8	0	23.17	3.839	2	0.2	-1	11	1	35.60	2.522	4	0.3	3	11	1	45.29	2.002	4	6.1
2	2	1	23.37	3.806	4	0.3	1	11	1	35.80	2.508	4	0.6	-4	2	2	45.31	2.001	4	0.3
0	0	2	24.35	3.655	2	0.8	-2	10	1	36.77	2.444	4	0.5	1	15	0	45.31	2.001	4	0.2
-2	4	1	24.92	3.573	4	0.5	-3	7	1	36.83	2.440	4	0.3	2	14	0	45.55	1.991	4	0.1
0	2	2	25.04	3.556	4	13.5	0	0	3	36.89	2.437	2	0.4	-3	9	2	45.86	1.979	4	0.2
-1	7	1	25.33	3.516	4	3.4	-1	9	2	37.08	2.425	4	0.1	2	6	3	45.93	1.976	4	0.3
2	4	1	25.47	3.497	4	6.8	-3	1	2	37.13	2.421	4	0.3	-4	8	1	46.35	1.959	4	0.9
2	6	0	25.59	3.481	4	16.0	2	10	1	37.16	2.419	4	1.1	-1	9	3	46.56	1.951	4	0.4
1	7	1	25.60	3.479	4	17.4	0	12	1	37.22	2.415	4	0.6	1	13	2	46.94	1.936	4	0.7
-1	1	2	26.02	3.424	4	5.0	0	2	3	37.37	2.407	4	0.6	1	9	3	47.04	1.932	4	2.1
0	8	1	26.22	3.399	4	3.2	3	7	1	37.41	2.404	4	1.4	-2	12	2	47.09	1.930	4	0.3
1	1	2	26.55	3.357	4	3.1	1	9	2	37.47	2.400	4	1.3	-2	14	1	47.15	1.927	4	0.3
0	4	2	27.02	3.300	4	8.2	-1	1	3	37.96	2.370	4	1.0	-3	3	3	47.23	1.924	4	0.6
-1	3	2	27.31	3.266	4	1.0	3	1	2	38.28	2.351	4	0.4	-2	8	3	47.73	1.905	4	0.5
1	9	0	27.78	3.211	4	0.6	0	10	2	38.28	2.351	4	0.7	5	1	0	47.99	1.896	4	0.3
1	3	2	27.81	3.207	4	1.1	4	2	0	38.37	2.346	4	0.9	0	14	2	48.39	1.881	4	0.3
-2	6	1	28.15	3.170	4	5.2	3	9	0	38.81	2.321	4	0.1	-4	6	2	48.48	1.878	4	0.1
3	1	0	28.34	3.149	4	0.3	-1	3	3	38.89	2.316	4	0.2	3	3	3	48.65	1.871	4	0.4
2	6	1	28.64	3.116	4	0.5	3	3	2	39.20	2.298	4	0.1	2	8	3	48.68	1.871	4	0.7
0	10	0	29.08	3.071	2	0.7	1	13	0	39.30	2.292	4	0.6	5	3	0	48.77	1.867	4	0.2
3	3	0	29.54	3.024	4	4.4	2	8	2	39.33	2.291	4	0.2	-3	5	3	48.79	1.867	4	0.3
0	6	2	30.04	2.974	4	1.0	1	3	3	39.45	2.284	4	0.3	0	16	1	49.07	1.856	4	0.3
1	5	2	30.20	2.959	4	2.7	-4	0	1	39.56	2.278	2	0.2	4	6	2	49.72	1.834	4	0.4
-1	9	1	30.29	2.951	4	1.0	-3	5	2	39.91	2.259	4	0.8	-4	10	1	49.84	1.830	4	0.2
-2	0	2	30.41	2.939	2	1.4	-4	2	1	40.01	2.253	4	0.2	3	13	1	49.98	1.825	4	0.6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MTN Dodecasil 3C

CHEMICAL COMPOSITION: $|((CH_3)_3N, CO_2)_y(N_2, Ar, CH_4)_x|$ $[Si_{136}O_{272}]$

REFINED COMPOSITION: $|N_{24}|$ $[Si_{136}O_{272}]$

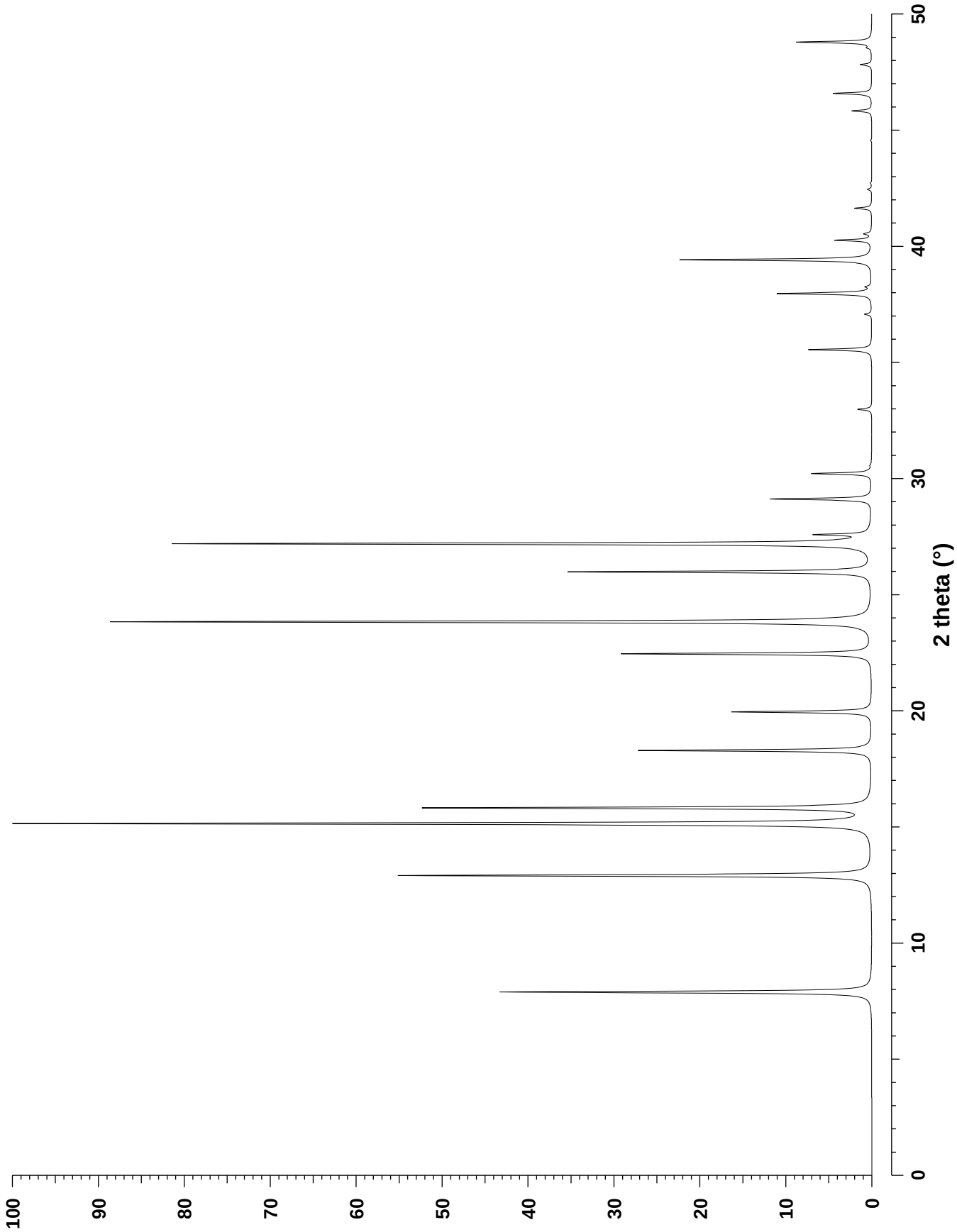
CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 19.402$ Å $b = 19.402$ Å $c = 19.402$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: H. Gies,
Z. Kristallogr. **167** 73–82 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	7.89	11.202	8	43.4	6	2	2	30.56	2.925	24	0.1	8	4	0	41.63	2.169	12	1.0
2	2	0	12.91	6.860	12	55.2	5	5	1	32.97	2.717	24	1.5	7	5	3	42.44	2.130	24	0.2
3	1	1	15.14	5.850	24	100.0	7	1	1	32.97	2.717	24	0.2	7	3	5	42.44	2.130	24	0.2
2	2	2	15.82	5.601	8	52.1	7	1	3	35.54	2.526	24	2.4	8	4	4	45.82	1.980	24	2.3
4	0	0	18.29	4.851	6	27.2	5	5	3	35.54	2.526	24	2.6	7	7	1	46.57	1.950	24	2.5
3	3	1	19.95	4.451	24	16.3	7	3	1	35.54	2.526	24	2.4	9	3	3	46.57	1.950	24	1.9
4	2	2	22.45	3.960	24	29.2	8	0	0	37.07	2.425	6	0.8	7	5	5	46.57	1.950	24	0.1
5	1	1	23.83	3.734	24	67.1	7	3	3	37.96	2.370	24	11.0	8	2	6	47.81	1.903	24	0.6
3	3	3	23.83	3.734	8	21.7	6	4	4	38.25	2.353	24	0.6	8	6	2	47.81	1.903	24	0.6
4	4	0	25.98	3.430	12	35.3	8	2	2	39.41	2.287	24	13.0	9	5	1	48.54	1.876	24	0.1
5	1	3	27.19	3.280	24	40.9	6	6	0	39.41	2.287	12	9.4	9	1	5	48.54	1.876	24	0.1
5	3	1	27.19	3.280	24	40.5	5	5	5	40.25	2.240	8	3.4	7	7	3	48.54	1.876	24	0.2
4	4	2	27.58	3.234	24	6.0	7	1	5	40.25	2.240	24	0.4	6	6	6	48.78	1.867	8	2.9
6	2	0	29.11	3.068	12	5.9	7	5	1	40.25	2.240	24	0.4	10	2	2	48.78	1.867	24	5.9
6	0	2	29.11	3.068	12	6.0	6	6	2	40.53	2.226	24	0.9							
5	3	3	30.21	2.959	24	7.0	8	0	4	41.63	2.169	12	1.0							

Dodecasil 3C

MTN



MTT Ammonium Fluoride ZSM-23

CHEMICAL COMPOSITION: $|(NH_4F)_{1.72}|\ [Si_{24}O_{48}]$

REFINED COMPOSITION: $|(NH_4F)_{1.72}|\ [Si_{24}O_{48}]$

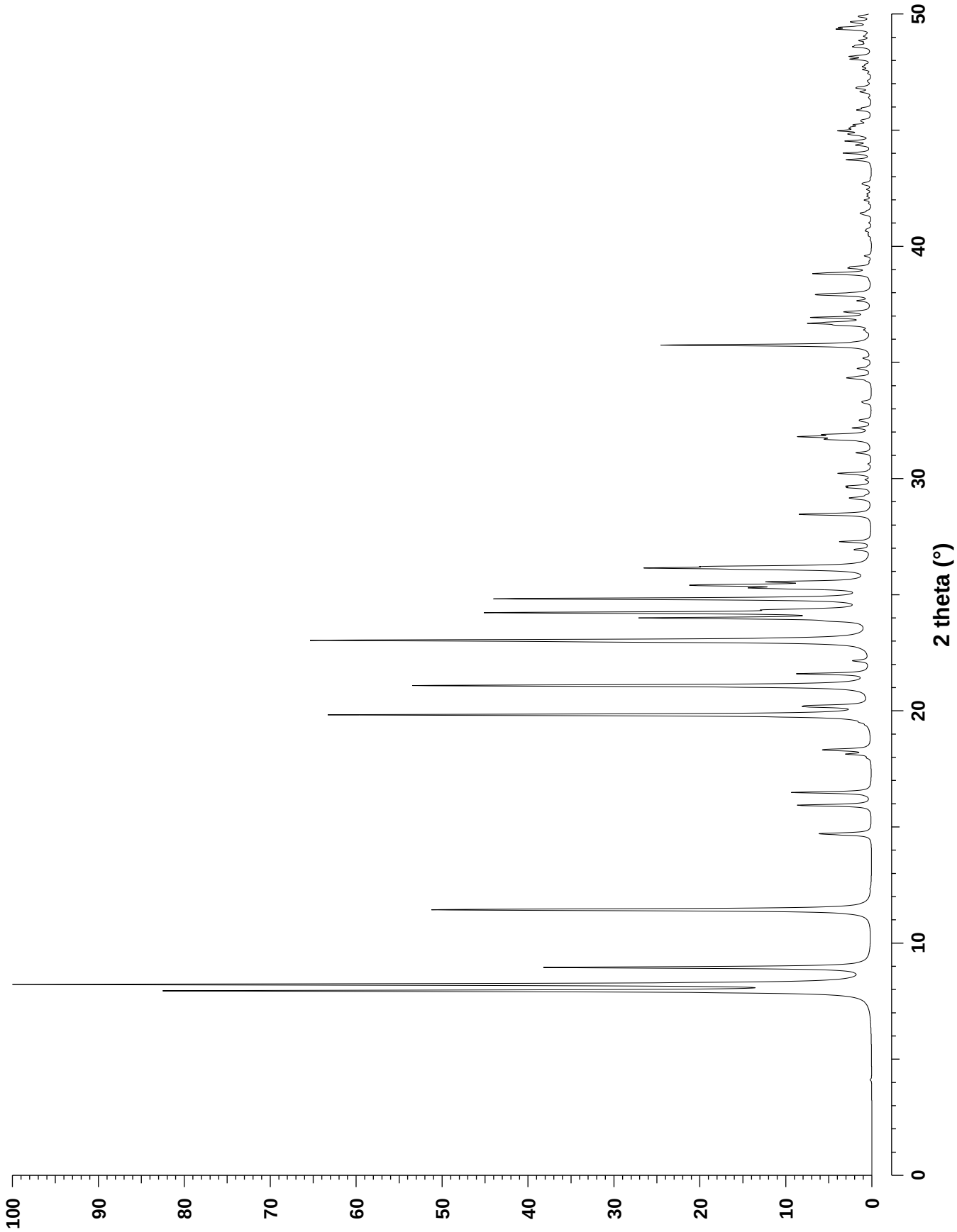
CRYSTAL DATA: $P12_11$ (No. 4) unique axis **b**
$a = 11.129$ Å $b = 5.025$ Å $c = 21.519$ Å
$\alpha = 90°$ $\beta = 89.85°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.033$, $R_{wp} = 0.085$, $R_F = 0.089$

REFERENCE: B. Marler, C. Deroche, H. Gies, C. A. Fyfe, H. Grondey, G. T. Kokotailo, Y. Feng, S. Ernst, J. Weitkamp and D. E. Cox, *J. Appl. Cryst.* **26** 636–644 (1993).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.94	11.129	2	81.9	1	1	5	28.44	3.138	4	4.8	4	1	3	39.05	2.307	4	2.0
0	0	2	8.22	10.759	2	100.0	-1	1	5	28.47	3.135	4	5.0	-4	1	3	39.11	2.303	4	1.8
1	0	1	8.94	9.896	2	21.8	2	1	4	29.11	3.067	4	1.2	4	1	4	40.65	2.220	4	0.6
-1	0	1	8.96	9.875	2	19.0	-2	1	4	29.16	3.062	4	2.0	2	1	8	41.35	2.183	4	0.5
1	0	2	11.42	7.746	2	33.2	2	0	6	29.60	3.018	2	2.3	0	0	10	41.98	2.152	2	0.8
-1	0	2	11.45	7.725	2	26.0	-2	0	6	29.67	3.011	2	2.4	-1	1	9	42.68	2.119	4	0.6
1	0	3	14.67	6.036	2	2.7	3	1	0	29.94	2.984	4	0.6	-4	1	5	42.72	2.117	4	0.5
-1	0	3	14.71	6.022	2	4.9	-1	0	7	30.18	2.961	2	0.5	3	2	1	43.71	2.071	4	1.1
2	0	0	15.93	5.564	2	8.8	3	1	1	30.22	2.957	4	3.3	-3	2	1	43.72	2.070	4	1.9
0	0	4	16.48	5.380	2	9.4	-3	1	2	31.11	2.874	4	1.6	0	2	6	44.00	2.058	4	3.2
0	1	1	18.13	4.893	4	2.7	1	1	6	31.67	2.825	4	3.3	3	2	2	44.34	2.043	4	0.8
1	0	4	18.30	4.848	2	3.7	-1	1	6	31.70	2.822	4	1.3	-3	2	2	44.36	2.042	4	1.0
-1	0	4	18.34	4.839	2	3.4	2	1	5	31.72	2.821	4	0.9	5	1	0	44.52	2.035	4	3.0
1	1	1	19.82	4.480	4	34.1	-2	1	5	31.78	2.816	4	1.9	2	2	5	44.81	2.022	4	1.5
-1	1	1	19.82	4.478	4	30.2	3	0	5	31.80	2.814	2	5.9	-2	2	5	44.85	2.021	4	1.2
2	0	3	20.17	4.402	2	5.2	-3	0	5	31.89	2.806	2	4.5	4	1	6	44.96	2.016	4	3.2
-2	0	3	20.22	4.391	2	4.9	4	0	0	32.17	2.782	2	2.1	2	1	9	45.00	2.014	4	0.6
1	1	2	21.07	4.216	4	30.6	3	1	3	32.47	2.758	4	0.9	-4	1	6	45.06	2.012	4	0.6
-1	1	2	21.09	4.212	4	27.0	-3	1	3	32.52	2.753	4	1.0	-2	1	9	45.08	2.011	4	0.8
0	1	3	21.59	4.116	4	8.4	4	0	2	33.24	2.695	2	0.5	2	0	10	45.13	2.009	2	1.4
1	0	5	22.12	4.018	2	0.7	0	0	8	33.31	2.690	2	0.6	-2	0	10	45.22	2.005	2	1.7
-1	0	5	22.16	4.011	2	1.4	1	0	8	34.28	2.616	2	0.8	-3	1	8	45.44	1.996	4	0.5
2	0	4	22.96	3.873	2	17.1	-1	0	8	34.32	2.613	2	0.6	5	0	5	45.85	1.979	2	1.0
-2	0	4	23.02	3.863	2	18.4	3	1	4	34.33	2.612	4	1.7	0	1	10	45.87	1.978	4	0.8
1	1	3	23.03	3.862	4	24.7	-3	1	4	34.39	2.607	4	1.0	-5	0	5	45.95	1.975	2	0.9
-1	1	3	23.05	3.858	4	25.2	-2	1	6	34.73	2.583	4	1.4	1	1	10	46.61	1.948	4	0.5
2	1	0	23.86	3.729	4	2.2	-1	1	7	35.18	2.551	4	0.7	-1	1	10	46.65	1.947	4	1.0
3	0	0	23.99	3.710	2	25.6	0	2	0	35.74	2.513	2	24.9	3	2	4	46.80	1.941	4	1.3
2	1	1	24.21	3.676	4	21.0	-4	0	4	36.39	2.469	2	0.5	-3	2	4	46.85	1.939	4	1.1
-2	1	1	24.23	3.674	4	25.8	3	1	5	36.60	2.455	4	2.8	4	1	7	47.60	1.910	4	0.9
3	0	1	24.34	3.657	2	4.2	1	2	0	36.67	2.451	4	1.1	5	1	4	47.74	1.905	4	0.6
-3	0	1	24.36	3.654	2	4.2	-3	1	5	36.68	2.450	4	5.0	-5	1	4	47.82	1.902	4	0.5
0	0	6	24.82	3.586	2	44.1	0	2	2	36.73	2.447	4	2.0	5	0	6	48.05	1.893	2	2.3
2	1	2	25.26	3.526	4	5.9	-1	2	1	36.92	2.435	4	0.5	-5	0	6	48.17	1.889	2	2.4
-2	1	2	25.29	3.522	4	7.0	4	1	0	36.93	2.434	4	6.0	3	2	5	48.58	1.874	4	1.8
3	0	2	25.38	3.510	2	11.6	4	1	1	37.16	2.419	4	2.1	-3	2	5	48.64	1.872	4	1.2
-3	0	2	25.42	3.504	2	12.3	-4	1	1	37.18	2.418	4	0.9	3	1	9	48.75	1.868	4	0.5
1	1	4	25.53	3.489	4	3.7	1	2	2	37.64	2.390	4	1.1	4	2	0	48.84	1.865	4	0.7
-1	1	4	25.56	3.485	4	7.7	4	1	2	37.88	2.375	4	1.3	-3	1	9	48.86	1.864	4	0.6
1	0	6	26.08	3.416	2	4.6	2	1	7	37.90	2.374	4	2.6	2	0	11	49.34	1.847	2	3.5
-1	0	6	26.12	3.411	2	4.7	-4	1	2	37.92	2.373	4	2.0	-2	0	11	49.42	1.844	2	3.1
2	0	5	26.14	3.409	2	18.1	0	1	8	37.94	2.371	4	0.6	0	2	8	49.65	1.836	4	1.1
-2	0	5	26.21	3.400	2	14.1	-2	1	7	37.96	2.370	4	2.5	-2	2	7	49.67	1.835	4	1.0
2	1	3	26.93	3.311	4	1.6	1	1	8	38.81	2.320	4	4.8	6	0	2	49.87	1.829	2	0.9
0	1	5	27.28	3.269	4	3.7	-1	1	8	38.84	2.318	4	2.4	-6	0	2	49.91	1.827	2	0.9

Ammonium Fluoride ZSM-23

MTT



MTW ZSM-12, Calcined

CHEMICAL COMPOSITION: $[Si_{56}O_{112}]$

REFINED COMPOSITION: $[Si_{56}O_{112}]$

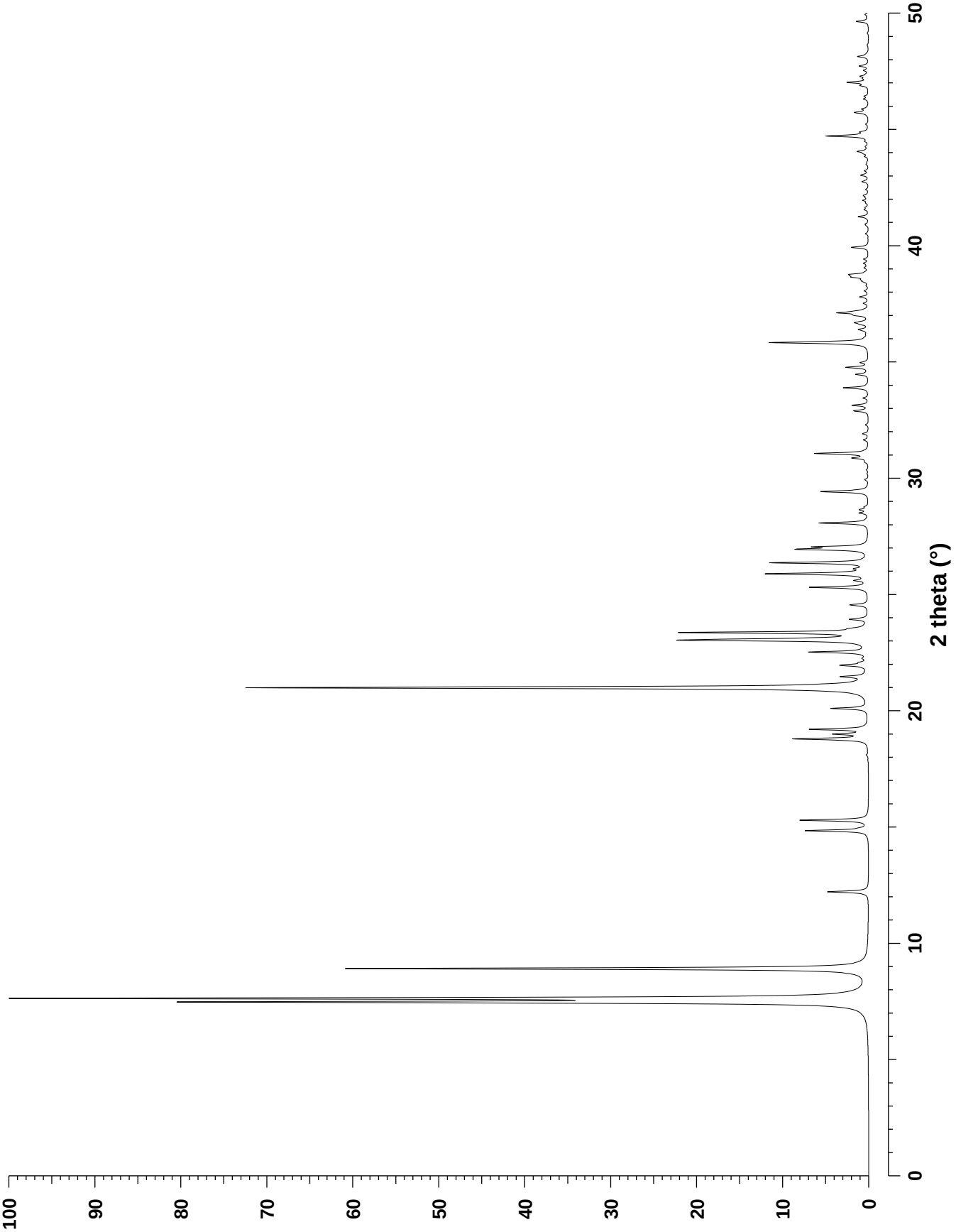
CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 24.8633$ Å $b = 5.01238$ Å $c = 24.3275$ Å
$\alpha = 90°$ $\beta = 107.7215°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.058$, $R_{wp} = 0.181$, $R_I = 0.069$

REFERENCE: C. A. Fyfe, H. Gies, G. T. Kokotailo, B. Marler and D. E. Cox, *J. Phys. Chem.* **94** 3718–3721 (1990).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	7.47	11.842	2	78.3	-8	0	2	28.76	3.104	2	0.4	7	1	4	39.06	2.306	4	0.2
0	0	2	7.63	11.587	2	100.0	-8	0	4	29.41	3.037	2	2.1	2	2	3	39.24	2.296	4	0.5
-2	0	2	8.91	9.929	2	63.6	-2	0	8	29.43	3.035	2	4.1	-9	1	6	39.42	2.286	4	0.5
2	0	2	12.21	7.251	2	5.0	-4	0	8	29.93	2.985	2	0.4	9	1	1	39.92	2.258	4	2.1
-2	0	4	14.84	5.971	2	7.7	1	1	6	30.35	2.945	4	0.2	3	1	8	40.51	2.227	4	0.3
4	0	0	14.96	5.921	2	0.4	5	1	3	30.68	2.914	4	0.3	-9	1	7	40.92	2.206	4	0.3
0	0	4	15.29	5.793	2	8.3	3	1	5	30.85	2.898	4	0.4	-10	0	8	41.24	2.189	2	0.9
1	1	0	18.09	4.904	4	0.2	-7	1	2	30.86	2.898	4	1.4	-3	1	10	41.25	2.188	4	0.3
1	1	1	18.73	4.737	4	1.0	6	0	4	31.06	2.880	2	3.9	-8	0	10	41.54	2.174	2	0.4
4	0	2	18.79	4.722	2	8.8	-7	1	3	31.06	2.879	4	2.7	7	1	5	41.64	2.169	4	0.3
2	0	4	18.99	4.673	2	3.8	-1	1	7	31.64	2.828	4	0.6	5	1	7	41.83	2.159	4	0.3
-1	1	2	19.20	4.622	4	7.0	7	1	0	31.91	2.804	4	0.7	2	0	10	41.94	2.154	2	0.6
1	1	2	20.10	4.417	4	4.4	-6	0	8	32.29	2.772	2	0.4	-1	1	10	42.06	2.148	4	0.2
-1	1	3	20.84	4.263	4	0.4	-7	1	5	32.89	2.723	4	1.8	-6	2	2	42.14	2.144	4	0.3
3	1	0	20.99	4.232	4	75.7	7	1	1	33.13	2.704	4	1.9	4	2	3	42.17	2.143	4	0.3
-3	1	2	21.14	4.202	4	1.1	8	0	2	33.44	2.679	2	0.6	-6	2	3	42.41	2.131	4	0.3
-6	0	2	21.46	4.141	2	2.9	3	1	6	33.88	2.646	4	3.1	6	2	0	42.74	2.116	4	0.7
-2	0	6	21.93	4.054	2	1.4	-7	1	6	34.46	2.603	4	1.5	0	2	6	43.02	2.102	4	0.7
3	1	1	21.96	4.048	4	2.3	7	1	2	34.76	2.581	4	2.7	-6	2	4	43.05	2.101	4	0.3
1	1	3	22.07	4.027	4	0.7	-1	1	8	34.97	2.566	4	0.9	-4	2	6	43.21	2.094	4	0.4
-3	1	3	22.25	3.996	4	0.4	5	1	5	35.77	2.511	4	0.6	9	1	3	43.49	2.081	4	0.3
6	0	0	22.52	3.947	2	7.0	-5	1	8	35.83	2.506	4	2.1	8	0	6	43.83	2.066	2	0.4
-1	1	4	23.01	3.865	4	0.5	0	2	0	35.83	2.506	2	9.8	-11	1	3	43.96	2.060	4	0.3
0	0	6	23.03	3.862	2	18.8	-10	0	2	36.33	2.473	2	0.3	-11	1	4	44.04	2.056	4	1.0
-6	0	4	23.08	3.853	2	9.7	-7	1	7	36.39	2.469	4	1.0	-11	1	5	44.48	2.037	4	0.3
-4	0	6	23.36	3.809	2	22.6	-2	2	1	36.61	2.455	4	0.6	-4	0	12	44.71	2.027	2	5.0
3	1	2	23.53	3.781	4	1.2	2	2	0	36.65	2.452	4	0.3	-12	0	6	44.76	2.025	2	0.2
-3	1	4	23.93	3.718	4	2.2	0	2	2	36.69	2.450	4	1.4	-11	1	1	44.88	2.020	4	0.7
1	1	4	24.51	3.632	4	0.5	-2	2	2	36.99	2.430	4	1.0	-10	0	10	45.69	1.986	2	0.4
4	0	4	24.55	3.626	2	2.0	1	1	8	37.03	2.428	4	0.7	9	1	4	45.72	1.984	4	1.3
-5	1	1	25.30	3.520	4	6.0	-4	0	10	37.11	2.423	2	1.8	11	1	0	45.87	1.978	4	0.7
-5	1	2	25.30	3.520	4	1.1	3	1	7	37.11	2.423	4	1.5	6	2	3	46.30	1.961	4	0.6
3	1	3	25.60	3.480	4	1.3	-9	1	3	37.18	2.418	4	0.7	-11	1	7	46.42	1.956	4	0.5
5	1	0	25.88	3.443	4	10.2	-9	1	4	37.52	2.397	4	0.6	-8	2	1	46.88	1.938	4	0.8
-5	1	3	25.90	3.440	4	2.6	-2	2	3	37.79	2.381	4	1.0	-8	2	4	47.01	1.933	4	1.9
6	0	2	25.97	3.431	2	0.5	-10	0	6	38.05	2.365	2	0.4	-2	2	8	47.02	1.932	4	0.6
-3	1	5	26.10	3.415	4	1.1	-9	1	5	38.28	2.351	4	0.2	-12	0	8	47.17	1.927	2	0.2
2	0	6	26.36	3.381	2	11.9	-1	1	9	38.45	2.341	4	0.6	11	1	1	47.19	1.926	4	0.3
-6	0	6	26.94	3.310	2	8.1	4	0	8	38.53	2.336	2	0.6	-9	1	10	47.28	1.922	4	0.9
5	1	1	27.01	3.301	4	0.2	9	1	0	38.64	2.330	4	1.2	8	2	0	47.53	1.913	4	0.5
-5	1	4	27.04	3.297	4	5.7	-7	1	8	38.64	2.330	4	0.2	3	1	10	47.72	1.906	4	1.1
3	1	4	28.07	3.179	4	6.0	5	1	6	38.70	2.327	4	1.2	6	2	4	48.13	1.890	4	1.3
-1	1	6	28.50	3.132	4	1.0	-4	2	1	38.75	2.324	4	0.2	-1	1	12	49.63	1.837	4	1.0
5	1	2	28.64	3.117	4	0.7	-5	1	9	38.76	2.323	4	1.6	-11	1	9	49.64	1.836	4	0.5
-3	1	6	28.64	3.117	4	0.3	4	2	0	39.03	2.308	4	0.3	-9	1	11	49.93	1.827	4	0.4

ZSM-12, Calcined

MTW



MWW ITQ-1, Calcined (Siliceous MCM-22)

CHEMICAL COMPOSITION: $[Si_{72}O_{144}]$

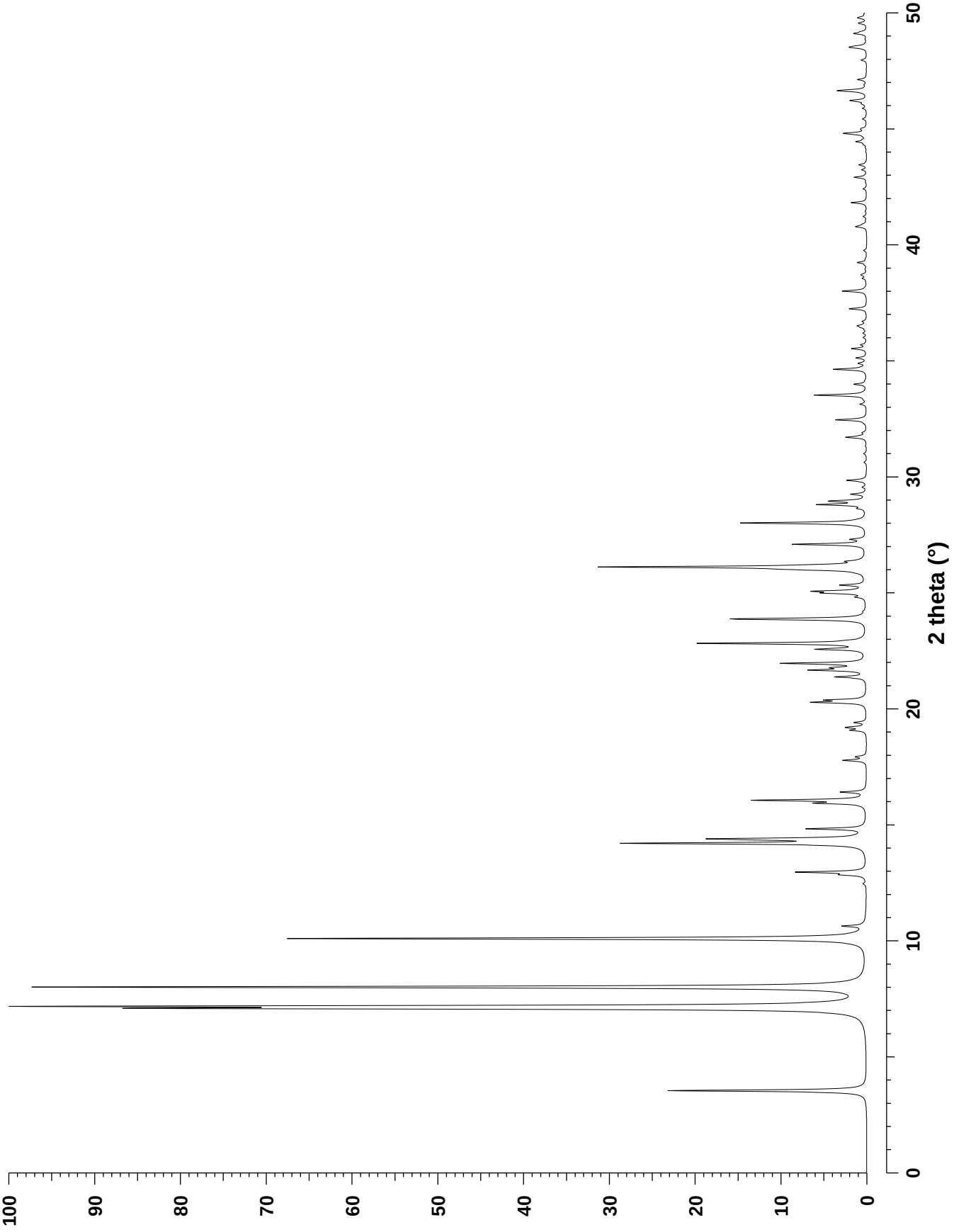
REFINED COMPOSITION: $[Si_{72}O_{144}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 14.2081$ Å $b = 14.2081$ Å $c = 24.945$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement. $R_{exp} = 0.103$, $R_{wp} = 0.159$, $R_F = 0.065$

REFERENCE: M. A. Camblor, A. Corma, M.-J. Diaz-Cabanas and Ch. Baerlocher, *J. Phys. Chem. B* **102** 44–51 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	3.54	24.945	2	23.9	2	2	3	27.30	3.266	12	1.7	5	1	0	40.83	2.210	12	0.4
0	0	2	7.09	12.472	2	74.3	1	1	7	28.01	3.185	12	15.1	5	0	5	40.89	2.207	12	0.3
1	0	0	7.18	12.305	6	90.6	3	0	5	28.16	3.168	12	0.2	4	0	8	41.22	2.190	12	0.4
1	0	1	8.01	11.035	12	100.0	0	0	8	28.63	3.118	2	0.8	4	2	4	41.44	2.179	24	0.1
1	0	2	10.10	8.759	12	69.6	2	1	6	28.80	3.100	24	5.7	1	1	11	41.81	2.160	12	1.9
0	0	3	10.64	8.315	2	2.6	2	0	7	28.95	3.084	12	4.2	3	0	10	42.41	2.131	12	0.4
1	1	0	12.46	7.104	6	0.3	4	0	1	29.25	3.053	12	1.8	4	2	5	42.91	2.108	24	1.5
1	0	3	12.85	6.889	12	2.4	1	0	8	29.55	3.023	12	0.4	3	2	8	43.23	2.093	24	0.6
1	1	1	12.96	6.832	12	8.3	3	1	4	29.84	2.994	24	2.4	5	1	4	43.44	2.083	24	0.9
0	0	4	14.20	6.236	2	28.6	3	0	6	30.62	2.920	12	0.3	6	0	1	44.32	2.044	12	0.3
1	1	2	14.35	6.173	12	6.0	4	0	3	31.00	2.885	12	0.3	2	1	11	44.44	2.038	24	1.2
2	0	0	14.40	6.152	6	15.8	1	1	8	31.33	2.855	12	0.1	4	1	8	44.53	2.035	24	0.3
2	0	1	14.83	5.973	12	7.0	3	2	0	31.70	2.823	12	2.4	4	2	6	44.65	2.029	24	0.1
1	0	4	15.93	5.563	12	5.3	3	1	5	31.77	2.817	24	0.4	5	0	7	44.75	2.025	12	0.7
2	0	2	16.06	5.518	12	13.4	3	2	1	31.90	2.805	24	0.5	6	0	2	44.79	2.024	12	0.1
1	1	3	16.41	5.401	12	3.0	0	0	9	32.30	2.772	2	0.1	4	3	0	44.80	2.023	12	2.3
0	0	5	17.78	4.989	2	2.8	4	0	4	32.45	2.759	12	3.7	5	1	5	44.86	2.021	24	0.1
2	0	3	17.93	4.946	12	1.2	1	0	9	33.13	2.704	12	0.7	4	3	1	44.96	2.016	24	0.3
2	1	0	19.08	4.651	12	1.8	3	0	7	33.31	2.690	12	0.2	3	1	10	45.01	2.014	24	0.5
1	0	5	19.20	4.623	12	2.4	3	2	3	33.52	2.673	24	6.3	4	3	2	45.42	1.997	24	0.5
2	1	1	19.41	4.572	24	1.4	3	1	6	33.99	2.638	24	1.5	3	2	9	45.88	1.978	24	0.4
2	0	4	20.28	4.380	12	6.2	2	1	8	34.63	2.590	24	4.0	5	2	0	46.07	1.970	12	0.4
2	1	2	20.38	4.358	24	4.4	1	1	9	34.74	2.582	12	0.2	4	3	3	46.18	1.966	24	0.6
0	0	6	21.37	4.157	2	3.6	3	2	4	34.89	2.572	24	0.9	5	2	1	46.22	1.964	24	1.7
3	0	0	21.67	4.102	6	6.4	4	1	3	35.12	2.555	24	1.3	5	1	6	46.54	1.951	24	0.2
1	1	5	21.77	4.083	12	3.1	2	0	9	35.52	2.527	12	1.8	6	0	4	46.62	1.948	12	1.0
2	1	3	21.90	4.059	24	0.7	2	2	7	35.69	2.516	12	0.7	4	2	7	46.64	1.947	24	2.1
3	0	1	21.96	4.047	12	9.9	0	0	10	36.00	2.494	2	0.4	5	2	2	46.67	1.946	24	1.0
1	0	6	22.57	3.939	12	5.7	3	0	8	36.19	2.482	12	0.4	4	0	10	46.89	1.938	12	0.2
3	0	2	22.82	3.896	12	20.2	4	0	6	36.33	2.473	12	0.2	4	1	9	47.12	1.929	24	1.1
2	0	5	22.95	3.875	12	0.9	4	1	4	36.43	2.466	24	0.2	6	0	5	47.96	1.897	12	0.5
2	1	4	23.87	3.728	24	16.4	3	1	7	36.45	2.465	24	0.3	1	0	13	47.98	1.896	12	0.1
3	0	3	24.20	3.678	12	0.2	5	0	0	36.51	2.461	6	0.9	5	1	7	48.47	1.878	24	0.2
1	1	6	24.81	3.588	12	1.0	3	2	5	36.57	2.457	24	0.2	6	1	0	48.51	1.876	12	1.7
0	0	7	24.99	3.564	2	4.3	5	0	1	36.69	2.449	12	0.5	4	3	5	48.56	1.875	24	0.8
2	2	0	25.07	3.552	6	5.7	5	0	2	37.24	2.414	12	2.1	4	2	8	48.86	1.864	24	0.1
2	2	1	25.33	3.517	12	3.0	3	3	0	38.00	2.368	6	2.9	6	1	2	49.10	1.856	24	1.5
2	0	6	25.86	3.445	12	0.2	3	2	6	38.55	2.335	24	0.5	1	1	13	49.18	1.852	12	0.5
3	0	4	26.00	3.427	12	4.4	4	0	7	38.67	2.329	12	0.3	5	0	9	49.53	1.840	12	0.4
1	0	7	26.03	3.423	12	2.4	4	2	0	38.72	2.325	12	0.5	6	0	6	49.56	1.839	12	0.7
2	2	2	26.08	3.416	12	0.6	2	0	10	38.96	2.312	12	0.2	5	2	5	49.75	1.833	24	0.2
3	1	0	26.11	3.413	12	30.4	3	1	8	39.13	2.302	24	0.1	2	0	13	49.78	1.832	12	0.9
2	1	5	26.20	3.402	24	2.8	3	0	9	39.23	2.296	12	1.1	6	1	3	49.82	1.830	24	0.2
3	1	1	26.36	3.381	24	1.6	0	0	11	39.75	2.268	2	0.4	4	1	10	49.90	1.828	24	0.1
3	1	2	27.09	3.292	24	8.8	3	2	7	40.78	2.213	24	1.1	4	0	11	49.96	1.825	12	0.2

ITQ-1, Calcined (Siliceous MCM-22) MWW



NAT Natrolite

CHEMICAL COMPOSITION: $|Na_{16}(H_2O)_{16}|\ [Si_{24}Al_{16}O_{80}]$
Aussig, Bohemia

REFINED COMPOSITION: $|Na_{16}(H_2O)_{16}|\ [Si_{24}Al_{16}O_{80}]$

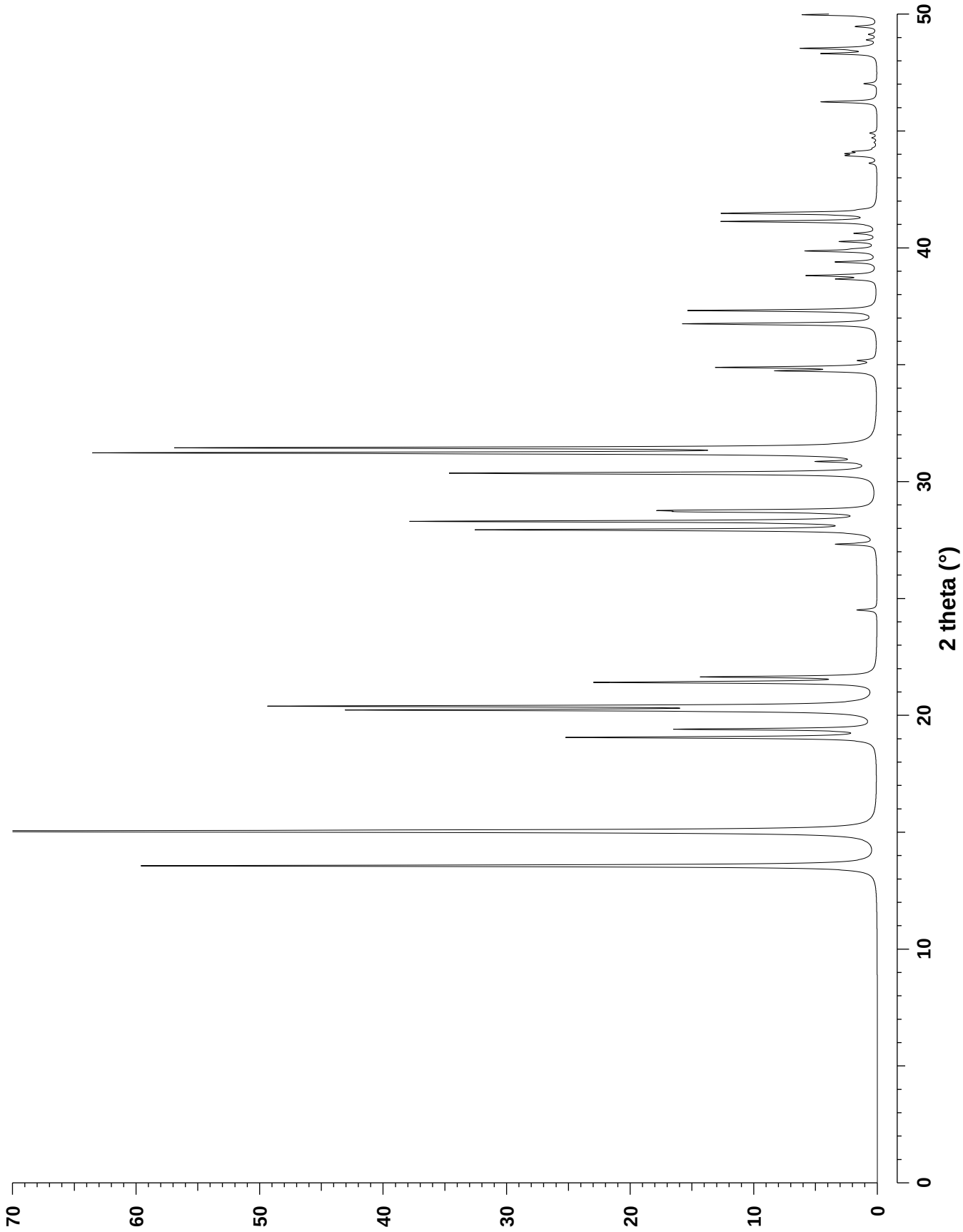
CRYSTAL DATA: $Fdd2$ (No. 43)
$a = 18.30$ Å $b = 18.63$ Å $c = 6.60$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{wp} = 0.08$

REFERENCE: W. M. Meier,
Z. Kristallogr. **113** 430–444 (1960).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	2	0	13.56	6.528	4	59.6	2	4	2	34.73	2.583	8	7.5	4	8	0	43.61	2.075	4	0.6
1	1	1	15.04	5.890	8	100.0	4	2	2	34.88	2.572	8	12.2	1	3	3	43.94	2.061	8	2.1
0	4	0	19.05	4.657	2	24.9	4	6	0	34.92	2.569	4	0.7	3	1	3	44.02	2.057	8	1.9
4	0	0	19.40	4.575	2	16.0	6	4	0	35.17	2.552	4	1.3	8	4	0	44.11	2.053	4	1.6
1	3	1	20.22	4.391	8	40.5	1	7	1	36.74	2.446	8	15.7	5	7	1	44.26	2.046	8	0.2
3	1	1	20.39	4.356	8	47.2	7	1	1	37.31	2.410	8	15.3	7	5	1	44.50	2.036	8	0.2
2	4	0	21.41	4.151	4	22.5	0	8	0	38.66	2.329	2	3.0	4	6	2	44.70	2.027	8	0.4
4	2	0	21.64	4.106	4	13.6	4	4	2	38.81	2.321	8	5.5	6	4	2	44.90	2.019	8	0.6
3	3	1	24.50	3.633	8	1.6	3	7	1	39.38	2.288	8	1.3	1	9	1	46.23	1.964	8	1.5
4	4	0	27.32	3.264	4	3.2	8	0	0	39.39	2.287	2	2.1	3	3	3	46.24	1.963	8	3.2
1	5	1	27.93	3.195	8	32.0	7	3	1	39.83	2.263	8	0.6	9	1	1	47.01	1.933	8	1.1
5	1	1	28.29	3.155	8	37.3	0	6	2	39.86	2.261	4	5.2	1	5	3	48.30	1.884	8	4.3
0	2	2	28.70	3.111	4	11.5	2	8	0	39.95	2.257	4	1.1	3	9	1	48.44	1.879	8	0.8
2	0	2	28.76	3.104	4	13.8	6	0	2	40.26	2.240	4	3.0	5	1	3	48.53	1.876	8	6.0
2	2	2	30.35	2.945	8	33.4	8	2	0	40.61	2.221	4	1.7	2	8	2	48.89	1.863	8	0.8
2	6	0	30.40	2.940	4	2.6	2	6	2	41.12	2.195	8	12.5	9	3	1	49.12	1.855	8	0.6
6	2	0	30.85	2.899	4	3.8	6	2	2	41.46	2.178	8	10.3	8	2	2	49.46	1.843	8	1.7
3	5	1	31.22	2.865	8	61.7	6	6	0	41.50	2.176	4	4.3	2	10	0	49.96	1.826	4	6.1
5	3	1	31.44	2.845	8	54.9	1	1	3	41.63	2.169	8	0.6							

Natrolite

NAT



NAT Gonnardite

CHEMICAL COMPOSITION: $|Na_{6.42}K_{0.01}Ca_{1.50}(H_2O)_{12.37}|\ [Si_{10.73}Al_{9.22}O_{40}]$
Tvedalen, Langesund District, Norway

REFINED COMPOSITION: $|Na_{6.528}Ca_{1.472}(H_2O)_{12}H_8|\ [Si_{10.25}Al_{9.75}O_{40}]$

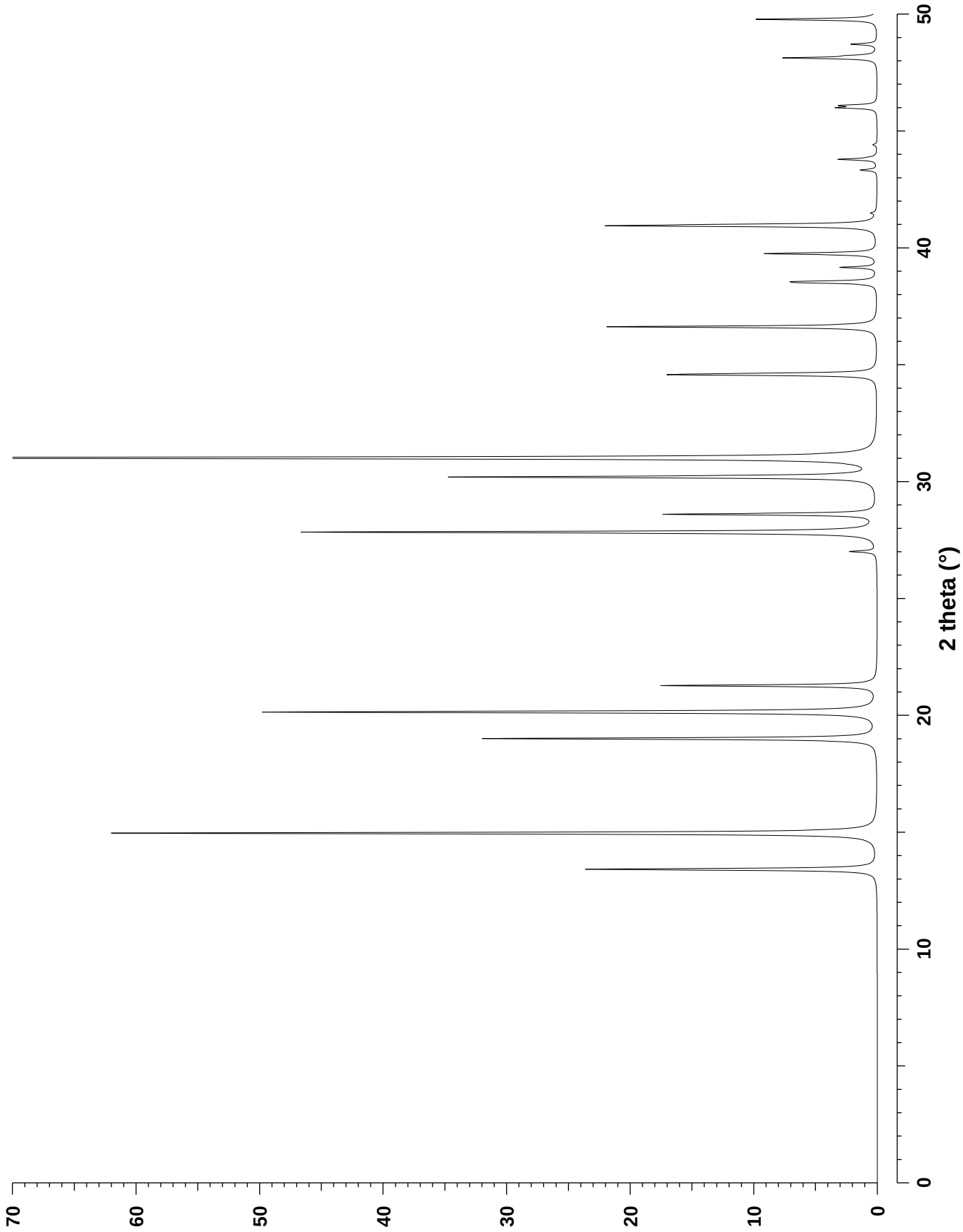
CRYSTAL DATA: $I\bar{4}2d$ (No. 122)
$a = 13.21$ Å $b = 13.21$ Å $c = 6.622$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.03$

REFERENCE: F. Mazzi, A. O. Larsen, G. Gottardi and E. Galli,
Neues Jarhb. Mineral. Monatsh. 219–228 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	13.41	6.605	4	23.6	3	1	2	34.57	2.595	16	15.2	6	2	0	43.32	2.089	8	1.4
1	0	1	14.96	5.920	8	62.1	5	1	0	34.62	2.591	8	4.8	2	1	3	43.78	2.068	16	3.1
2	2	0	19.00	4.670	4	31.9	4	3	1	36.62	2.454	16	21.9	6	1	1	43.87	2.064	16	0.3
2	1	1	20.14	4.408	16	49.8	4	0	2	38.50	2.338	8	4.6	5	1	2	44.40	2.040	16	0.3
3	1	0	21.27	4.177	8	17.5	4	4	0	38.55	2.335	4	5.1	3	0	3	45.99	1.973	8	3.0
4	0	0	27.00	3.303	4	2.1	5	2	1	39.16	2.300	16	3.0	5	4	1	46.08	1.970	16	2.7
3	2	1	27.83	3.206	16	46.6	3	3	2	39.74	2.268	8	8.7	3	2	3	48.12	1.891	16	7.4
1	1	2	28.60	3.121	8	17.2	5	3	0	39.79	2.265	8	1.0	6	3	1	48.21	1.888	16	1.5
2	0	2	30.19	2.960	8	33.4	4	2	2	40.94	2.204	16	19.7	5	3	2	48.70	1.870	16	2.1
4	2	0	30.26	2.954	8	4.4	6	0	0	40.99	2.202	4	6.0	6	4	0	49.77	1.832	8	9.8
4	1	1	31.01	2.884	16	100.0	1	0	3	41.47	2.177	8	0.4							

Gonnardite

NAT



NAT Mesolite

CHEMICAL COMPOSITION: $|Na_{16}Ca_{16}(H_2O)_{64}|\ [Si_{72}Al_{48}O_{240}]$
Poona, India

REFINED COMPOSITION: $|Na_{16}Ca_{16}(H_2O)_{64}|\ [Si_{72}Al_{48}O_{240}]$

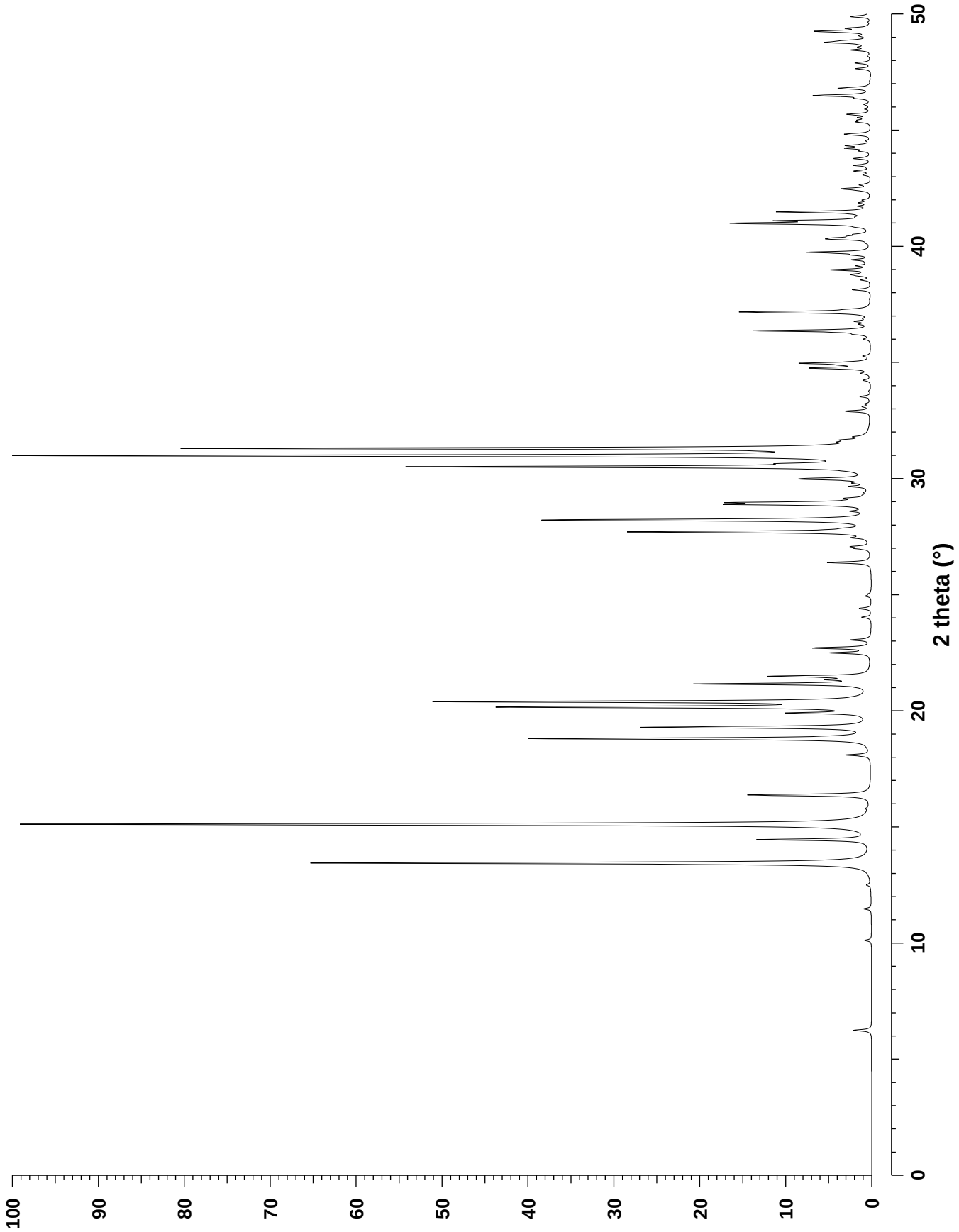
CRYSTAL DATA: *Fdd*2 (No. 43)
$a = 18.4049$ Å $b = 56.655$ Å $c = 6.5443$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.052$

REFERENCE: G. Artioli, J. V. Smith and J. J. Pluth,
Acta Cryst. **C42** 937–942 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	4	0	6.24	14.164	2	2.2	0	10	2	31.57	2.834	4	1.4	1	3	3	41.98	2.152	8	0.8
2	2	0	10.11	8.752	4	0.8	2	8	2	31.65	2.827	8	2.0	8	10	0	42.40	2.132	4	0.7
2	4	0	11.47	7.717	4	0.9	6	8	0	31.79	2.815	4	1.2	7	13	1	42.46	2.129	8	1.8
0	8	0	12.50	7.082	2	0.5	5	11	1	32.89	2.723	8	2.9	1	5	3	42.48	2.128	8	1.2
2	6	0	13.44	6.590	4	65.9	2	20	0	33.09	2.707	4	0.7	1	25	1	42.50	2.127	8	0.4
1	1	1	14.45	6.130	8	13.1	6	10	0	33.21	2.697	4	0.6	2	26	0	42.64	2.120	4	1.2
1	3	1	15.11	5.862	8	100.0	3	17	1	33.52	2.673	8	1.3	4	24	0	43.07	2.100	4	0.8
1	5	1	16.37	5.416	8	14.4	4	4	2	34.22	2.621	8	0.9	1	7	3	43.23	2.093	8	1.9
1	7	1	18.09	4.905	8	2.9	4	18	0	34.52	2.598	4	1.0	6	10	2	43.48	2.081	8	0.4
0	12	0	18.80	4.721	2	40.0	5	13	1	34.72	2.584	8	1.5	6	20	0	43.48	2.081	4	1.6
4	0	0	19.29	4.601	2	26.7	2	12	2	34.75	2.581	8	5.9	8	12	0	43.77	2.068	4	2.0
3	1	1	19.90	4.462	8	8.7	6	12	0	34.88	2.572	4	1.9	3	1	3	44.09	2.054	8	1.2
1	9	1	20.16	4.405	8	42.3	4	6	2	34.96	2.566	8	7.9	7	15	1	44.19	2.049	8	0.6
4	4	0	20.29	4.376	4	0.5	0	14	2	35.27	2.544	4	0.8	1	9	3	44.22	2.048	8	2.4
3	3	1	20.39	4.355	8	50.1	4	8	2	35.99	2.496	8	0.7	3	3	3	44.33	2.043	8	2.7
2	12	0	21.15	4.201	4	20.4	3	19	1	36.20	2.482	8	1.0	4	18	2	44.53	2.035	8	0.4
3	5	1	21.34	4.163	8	3.7	1	21	1	36.35	2.472	8	13.7	0	22	2	44.78	2.024	4	0.4
4	6	0	21.48	4.136	4	11.5	2	14	2	36.64	2.452	8	1.0	3	5	3	44.81	2.022	8	1.8
1	11	1	22.49	3.953	8	4.7	6	14	0	36.76	2.445	4	1.3	6	12	2	44.82	2.022	8	0.5
3	7	1	22.70	3.917	8	6.7	7	1	1	36.88	2.437	8	0.5	3	25	1	44.83	2.022	8	0.6
4	8	0	23.05	3.858	4	2.4	7	3	1	37.16	2.420	8	15.3	8	14	0	45.34	2.000	4	1.5
2	14	0	24.02	3.704	4	1.1	4	10	2	37.27	2.413	8	1.0	1	11	3	45.42	1.997	8	1.2
3	9	1	24.40	3.648	8	1.4	4	20	0	37.27	2.412	4	0.5	3	7	3	45.53	1.992	8	1.3
4	10	0	24.93	3.572	4	0.7	0	24	0	38.12	2.361	2	2.2	1	27	1	45.67	1.986	8	2.7
3	11	1	26.38	3.378	8	5.2	7	7	1	38.54	2.336	8	1.1	2	22	2	45.91	1.976	8	0.7
2	16	0	26.98	3.305	4	1.5	2	16	2	38.72	2.325	8	1.0	4	26	0	46.09	1.969	4	0.5
4	12	0	27.06	3.295	4	2.0	4	12	2	38.78	2.322	8	1.9	6	14	2	46.36	1.958	8	1.4
0	2	2	27.44	3.251	4	1.6	5	17	1	38.97	2.311	8	2.3	3	9	3	46.48	1.954	8	5.8
1	15	1	27.70	3.221	8	28.3	3	21	1	38.98	2.311	8	2.4	5	23	1	46.48	1.954	8	0.8
5	1	1	27.85	3.203	8	1.2	8	0	0	39.16	2.301	2	1.5	4	20	2	46.79	1.942	8	1.3
5	3	1	28.21	3.163	8	38.4	2	24	0	39.41	2.287	4	1.9	9	3	1	46.79	1.942	8	2.1
3	13	1	28.59	3.122	8	1.6	7	9	1	39.62	2.275	8	1.4	1	13	3	46.83	1.940	8	0.9
0	6	2	28.88	3.092	4	14.1	0	18	2	39.73	2.268	4	7.3	3	11	3	47.64	1.909	8	1.8
5	5	1	28.92	3.087	8	0.4	6	0	2	40.30	2.238	4	3.9	3	27	1	47.88	1.900	8	1.8
2	0	2	28.96	3.083	4	13.9	8	6	0	40.35	2.235	4	2.8	1	15	3	48.44	1.879	8	2.2
2	2	2	29.14	3.065	8	2.1	6	2	2	40.43	2.231	8	1.6	2	24	2	48.57	1.874	8	1.0
2	4	2	29.65	3.013	8	2.1	4	14	2	40.51	2.227	8	1.4	5	3	3	48.76	1.867	8	4.5
6	4	0	29.80	2.998	4	1.3	6	4	2	40.82	2.210	8	0.7	8	4	2	48.81	1.866	8	1.6
5	7	1	29.96	2.983	8	5.5	7	11	1	40.93	2.205	8	0.9	9	9	1	48.85	1.864	8	1.7
2	18	0	30.00	2.978	4	4.2	2	18	2	40.98	2.202	8	15.0	8	18	0	49.05	1.857	4	0.9
1	17	1	30.49	2.932	8	2.5	6	18	0	41.09	2.197	4	9.6	5	5	3	49.21	1.851	8	1.1
2	6	2	30.50	2.931	8	51.0	8	8	0	41.26	2.188	4	0.7	5	25	1	49.22	1.851	8	0.6
6	6	0	30.64	2.917	4	5.6	6	6	2	41.47	2.178	8	10.9	2	30	0	49.25	1.850	4	5.5
3	15	1	30.98	2.887	8	99.2	1	1	3	41.72	2.165	8	1.2	8	6	2	49.38	1.846	8	2.5
5	9	1	31.29	2.858	8	79.3	3	23	1	41.86	2.158	8	1.2	5	7	3	49.88	1.828	8	2.4

Mesolite

NAT



NAT Scolecite

CHEMICAL COMPOSITION: $|Ca_4(H_2O)_{12}|\ [Si_{12}Al_8O_{40}]$
Bombay, India

REFINED COMPOSITION: $|Ca_4(H_2O)_{12}|\ [Si_{12}Al_8O_{40}]$

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 6.5222$ Å $b = 18.9678$ Å $c = 9.8398$ Å
$\alpha = 90°$ $\beta = 109.972°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.031$

REFERENCE: J. V. Smith, J. J. Pluth, G. Artioli and F. K. Ross,
in *Proceedings of the 6th International Zeolite Conference, Reno 1983*,
Ed. by D. H. Olson and A. Bisio (Butterworth: Guildford) 842–850 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	1	13.37	6.621	4	49.3	0	4	3	34.71	2.585	4	2.0	-1	5	4	43.89	2.063	4	1.0
-1	1	1	15.10	5.869	4	100.0	-2	2	3	34.80	2.578	4	2.8	1	5	3	44.13	2.052	4	1.5
1	1	0	15.19	5.833	4	13.1	2	4	0	34.85	2.574	4	1.2	-3	3	2	44.28	2.046	4	2.4
0	4	0	18.71	4.742	2	37.5	2	2	1	35.14	2.554	4	2.0	-3	1	3	44.29	2.045	4	0.1
0	0	2	19.19	4.624	2	35.1	-1	7	1	36.20	2.481	4	3.0	-2	6	3	44.32	2.044	4	0.5
-1	3	1	20.11	4.416	4	26.1	1	7	0	36.25	2.478	4	5.2	-3	3	1	44.38	2.041	4	2.7
1	3	0	20.18	4.401	4	24.4	-1	5	3	36.52	2.460	4	0.6	-2	4	4	44.53	2.034	4	2.6
-1	1	2	20.26	4.383	4	42.7	1	5	2	36.72	2.447	4	3.3	3	1	0	44.60	2.032	4	5.0
1	1	1	20.47	4.338	4	10.3	-1	1	4	36.87	2.438	4	6.3	2	6	1	44.60	2.032	4	1.7
0	4	1	21.05	4.220	4	12.3	1	1	3	37.15	2.420	4	9.5	2	4	2	44.95	2.017	4	0.2
0	2	2	21.38	4.156	4	7.8	0	8	0	37.95	2.371	2	0.9	-1	9	1	45.48	1.994	4	2.2
-1	3	2	24.26	3.669	4	4.6	-2	4	3	38.60	2.332	4	2.8	1	9	0	45.51	1.993	4	0.6
1	3	1	24.44	3.642	4	10.6	-1	7	2	38.78	2.322	4	4.1	-3	3	3	46.42	1.956	4	8.4
0	4	2	26.93	3.311	4	2.2	1	7	1	38.90	2.315	4	1.3	-1	1	5	46.43	1.956	4	1.3
-1	5	1	27.60	3.232	4	10.4	2	4	1	38.92	2.314	4	1.0	3	3	0	46.72	1.944	4	0.7
1	5	0	27.65	3.226	4	9.0	0	0	4	38.95	2.312	2	2.3	1	1	4	46.73	1.944	4	0.3
-1	1	3	28.00	3.187	4	9.6	0	8	1	39.22	2.297	4	4.0	-2	8	1	47.41	1.918	4	1.2
0	6	0	28.23	3.161	2	0.2	-1	3	4	39.32	2.291	4	0.9	-1	9	2	47.64	1.909	4	0.5
1	1	2	28.26	3.158	4	15.2	1	3	3	39.59	2.276	4	0.8	1	9	1	47.74	1.905	4	3.9
-2	0	2	28.93	3.086	2	6.1	-2	6	1	39.71	2.270	4	8.0	0	10	0	47.96	1.897	2	1.4
-2	2	1	28.95	3.084	4	9.3	-2	0	4	40.03	2.252	2	3.4	-2	8	2	48.41	1.880	4	1.5
2	0	0	29.13	3.065	2	7.3	0	2	4	40.14	2.246	4	4.7	0	8	3	48.43	1.879	4	0.9
0	6	1	29.87	2.991	4	6.3	2	0	2	40.48	2.228	2	0.5	-1	3	5	48.48	1.878	4	0.8
-2	2	2	30.46	2.934	4	31.5	-2	6	2	40.87	2.208	4	9.7	2	8	0	48.54	1.875	4	0.1
0	2	3	30.49	2.932	4	11.5	0	6	3	40.89	2.207	4	9.9	-3	5	1	48.56	1.875	4	1.7
2	2	0	30.65	2.916	4	13.1	2	6	0	41.01	2.201	4	3.0	-3	1	4	48.58	1.874	4	1.7
-1	5	2	30.81	2.902	4	33.9	-2	2	4	41.19	2.191	4	4.7	1	3	4	48.78	1.867	4	3.0
1	5	1	30.96	2.889	4	54.7	2	2	2	41.64	2.169	4	8.0	0	6	4	48.80	1.866	4	2.6
-1	3	3	31.07	2.878	4	26.2	-3	1	2	42.07	2.148	4	1.2	0	10	1	49.02	1.858	4	3.5
1	3	2	31.31	2.857	4	52.9	-3	1	1	42.18	2.143	4	3.0	3	1	1	49.07	1.857	4	3.2
-2	4	1	33.35	2.687	4	1.0	0	8	2	42.86	2.110	4	1.3	2	2	3	49.51	1.841	4	4.3
0	6	2	34.36	2.610	4	1.6	0	4	4	43.55	2.078	4	3.3	-2	6	4	49.70	1.834	4	0.5
-2	4	2	34.68	2.586	4	3.6	1	7	2	43.76	2.069	4	0.9							

Scolecite

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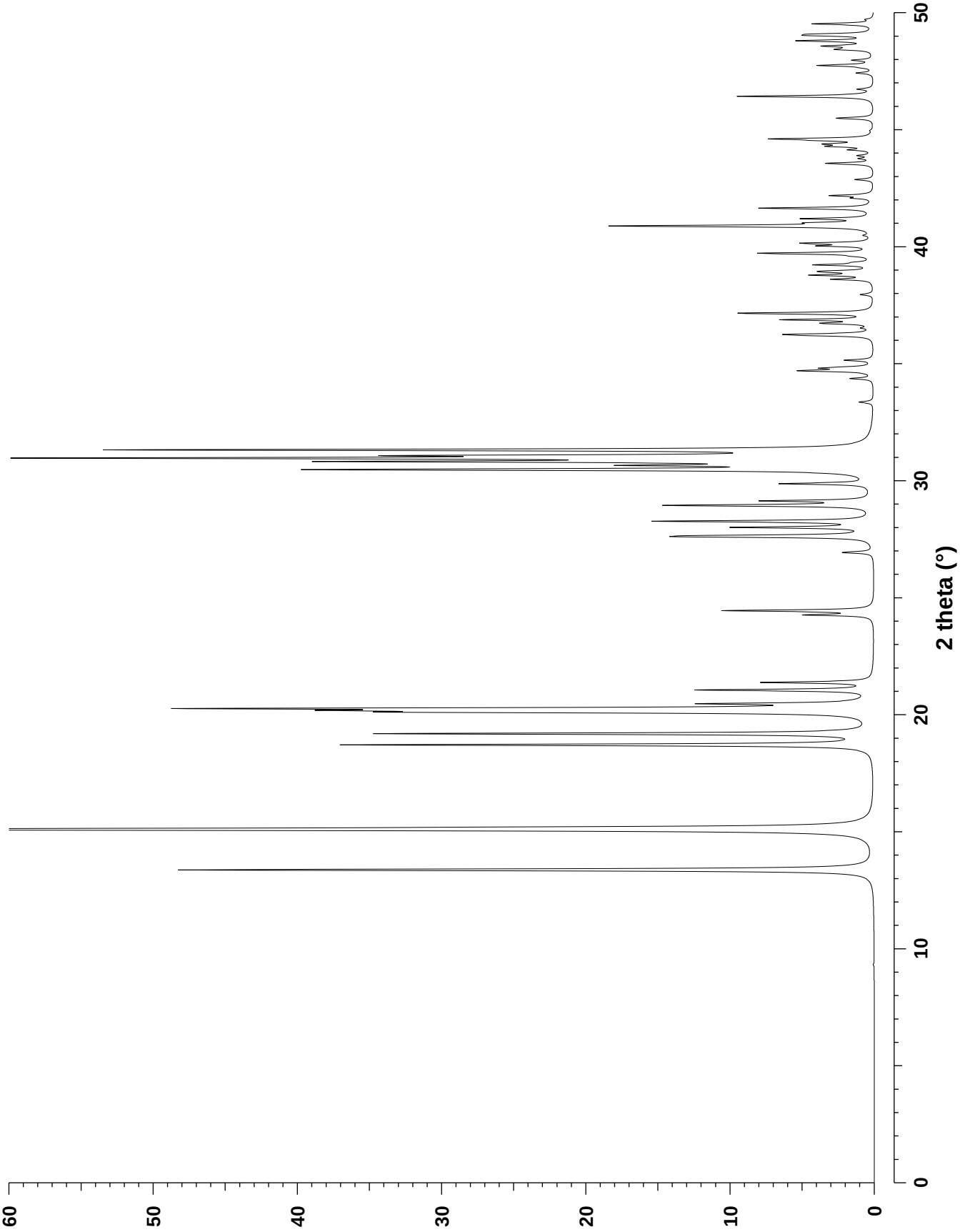


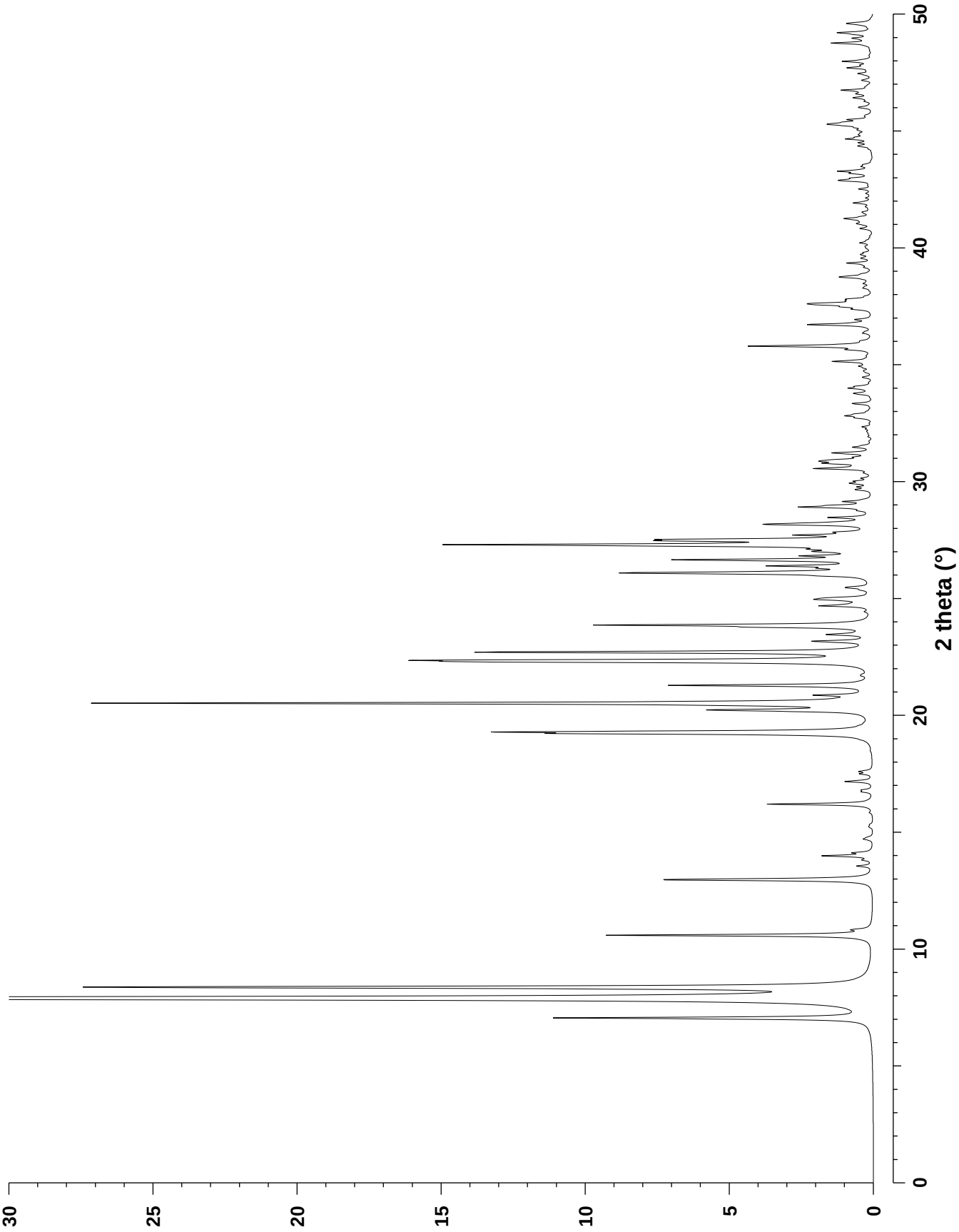
CHEMICAL COMPOSITION: $|(H_2O)_{20}|\ [Si_{68}O_{136}]$

REFINED COMPOSITION: $|(H_2O)_{20}|\ [Si_{68}O_{136}]$

CRYSTAL DATA: $P1\,2_1/c\,1$ (No. 14) unique axis **b**, cell choice 1
$a = 14.324$ Å $b = 22.376$ Å $c = 25.092$ Å
$\alpha = 90°$ $\beta = 151.515°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.075$, $R_{wp} = 0.14$, $R_I = 0.065$

REFERENCE: M. D. Shannon, J. L. Casci, P. A. Cox and S. J. Andrews, *Nature* **353** 417–420 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
-1	0	2	7.05	12.546	2	10.9	-4	2	6	26.15	3.407	4	1.1	-1	0	6	33.99	2.637	2	0.7
0	2	0	7.90	11.188	2	100.0	-2	2	6	26.29	3.389	4	1.0	-3	7	4	34.07	2.632	4	0.5
-1	1	1	8.34	10.597	4	12.9	2	1	0	26.39	3.377	4	3.1	-2	8	4	35.13	2.555	4	1.2
0	1	1	8.38	10.553	4	19.6	-3	4	6	26.61	3.349	4	1.3	2	6	0	35.64	2.519	4	0.7
-1	2	2	10.59	8.350	4	9.3	-4	1	5	26.65	3.345	4	6.0	-5	0	10	35.79	2.509	2	3.9
0	2	1	10.83	8.173	4	0.5	-1	1	5	26.82	3.324	4	1.9	-4	6	5	35.83	2.506	4	0.7
1	0	0	12.96	6.832	2	5.7	-1	6	3	26.99	3.303	4	0.5	-5	2	10	36.71	2.448	4	2.2
-2	1	3	12.99	6.814	4	2.4	-3	0	2	27.01	3.301	2	0.9	0	9	1	36.93	2.434	4	0.4
1	1	0	13.55	6.534	4	0.5	1	0	2	27.10	3.290	2	1.1	-3	8	5	37.37	2.406	4	0.5
-1	3	1	13.97	6.339	4	0.3	1	6	0	27.24	3.273	4	3.5	-4	6	8	37.47	2.400	4	0.7
0	3	1	13.99	6.330	4	1.4	2	2	0	27.30	3.267	4	13.2	-3	8	4	37.56	2.395	4	0.9
-2	0	4	14.12	6.273	2	0.6	0	4	3	27.46	3.248	4	0.5	-5	1	5	37.59	2.393	4	0.8
-2	2	4	16.20	5.472	4	3.7	-3	5	5	27.46	3.248	4	4.4	-1	8	4	37.62	2.391	4	1.0
-2	3	3	17.17	5.163	4	1.0	-2	5	5	27.52	3.241	4	5.3	-4	7	6	37.74	2.383	4	0.4
1	3	0	17.60	5.038	4	0.4	-1	2	5	27.71	3.220	4	1.9	0	1	5	37.80	2.380	4	0.6
-3	0	4	19.15	4.635	2	0.4	-2	6	4	27.83	3.206	4	0.8	-3	8	6	38.73	2.325	4	0.6
-3	1	5	19.22	4.619	4	8.3	-2	6	2	28.15	3.170	4	0.7	-3	5	1	38.76	2.323	4	0.5
-2	1	5	19.29	4.600	4	11.1	-2	5	1	28.16	3.168	4	1.8	2	5	1	38.80	2.321	4	0.3
-2	1	1	20.19	4.399	4	1.9	-3	2	2	28.18	3.166	4	0.4	-5	3	5	39.34	2.290	4	0.8
1	1	1	20.23	4.389	4	4.1	0	6	2	28.20	3.165	4	0.5	-5	4	5	40.82	2.211	4	0.4
-3	2	5	20.42	4.349	4	1.6	1	5	1	28.20	3.165	4	1.1	-5	5	10	41.25	2.189	4	0.7
-2	2	5	20.49	4.334	4	0.4	1	2	2	28.27	3.157	4	0.5	-4	8	5	41.91	2.156	4	0.6
1	4	0	20.52	4.328	4	26.6	-4	0	8	28.46	3.136	2	1.3	1	10	0	42.51	2.126	4	0.4
-1	2	4	20.86	4.259	4	1.6	-1	7	1	28.90	3.089	4	1.0	0	5	5	42.85	2.111	4	0.4
-2	4	4	21.28	4.175	4	6.7	0	7	1	28.91	3.088	4	1.3	3	4	0	42.88	2.109	4	0.6
-3	3	5	22.29	3.989	4	10.7	-4	3	5	28.98	3.081	4	1.0	-6	5	9	42.98	2.105	4	0.5
-2	3	5	22.35	3.977	4	12.5	-1	3	5	29.14	3.065	4	0.9	-3	5	9	43.18	2.095	4	0.5
-1	3	4	22.69	3.919	4	0.5	-4	4	6	29.64	3.014	4	0.4	-6	0	12	43.27	2.091	2	1.1
-3	2	6	22.70	3.917	4	13.1	-2	4	6	29.77	3.001	4	0.4	-7	1	11	44.49	2.036	4	0.4
-2	3	1	23.14	3.844	4	0.7	-3	5	3	29.92	2.987	4	0.7	3	5	0	44.65	2.030	4	0.8
1	3	1	23.17	3.838	4	1.4	0	5	3	30.01	2.978	4	0.5	-4	1	11	44.73	2.026	4	0.4
-2	5	3	23.45	3.794	4	1.2	-3	6	5	30.55	2.926	4	1.8	-4	9	5	45.26	2.003	4	0.6
-1	5	3	23.49	3.788	4	0.4	-3	6	4	30.77	2.906	4	0.9	-2	10	1	45.29	2.002	4	0.4
1	5	0	23.77	3.743	4	2.9	-4	2	4	30.78	2.905	4	0.5	-1	9	5	45.37	1.999	4	0.5
0	6	0	23.86	3.729	2	9.2	-1	6	4	30.85	2.898	4	0.9	0	0	6	45.48	1.995	2	0.6
-3	4	5	24.68	3.608	4	1.6	-4	4	5	30.89	2.895	4	0.6	3	6	0	46.74	1.944	4	1.0
-2	4	5	24.74	3.599	4	0.4	-4	3	8	30.93	2.891	4	0.5	0	7	5	47.45	1.916	4	0.4
-3	4	4	24.95	3.569	4	1.4	-1	4	5	31.04	2.881	4	0.4	-7	4	10	47.69	1.907	4	0.7
-1	6	1	25.00	3.562	4	0.8	1	6	1	31.22	2.865	4	1.2	-3	4	10	47.97	1.897	4	1.0
-1	4	4	25.04	3.556	4	0.4	-3	4	2	31.47	2.843	4	0.4	-5	8	10	48.75	1.868	4	1.2
-2	4	1	25.45	3.500	4	0.6	-4	4	8	32.73	2.736	4	0.3	-7	5	11	48.97	1.860	4	0.4
1	4	1	25.49	3.495	4	0.5	-1	8	2	32.81	2.730	4	0.8	3	7	0	49.12	1.855	4	0.4
-4	1	7	25.96	3.432	4	0.9	0	6	3	32.88	2.724	4	0.3	-4	5	11	49.20	1.852	4	0.5
-3	1	7	26.05	3.421	4	1.7	-1	5	5	33.33	2.688	4	0.7	1	11	1	49.20	1.852	4	0.4
2	0	0	26.09	3.416	2	7.4	-5	0	6	33.77	2.654	2	0.5	-3	5	10	49.59	1.838	4	0.3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CHEMICAL COMPOSITION: $|Na_{2.5}K_{0.2}Mg_{3.1}Ca_{4.9}(H_2O)_{93}|\ [Si_{117.2}Al_{18.8}O_{272}]$
Mt. Adamson, Northern Victoria Land, Antarctica

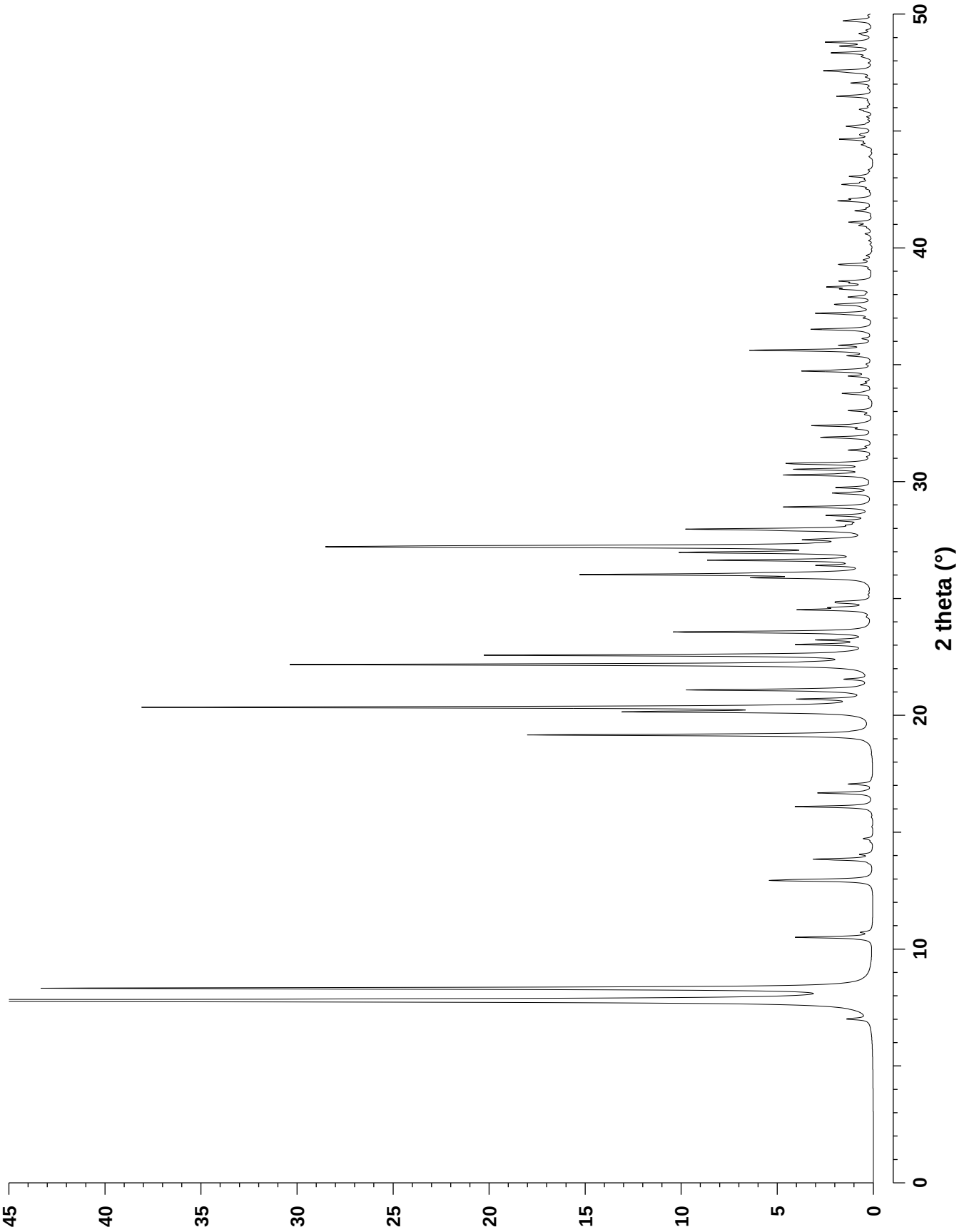
REFINED COMPOSITION: $|Na_{66.8}|^{\dagger}\ [Si_{115.6}Al_{20.4}O_{272}]$

CRYSTAL DATA: *Cmce* (No. 64)
$a = 13.698$ Å $b = 25.213$ Å $c = 22.660$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_F = 0.1195$, $R_w = 0.0968$

REFERENCE: A. Alberti, G. Vezzalini, E. Galli and S. Quartieri, *Eur. J. Mineral.* **8** 69–75 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	7.01	12.606	2	1.1	3	1	5	27.96	3.191	8	9.0	5	1	5	38.57	2.334	8	1.6
0	0	2	7.80	11.330	2	100.0	4	2	2	28.13	3.173	8	0.6	5	5	3	39.28	2.294	8	1.8
1	1	1	8.32	10.630	8	42.9	1	7	3	28.21	3.163	8	0.4	6	0	0	39.47	2.283	2	0.3
0	2	2	10.50	8.427	4	4.0	0	8	0	28.32	3.152	2	1.6	4	8	2	39.67	2.272	8	0.3
1	1	2	10.72	8.250	8	0.5	1	1	7	28.55	3.126	8	2.2	1	5	9	40.59	2.223	8	0.4
2	0	0	12.93	6.849	2	3.6	3	5	3	28.91	3.089	8	4.5	0	10	5	40.96	2.203	4	0.3
1	3	1	12.96	6.830	8	2.5	2	6	4	29.50	3.027	8	1.9	3	1	9	41.09	2.196	8	1.2
1	1	3	13.84	6.398	8	3.1	3	3	5	29.74	3.004	8	1.8	3	5	8	41.57	2.172	8	0.3
0	4	0	14.05	6.303	2	0.6	1	5	6	30.28	2.952	8	4.4	4	6	6	41.58	2.172	8	0.7
2	2	0	14.72	6.018	4	0.5	2	4	6	30.52	2.929	8	3.9	1	11	3	41.70	2.166	8	0.2
0	4	2	16.09	5.508	4	4.1	4	4	2	30.74	2.908	8	1.0	2	0	10	42.00	2.151	4	1.6
2	2	2	16.68	5.315	8	2.9	3	5	4	30.77	2.906	8	3.7	6	4	0	42.09	2.147	4	0.8
1	3	3	17.06	5.198	8	1.3	4	2	4	31.34	2.855	8	1.2	5	5	5	42.52	2.126	8	0.3
1	5	1	19.16	4.632	8	17.9	2	8	1	31.50	2.840	8	0.3	2	2	10	42.63	2.121	8	0.2
3	1	1	20.15	4.407	8	11.4	2	6	5	31.84	2.810	8	0.3	6	0	4	42.70	2.118	4	1.5
1	5	2	20.34	4.367	8	1.4	3	7	1	31.89	2.806	8	2.6	3	9	5	42.80	2.113	8	0.4
2	0	4	20.34	4.365	4	36.1	2	8	2	32.25	2.776	8	0.7	0	8	8	42.93	2.107	4	0.2
2	4	2	20.69	4.292	8	3.3	0	2	8	32.39	2.764	4	2.9	0	12	0	43.05	2.101	2	1.2
0	4	4	21.08	4.213	4	9.4	1	7	5	32.42	2.762	8	0.3	3	11	1	44.40	2.040	8	0.5
0	6	0	21.14	4.202	2	0.3	1	9	1	32.87	2.725	8	0.3	2	4	10	44.50	2.036	8	0.3
2	2	4	21.54	4.125	8	1.2	3	5	5	33.03	2.712	8	1.3	5	5	6	44.64	2.030	8	1.0
1	5	3	22.17	4.010	8	30.2	4	6	0	33.76	2.655	4	1.5	5	3	7	44.65	2.029	8	0.4
0	6	2	22.57	3.940	4	19.9	3	1	7	34.14	2.626	8	0.6	4	10	1	44.82	2.022	8	0.3
3	1	3	23.03	3.861	8	3.7	2	0	8	34.26	2.617	4	0.3	3	5	9	44.87	2.020	8	0.4
1	3	5	23.22	3.830	8	2.6	2	6	6	34.51	2.599	8	1.1	2	12	0	45.14	2.009	4	0.4
0	0	6	23.56	3.777	2	10.3	4	6	2	34.71	2.585	8	0.4	6	6	0	45.20	2.006	4	1.2
1	5	4	24.51	3.632	8	3.6	0	4	8	34.72	2.584	4	3.1	0	10	7	45.60	1.989	4	0.3
2	2	5	24.59	3.620	8	0.2	1	9	3	34.78	2.580	8	0.6	1	3	11	45.83	1.980	8	0.3
0	2	6	24.61	3.618	4	1.5	4	0	6	35.38	2.537	4	1.1	4	8	6	45.92	1.976	8	0.5
2	4	4	24.81	3.589	8	1.2	0	10	0	35.61	2.521	2	5.9	6	0	6	46.48	1.954	4	1.8
2	6	0	24.86	3.582	4	1.3	3	5	6	35.62	2.521	8	0.5	5	5	7	47.04	1.932	8	1.1
1	7	1	25.88	3.443	8	5.2	0	10	1	35.83	2.506	4	1.6	3	9	7	47.30	1.922	8	0.3
4	0	0	26.02	3.424	2	14.1	4	2	6	36.11	2.487	8	0.5	2	6	10	47.48	1.915	8	0.5
2	6	2	26.09	3.415	8	2.7	0	10	2	36.51	2.461	4	3.1	1	13	1	47.52	1.913	8	0.6
0	6	4	26.41	3.375	4	2.4	1	5	8	36.99	2.430	8	0.4	4	10	4	47.57	1.911	8	2.1
3	5	1	26.63	3.347	8	8.2	0	8	6	37.15	2.420	4	0.2	7	1	3	48.17	1.889	8	0.2
2	0	6	26.96	3.307	4	7.8	2	4	8	37.19	2.417	8	2.8	0	10	8	48.33	1.883	4	1.7
4	2	0	26.98	3.305	4	1.6	5	5	1	37.57	2.394	8	1.8	3	5	10	48.34	1.883	8	0.3
4	0	2	27.20	3.278	4	22.6	0	10	3	37.61	2.392	4	0.2	3	1	11	48.62	1.873	8	1.6
1	5	5	27.25	3.273	8	13.9	3	9	1	37.89	2.375	8	1.0	3	11	5	48.79	1.867	8	2.3
3	5	2	27.50	3.243	8	2.2	5	5	2	38.22	2.355	8	0.8	1	9	9	49.10	1.855	8	0.3
2	4	5	27.52	3.241	8	0.2	2	10	1	38.24	2.353	8	0.6	1	11	7	49.16	1.853	8	0.6
0	4	6	27.53	3.240	4	0.3	0	6	8	38.32	2.349	4	1.6	7	3	3	49.31	1.848	8	0.2
2	6	3	27.56	3.236	8	0.6	1	9	5	38.34	2.348	8	0.6	5	5	8	49.70	1.834	8	1.3
2	2	6	27.89	3.199	8	2.3	3	5	7	38.48	2.339	8	0.7	3	3	11	49.75	1.833	8	0.5

The space group symbol *Cmce* now replaces the older form, *Cmca*.
†Na atoms represent unresolved cations and water in the channels.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NON 2-aminopentane Nonasil

CHEMICAL COMPOSITION: $|(C_5H_{11}NH_2)_4|$ $[Si_{88}O_{176}]$
$C_5H_{11}NH_2$ = 2-aminopentane

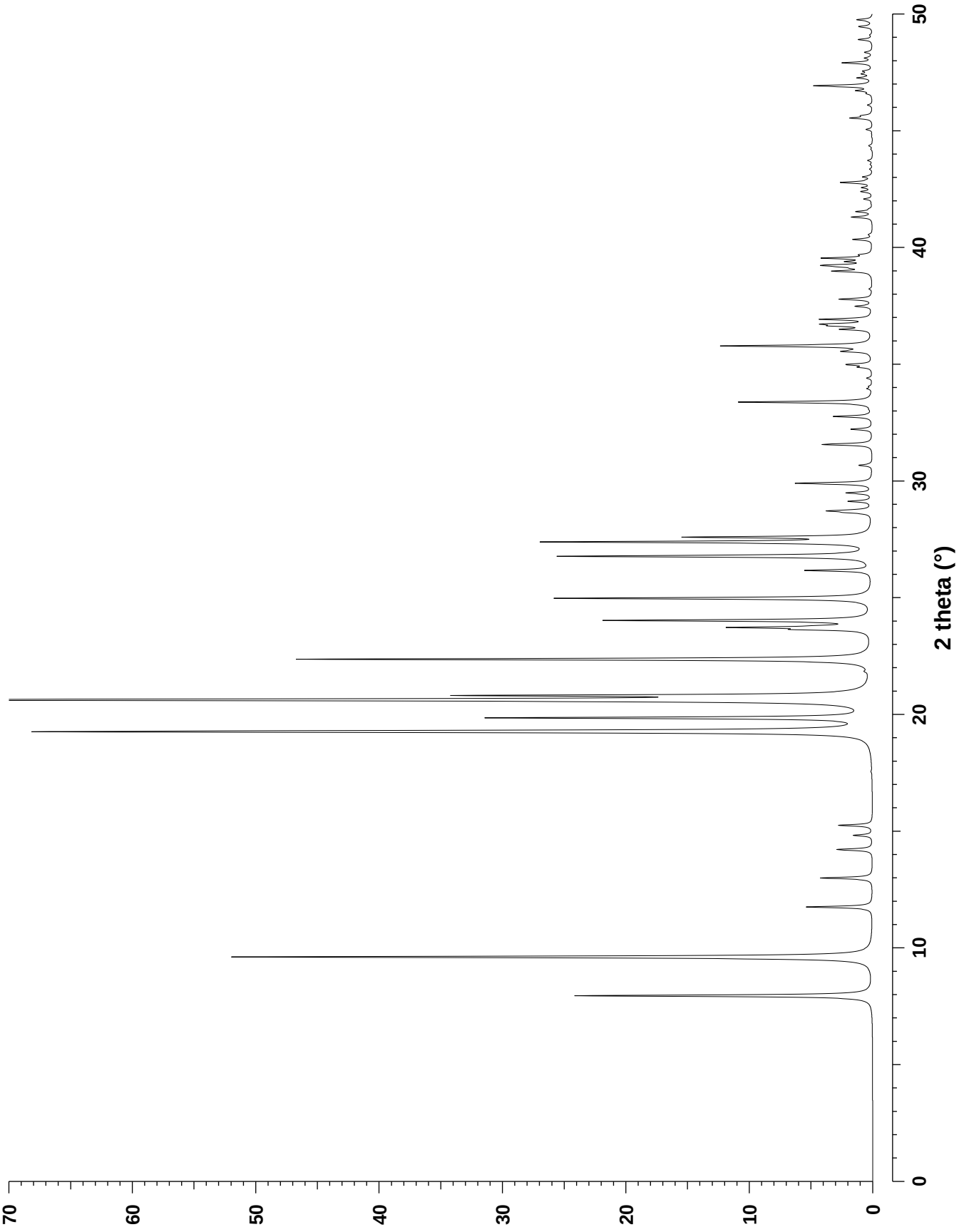
REFINED COMPOSITION: $|C_{36}|$ $[Si_{88}O_{176}]$

CRYSTAL DATA: *Fmmm* (No. 69)
$a = 22.232$ Å $b = 15.058$ Å $c = 13.627$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.125$

REFERENCE: B. Marler, N. Dehnbostel, H. H. Eulert, H. Gies and F. Liebau, *J. Inclusion Phenomena* **4** 339–349 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	7.95	11.116	2	24.5	8	0	0	32.21	2.779	2	1.7	10	2	0	42.39	2.132	4	0.8
1	1	1	9.61	9.198	8	52.7	3	5	1	32.76	2.733	8	3.2	8	4	2	42.56	2.124	8	0.8
0	2	0	11.75	7.529	2	5.4	5	3	3	33.37	2.685	8	11.0	1	7	1	42.75	2.115	8	0.5
0	0	2	12.99	6.814	2	4.3	6	4	0	33.95	2.641	4	0.4	10	0	2	42.78	2.114	4	2.3
2	2	0	14.21	6.234	4	2.9	7	3	1	34.05	2.633	8	0.2	5	3	5	42.89	2.109	8	0.2
3	1	1	14.82	5.976	8	1.6	8	2	0	34.40	2.607	4	0.5	4	0	6	43.02	2.102	4	0.7
2	0	2	15.25	5.809	4	2.8	8	0	2	34.87	2.573	4	1.0	6	4	4	43.35	2.087	8	0.2
1	3	1	19.26	4.608	8	61.7	7	1	3	34.98	2.565	8	2.0	6	6	0	43.55	2.078	4	0.2
2	2	2	19.30	4.599	8	14.4	0	4	4	35.54	2.526	4	2.1	8	2	4	43.72	2.070	8	0.4
4	2	0	19.85	4.472	4	31.2	3	1	5	35.60	2.522	8	0.7	7	1	5	44.20	2.049	8	0.1
4	0	2	20.62	4.307	4	100.0	0	6	0	35.78	2.510	2	11.4	3	7	1	44.35	2.043	8	0.3
1	1	3	20.81	4.268	8	30.3	6	0	4	35.80	2.508	4	1.3	1	5	5	45.05	2.012	8	0.5
5	1	1	21.84	4.070	8	0.2	6	4	2	36.49	2.462	8	2.3	9	3	3	45.54	1.992	8	1.8
3	3	1	22.36	3.975	8	47.3	5	5	1	36.64	2.453	8	2.6	2	6	4	45.63	1.988	8	0.4
0	4	0	23.63	3.764	2	4.7	2	6	0	36.71	2.448	4	3.5	6	6	2	45.64	1.988	8	0.4
3	1	3	23.72	3.751	8	10.4	8	2	2	36.92	2.435	8	4.2	7	5	3	46.09	1.969	8	0.4
4	2	2	23.80	3.738	8	2.0	9	1	1	37.48	2.400	8	1.4	3	5	5	46.58	1.950	8	0.4
6	0	0	24.02	3.705	2	21.8	1	3	5	37.78	2.381	8	2.6	0	4	6	46.71	1.945	4	1.2
2	4	0	24.97	3.566	4	26.1	6	2	4	37.81	2.379	8	0.2	1	7	3	46.91	1.937	8	2.4
0	0	4	26.16	3.407	2	5.4	0	6	2	38.22	2.355	4	0.2	6	0	6	46.92	1.936	4	2.5
1	3	3	26.77	3.330	8	24.4	7	3	3	38.98	2.311	8	3.1	1	1	7	47.26	1.923	8	1.2
6	2	0	26.82	3.325	4	3.5	2	6	2	39.10	2.304	8	0.8	5	7	1	47.42	1.917	8	0.7
2	0	4	27.38	3.257	4	26.4	4	4	4	39.17	2.300	8	1.5	2	4	6	47.46	1.916	8	0.1
6	0	2	27.40	3.255	4	0.4	5	1	5	39.23	2.296	8	3.5	10	4	0	47.49	1.914	4	0.1
5	3	1	27.59	3.233	8	14.7	4	6	0	39.39	2.287	4	1.8	7	3	5	47.55	1.912	8	0.6
4	4	0	28.64	3.117	4	1.6	3	3	5	39.54	2.279	8	4.0	4	6	4	47.90	1.899	8	2.5
5	1	3	28.71	3.109	8	3.2	0	0	6	39.68	2.271	2	0.8	9	5	1	48.11	1.891	8	0.6
0	2	4	28.76	3.104	4	0.5	8	4	0	40.34	2.236	4	1.6	0	8	0	48.35	1.882	2	0.6
3	3	3	29.12	3.066	8	1.9	2	0	6	40.54	2.225	4	0.3	8	6	0	48.90	1.863	4	1.2
7	1	1	29.48	3.030	8	2.1	5	5	3	41.30	2.186	8	1.7	2	8	0	49.09	1.856	4	0.2
2	2	4	29.89	2.989	8	4.5	0	2	6	41.53	2.174	4	1.3	10	4	2	49.45	1.843	8	1.1
6	2	2	29.90	2.988	8	1.9	4	6	2	41.65	2.168	8	0.2	4	4	6	49.67	1.836	8	0.2
1	5	1	30.67	2.915	8	1.1	9	1	3	42.07	2.148	8	0.7	11	1	3	49.75	1.833	8	1.3
4	4	2	31.56	2.834	8	4.2	2	2	6	42.35	2.134	8	0.1							

2-aminopentane Nonasil NON



CHEMICAL COMPOSITION: $|Na_{0.1}K_{1.09}Mg_{1.11}Ca_{1.07}Sr_{0.01}Ba_{0.01}(H_2O)_{17.63}|\ [Al_{5.52}Fe^{3+}_{0.01}Si_{12.49}O_{36}]$
Poia Creek, Adamello, Italy

REFINED COMPOSITION: $|KMgCa_{1.32}O_{16.04}|\ [Si_{12.6}Al_{5.4}O_{36}]$

CRYSTAL DATA: $P\overline{6}m2$ (No. 187)
$a = 13.331$ Å $b = 13.291$ Å $c = 7.593$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.058$, $R_w = 0.038$

REFERENCE: A. Alberti, G. Cruciani, E. Galli and G. Vezzalini,
Zeolites **17** 457–461 (1996).

h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$
1	0	0	7.66	11.545	6	100.0	2	1	2	31.24	2.863	24	46.9	3	3	1	42.45	2.129	12	3.4
0	0	1	11.65	7.593	2	13.8	3	0	2	33.15	2.703	12	1.3	3	0	3	42.76	2.115	12	4.8
1	1	0	13.30	6.655	6	12.1	4	0	1	33.21	2.698	12	8.8	4	1	2	43.10	2.099	24	1.0
1	0	1	13.96	6.344	12	9.7	3	2	0	33.88	2.646	12	1.5	4	2	1	43.18	2.095	24	3.4
2	0	0	15.35	5.772	6	19.3	0	0	3	35.47	2.531	2	1.3	5	1	0	43.67	2.073	12	0.4
2	0	1	19.31	4.595	12	23.1	4	1	0	35.65	2.518	12	15.5	2	2	3	45.00	2.015	12	0.1
2	1	0	20.37	4.360	12	31.9	2	2	2	35.88	2.502	12	0.5	5	1	1	45.35	2.000	24	3.9
3	0	0	23.11	3.848	6	20.0	3	2	1	35.95	2.498	24	4.9	3	1	3	45.70	1.985	24	1.0
0	0	2	23.43	3.796	2	3.0	1	0	3	36.34	2.472	12	0.4	5	0	2	46.00	1.973	12	3.0
2	1	1	23.53	3.781	24	57.1	3	1	2	36.73	2.447	24	1.1	3	3	2	47.46	1.915	12	0.4
1	0	2	24.68	3.607	12	37.0	4	1	1	37.63	2.390	24	0.1	4	0	3	47.80	1.903	12	3.0
3	0	1	25.96	3.433	12	3.1	2	0	3	38.85	2.318	12	1.5	0	0	4	47.92	1.898	2	7.7
2	2	0	26.79	3.328	6	7.6	5	0	0	39.01	2.309	6	1.2	4	2	2	48.13	1.890	24	0.3
1	1	2	27.04	3.298	12	2.0	4	0	2	39.21	2.298	12	0.2	1	0	4	48.61	1.873	12	2.5
3	1	0	27.88	3.200	12	3.5	3	3	0	40.67	2.218	6	7.6	6	0	1	48.83	1.865	12	0.3
2	0	2	28.13	3.172	12	8.1	5	0	1	40.85	2.209	12	0.9	5	2	0	49.33	1.847	12	1.2
2	2	1	29.30	3.048	12	0.6	2	1	3	41.24	2.189	24	1.0	4	3	1	49.56	1.839	24	0.6
3	1	1	30.31	2.949	24	7.4	4	2	0	41.42	2.180	12	0.8							
4	0	0	30.98	2.886	6	25.3	3	2	2	41.61	2.171	24	0.1							

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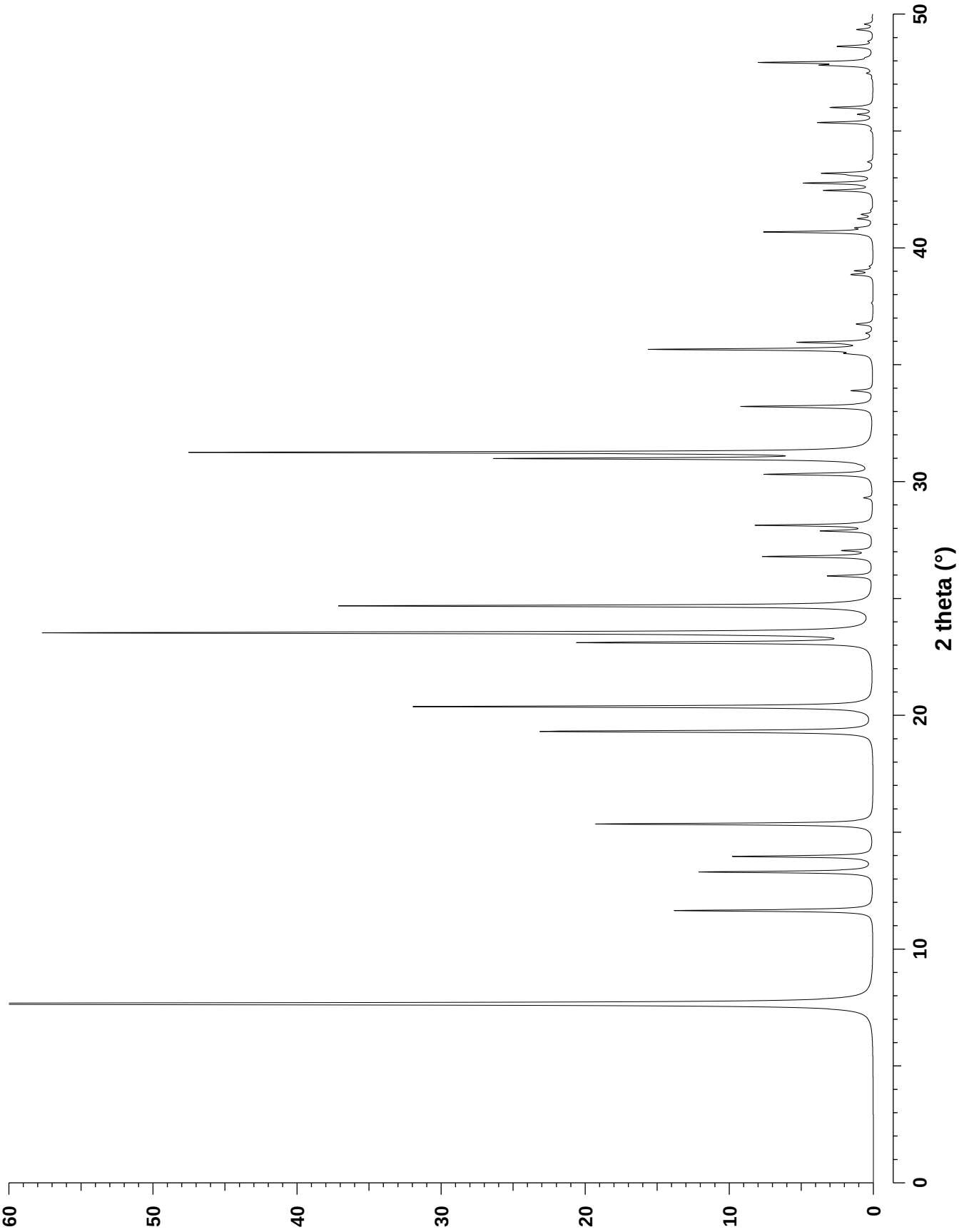


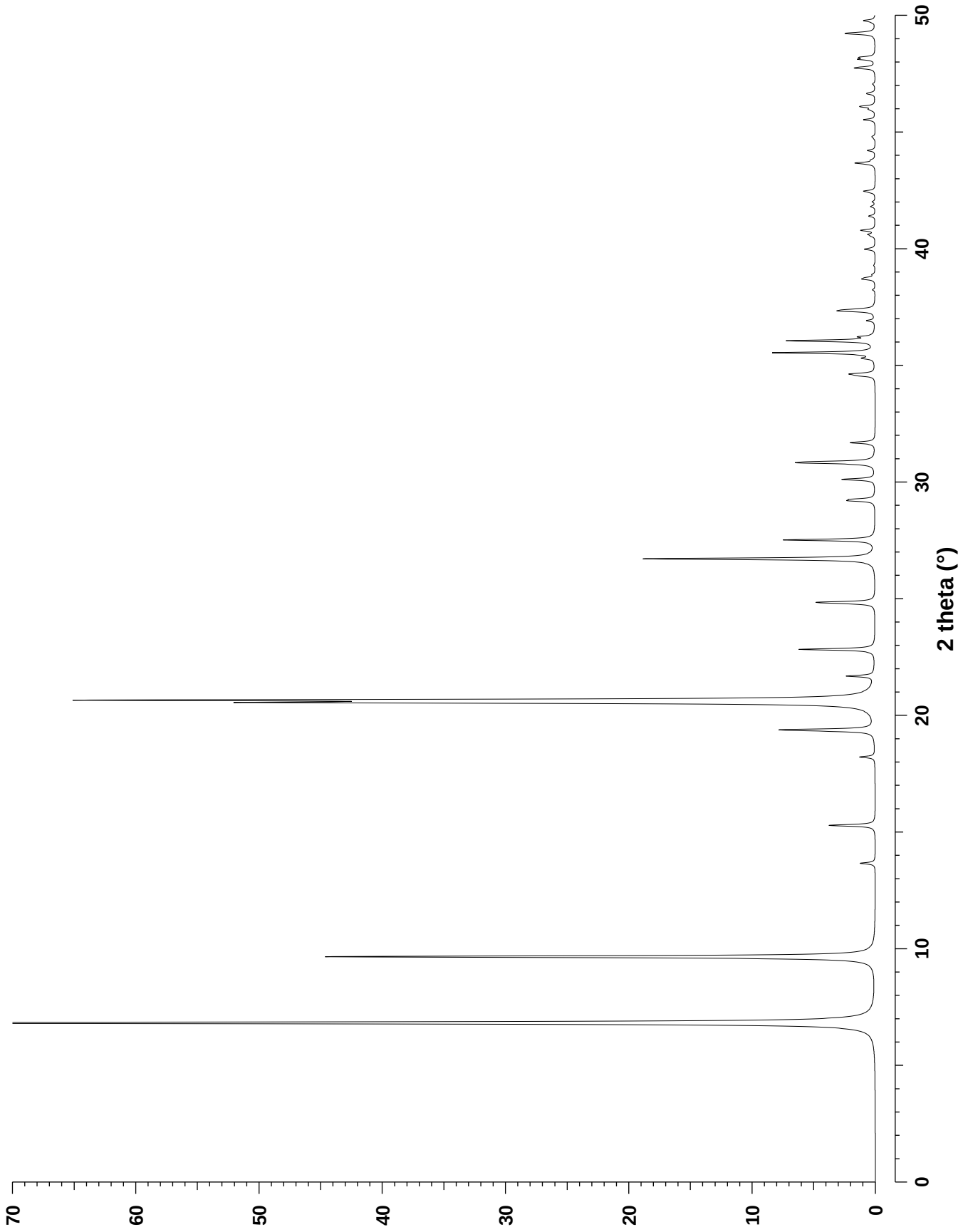
CHEMICAL COMPOSITION: $[Al_{16}P_{16}O_{64}]$

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: $Imm2$ (No. 44)
$a = 18.3549$ Å $b = 18.3206$ Å $c = 5.0530$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.044$, $R_{wp} = 0.059$

REFERENCE: D. E. Akporiaye, H. Fjellvåg, E. N. Halvorsen, T. Haug, A. Karlsson, and K. P Lillerud, *J. Chem. Soc., Chem. Commun.* 1553–1554 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.82	12.967	4	100.0	2	5	1	31.70	2.823	8	0.6	4	2	2	42.00	2.151	8	0.2
2	0	0	9.64	9.177	2	16.9	7	1	0	34.55	2.596	4	0.9	7	5	0	42.39	2.132	4	0.2
0	2	0	9.66	9.160	2	30.5	5	5	0	34.59	2.593	4	0.3	6	5	1	42.45	2.130	8	0.2
2	2	0	13.66	6.483	4	1.2	1	7	0	34.62	2.591	4	1.1	5	6	1	42.46	2.129	8	0.7
3	1	0	15.27	5.803	4	1.6	6	1	1	34.62	2.591	8	0.6	8	1	1	43.60	2.076	8	0.2
1	3	0	15.29	5.795	4	2.4	1	6	1	34.67	2.587	8	0.1	7	4	1	43.62	2.075	8	0.1
1	0	1	18.21	4.872	4	1.1	6	4	0	35.28	2.544	4	0.4	4	7	1	43.66	2.073	8	1.3
0	1	1	18.21	4.871	4	0.2	4	6	0	35.31	2.542	4	0.6	1	8	1	43.67	2.073	8	0.2
4	0	0	19.34	4.589	2	3.3	0	0	2	35.53	2.526	2	8.3	1	5	2	43.80	2.067	8	0.2
0	4	0	19.38	4.580	2	5.9	5	4	1	36.04	2.492	8	3.1	4	8	0	44.20	2.049	4	0.6
3	3	0	20.55	4.322	4	43.0	4	5	1	36.05	2.491	8	4.2	1	9	0	44.79	2.023	4	0.3
2	1	1	20.64	4.303	8	32.1	1	1	2	36.22	2.480	8	1.1	4	4	2	45.52	1.993	8	1.0
1	2	1	20.65	4.301	8	27.6	2	0	2	36.90	2.436	4	0.1	8	3	1	45.91	1.977	8	0.2
2	4	0	21.68	4.098	4	2.2	0	2	2	36.91	2.436	4	0.5	3	8	1	45.97	1.974	8	0.4
3	0	1	22.82	3.896	4	5.9	7	3	0	37.32	2.409	4	2.4	5	3	2	46.07	1.970	8	0.5
0	3	1	22.84	3.893	4	0.3	3	7	0	37.37	2.406	4	1.5	3	5	2	46.09	1.969	8	0.8
1	5	0	24.78	3.593	4	0.7	6	3	1	37.39	2.405	8	0.2	6	0	2	46.62	1.948	4	0.4
3	2	1	24.83	3.585	8	2.3	3	6	1	37.42	2.403	8	0.4	0	6	2	46.66	1.947	4	0.4
2	3	1	24.84	3.584	8	2.3	2	2	2	38.23	2.354	8	0.2	3	9	0	47.05	1.932	4	0.2
4	1	1	26.69	3.340	8	7.0	7	0	1	38.69	2.327	4	0.9	6	2	2	47.73	1.905	8	1.2
1	4	1	26.71	3.337	8	13.0	0	7	1	38.75	2.324	4	0.6	2	6	2	47.76	1.904	8	0.7
4	4	0	27.51	3.242	4	7.4	3	1	2	38.88	2.316	8	0.2	9	0	1	48.11	1.891	4	1.2
6	0	0	29.19	3.059	2	1.8	8	0	0	39.27	2.294	2	0.1	0	9	1	48.19	1.888	4	1.1
0	6	0	29.25	3.053	2	1.6	7	2	1	39.97	2.256	8	0.8	7	7	0	49.19	1.852	4	0.5
5	0	1	30.09	2.970	4	0.5	2	7	1	40.02	2.253	8	0.1	9	2	1	49.19	1.852	8	0.6
4	3	1	30.10	2.969	8	0.9	8	2	0	40.53	2.226	4	0.2	7	6	1	49.22	1.851	8	1.2
3	4	1	30.11	2.968	8	1.0	2	8	0	40.60	2.222	4	0.5	6	7	1	49.24	1.851	8	0.5
0	5	1	30.13	2.966	4	0.5	4	0	2	40.77	2.213	4	0.7	2	9	1	49.27	1.849	8	0.2
6	2	0	30.81	2.902	4	5.0	0	4	2	40.79	2.212	4	0.5	10	0	0	49.67	1.835	2	0.1
2	6	0	30.86	2.897	4	3.7	3	3	2	41.39	2.181	8	0.5	6	8	0	49.73	1.833	4	0.2
5	2	1	31.67	2.825	8	1.6	6	6	0	41.80	2.161	4	0.4	0	10	0	49.77	1.832	2	0.8


0
10
20
30
40
50
2 theta (°)
0
10
20
30
40
50
60
70

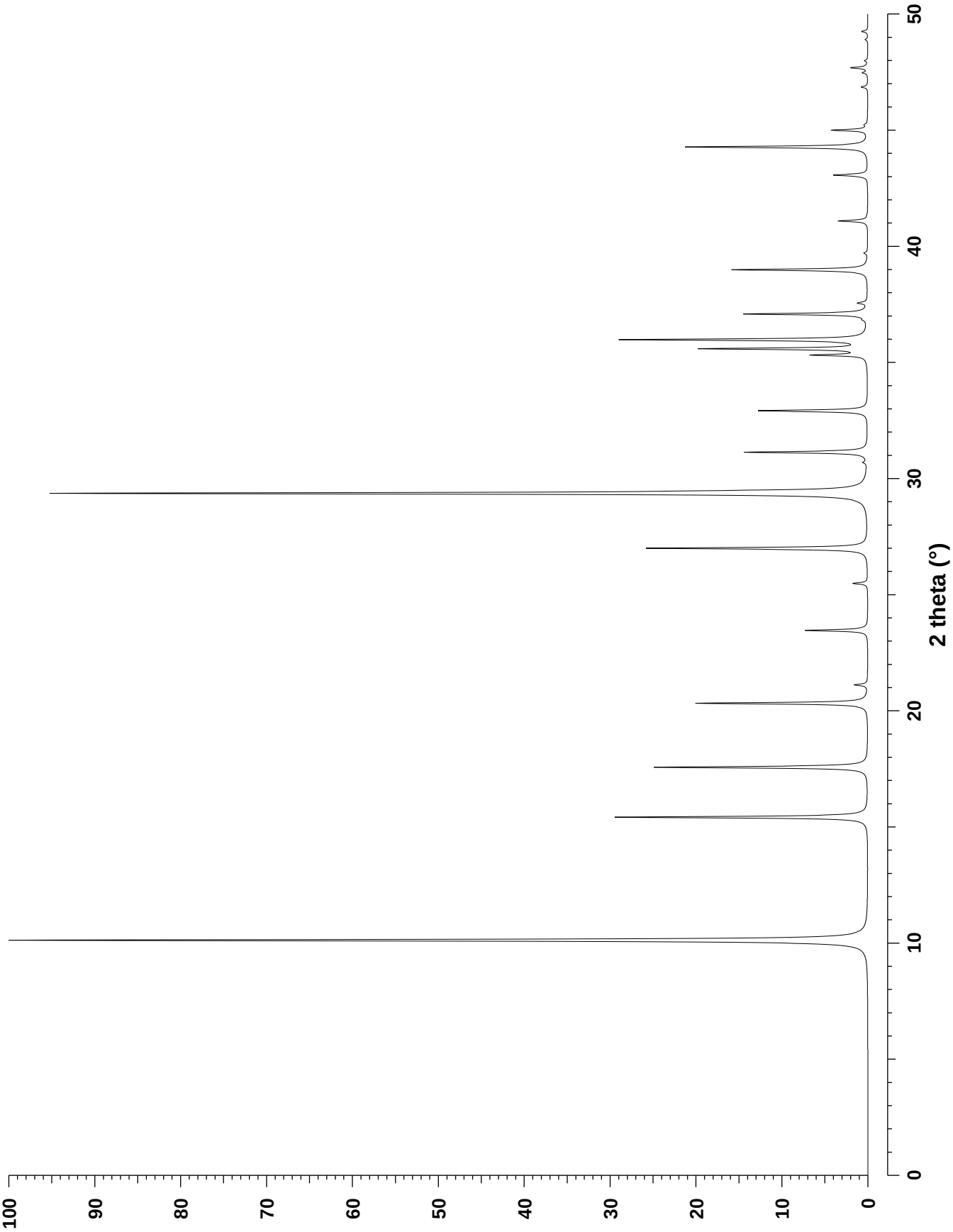
CHEMICAL COMPOSITION: $|K_6(H_2O)_9|\ [Be_3Si_6O_{18}]$

REFINED COMPOSITION: $|K_{5.37}(H_2O)_9|\ [Be_{3.51}Si_{5.52}O_{18}]$

CRYSTAL DATA: $P3_2$ (No. 145)
$a = 10.0928$ Å $b = 10.0928$ Å $c = 7.6264$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.0596$

REFERENCE: K. O. Kongshaug, H. Fjellvåg, K. P. Lillerud, T. E. Gier, G. D. Stucky and A. K. Cheetham, Private communication (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	10.12	8.741	6	100.0	2	2	0	35.58	2.523	6	19.3	3	1	2	44.27	2.046	6	5.8
1	0	1	15.42	5.746	6	15.5	3	-2	2	35.97	2.497	6	7.0	1	3	2	44.27	2.046	6	4.6
0	1	1	15.42	5.746	6	13.9	1	2	2	35.97	2.497	6	7.7	3	-2	3	44.99	2.015	6	0.9
1	1	0	17.57	5.046	6	24.9	3	-1	2	35.97	2.497	6	8.2	1	2	3	44.99	2.015	6	0.8
0	2	0	20.32	4.370	6	20.1	2	1	2	35.97	2.497	6	5.7	3	-1	3	44.99	2.015	6	1.3
2	-1	1	21.11	4.208	6	1.1	1	0	3	36.82	2.441	6	0.2	2	1	3	44.99	2.015	6	1.2
1	1	1	21.11	4.208	6	0.4	1	3	0	37.08	2.424	6	8.2	2	3	0	45.22	2.005	6	0.2
0	2	1	23.46	3.792	6	3.3	3	1	0	37.08	2.424	6	6.2	3	2	0	45.22	2.005	6	0.1
2	0	1	23.46	3.792	6	4.0	2	2	1	37.55	2.395	6	0.7	2	3	1	46.85	1.939	6	0.3
0	1	2	25.48	3.495	6	1.0	4	-2	1	37.55	2.395	6	0.4	5	-3	1	46.85	1.939	6	0.2
1	0	2	25.48	3.495	6	0.8	3	0	2	38.90	2.315	6	0.2	3	2	1	46.85	1.939	6	0.1
1	2	0	26.99	3.304	6	13.0	0	3	2	38.90	2.315	6	0.2	5	-2	1	46.85	1.939	6	0.2
2	1	0	26.99	3.304	6	12.8	4	-3	1	38.98	2.310	6	4.5	3	0	3	47.46	1.915	6	0.3
1	1	2	29.36	3.042	6	50.3	1	3	1	38.98	2.310	6	3.3	0	3	3	47.46	1.915	6	0.3
2	-1	2	29.36	3.042	6	43.7	4	-1	1	38.98	2.310	6	2.7	4	1	0	47.68	1.907	6	1.0
3	-2	1	29.46	3.031	6	2.2	3	1	1	38.98	2.310	6	5.2	1	4	0	47.68	1.907	6	1.0
3	-1	1	29.46	3.031	6	2.1	2	-1	3	39.70	2.270	6	0.3	0	4	2	47.98	1.896	6	0.1
1	2	1	29.46	3.031	6	2.2	2	0	3	41.08	2.197	6	1.9	4	0	2	47.98	1.896	6	0.2
2	1	1	29.46	3.031	6	2.7	0	2	3	41.08	2.197	6	1.6	0	1	4	48.89	1.863	6	0.1
0	3	0	30.69	2.914	6	0.4	4	-2	2	42.98	2.104	6	0.2	1	0	4	48.89	1.863	6	0.2
2	0	2	31.13	2.873	6	8.5	2	2	2	42.98	2.104	6	0.1	5	-4	1	49.24	1.850	6	0.2
0	2	2	31.13	2.873	6	5.8	0	4	1	43.06	2.101	6	1.8	4	1	1	49.24	1.850	6	0.3
3	0	1	32.91	2.722	6	4.7	4	0	1	43.06	2.101	6	2.1	5	-1	1	49.24	1.850	6	0.2
0	3	1	32.91	2.722	6	8.0	4	-3	2	44.27	2.046	6	6.2							
0	0	3	35.31	2.542	2	6.3	4	-1	2	44.27	2.046	6	4.8							


100
90
80
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60
50
40
30
20
10
0
0
10
20
30
40
50
2 theta (°)

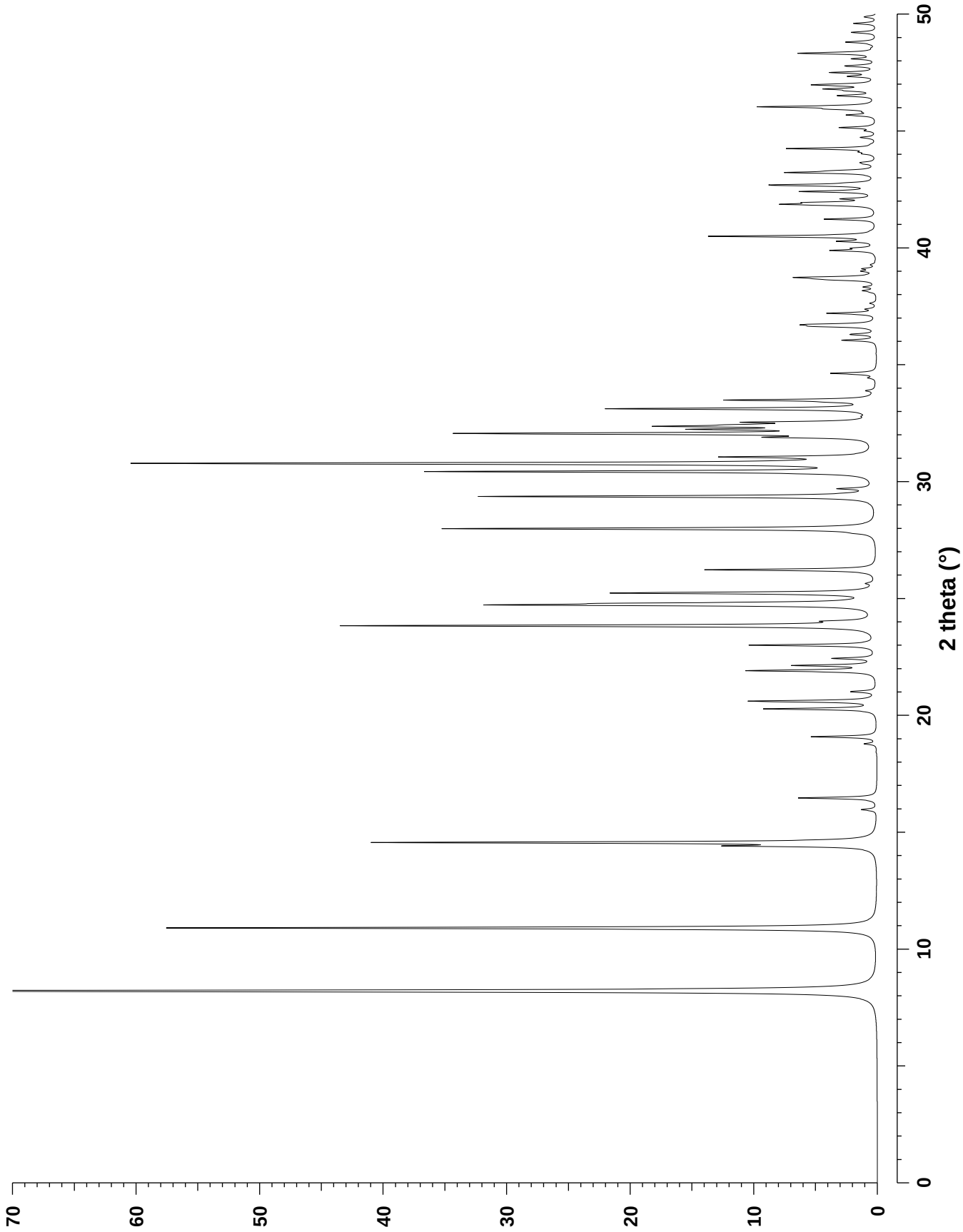
CHEMICAL COMPOSITION: $|Ca_8(H_2O)_{16}|\ [Si_{16}Al_{16}O_{60}(OH)_8]$
Taurus Mountains, Turkey

REFINED COMPOSITION: $|Ca_8(H_2O)_{16}|\ [Si_{16}Al_{16}O_{60}(OH)_8]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 21.555$ Å $b = 8.761$ Å $c = 9.304$ Å
$\alpha = 90°$ $\beta = 91.55°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: N. Engel and K. Yvon,
Z. Kristallogr. **169** 165–175 (1984).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
2	0	0	8.21	10.774	2	100.0	-3	1	3	32.79	2.731	4	0.3	-2	4	1	43.21	2.094	4	6.8
1	1	0	10.90	8.116	4	57.5	4	2	2	32.91	2.722	4	0.1	-6	2	3	43.28	2.090	4	1.8
-1	1	1	14.41	6.146	4	9.9	3	3	0	33.11	2.705	4	21.6	2	4	1	43.31	2.089	4	0.8
1	1	1	14.56	6.084	4	40.3	3	1	3	33.39	2.683	4	1.9	-8	2	2	43.58	2.077	4	0.7
3	1	0	15.96	5.554	4	1.2	-6	2	1	33.48	2.676	4	11.8	-7	3	1	43.64	2.074	4	1.0
4	0	0	16.46	5.387	2	6.4	6	2	1	33.88	2.646	4	0.7	7	3	1	44.01	2.057	4	0.8
3	1	1	18.78	4.725	4	1.0	-3	3	1	34.43	2.605	4	0.5	0	2	4	44.09	2.054	4	0.9
0	0	2	19.08	4.650	2	5.3	3	3	1	34.62	2.591	4	3.7	6	2	3	44.24	2.047	4	2.9
0	2	0	20.27	4.380	2	9.1	-7	1	2	36.04	2.492	4	2.8	9	1	2	44.24	2.047	4	4.3
-2	0	2	20.60	4.312	2	10.3	-2	2	3	36.29	2.476	4	2.0	8	2	2	44.43	2.039	4	0.1
2	0	2	21.01	4.228	2	2.0	1	3	2	36.63	2.453	4	3.0	-2	2	4	44.72	2.026	4	1.2
2	2	0	21.90	4.058	4	9.4	2	2	3	36.66	2.451	4	1.8	-5	1	4	45.00	2.014	4	0.8
-1	1	2	21.93	4.053	4	1.6	-5	1	3	36.71	2.448	4	4.8	2	2	4	45.14	2.009	4	3.0
1	1	2	22.13	4.017	4	6.5	5	3	0	37.19	2.418	4	4.0	-4	4	1	45.67	1.987	4	2.2
0	2	1	22.43	3.963	4	3.4	-6	2	2	37.37	2.407	4	0.8	0	4	2	45.79	1.981	4	0.5
5	1	0	23.00	3.867	4	10.2	5	1	3	37.62	2.391	4	0.5	4	4	1	45.87	1.978	4	0.1
-2	2	1	23.83	3.733	4	43.2	6	2	2	38.09	2.363	4	0.3	-6	0	4	45.92	1.976	2	1.2
2	2	1	24.02	3.705	4	2.7	-8	0	2	38.16	2.359	2	1.0	-10	0	2	45.94	1.976	2	1.8
-3	1	2	24.71	3.603	4	0.2	-3	3	2	38.32	2.349	4	0.9	5	1	4	46.03	1.972	4	9.2
-5	1	1	24.72	3.602	4	27.6	5	3	1	38.62	2.331	4	2.2	-2	4	2	46.50	1.953	4	3.0
6	0	0	24.79	3.591	2	15.5	3	3	2	38.67	2.328	4	2.5	2	4	2	46.71	1.945	4	1.7
-4	0	2	24.95	3.568	2	0.1	0	0	4	38.73	2.325	2	5.7	-7	3	2	46.79	1.942	4	3.7
5	1	1	25.15	3.540	4	0.9	-4	2	3	38.99	2.310	4	0.7	10	0	2	46.95	1.935	2	2.8
3	1	2	25.23	3.529	4	21.1	9	1	0	39.00	2.309	4	0.3	-4	2	4	46.97	1.934	4	2.1
4	0	2	25.64	3.474	2	0.6	8	0	2	39.10	2.304	2	1.0	10	2	0	47.00	1.933	4	0.8
4	2	0	26.22	3.399	4	13.9	8	2	0	39.27	2.294	4	0.4	-5	3	3	47.33	1.921	4	2.1
-4	2	1	27.79	3.210	4	0.6	2	0	4	39.88	2.260	2	3.5	7	3	2	47.49	1.915	4	3.6
0	2	2	27.98	3.189	4	35.1	-9	1	1	39.98	2.255	4	1.6	4	2	4	47.77	1.904	4	2.4
2	2	2	29.36	3.042	4	32.1	-8	2	1	40.27	2.240	4	2.7	-10	2	1	47.82	1.902	4	0.2
-5	1	2	29.69	3.009	4	2.6	1	1	4	40.46	2.229	4	0.1	5	3	3	48.08	1.893	4	1.8
5	1	2	30.42	2.938	4	35.8	9	1	1	40.49	2.228	4	13.4	10	2	1	48.31	1.884	4	5.7
-1	1	3	30.77	2.906	4	59.2	8	2	1	40.72	2.216	4	0.1	-11	1	1	48.35	1.882	4	1.2
7	1	0	30.79	2.904	4	0.4	0	4	0	41.22	2.190	2	4.2	-9	1	3	48.54	1.876	4	0.2
1	3	0	30.90	2.894	4	0.9	-3	1	4	41.80	2.161	4	0.4	6	4	0	48.69	1.870	4	0.2
1	1	3	30.98	2.886	4	1.1	-5	3	2	41.85	2.158	4	6.5	-4	4	2	48.79	1.867	4	2.3
-6	0	2	31.05	2.880	2	11.1	-4	0	4	41.90	2.156	2	0.7	-8	2	3	48.83	1.865	4	0.3
6	0	2	31.89	2.806	2	6.9	10	0	0	41.93	2.155	2	4.0	4	4	2	49.18	1.853	4	0.3
-7	1	1	32.05	2.792	4	32.9	-7	1	3	42.09	2.147	4	2.4	9	3	0	49.21	1.851	4	1.9
6	2	0	32.23	2.777	4	12.1	5	3	2	42.40	2.132	4	5.9	-6	4	1	49.59	1.838	4	1.4
-4	2	2	32.36	2.767	4	13.7	3	1	4	42.46	2.129	4	0.4	-7	1	4	49.59	1.838	4	0.5
-1	3	1	32.37	2.766	4	0.7	-1	3	3	42.66	2.119	4	1.7	9	1	3	49.85	1.829	4	0.3
1	3	1	32.43	2.760	4	6.6	7	3	0	42.68	2.119	4	7.0	6	4	1	49.88	1.828	4	0.8
7	1	1	32.53	2.752	4	8.8	4	0	4	42.77	2.114	2	1.2							


0
10
20
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40
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2 theta (°)
70
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50
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30
20
10
0

PAU Paulingite

CHEMICAL COMPOSITION: $|Na_{13}K_{68}Ca_{36}Ba_{1.5}(H_2O)_{705}|\ [Si_{520}Al_{152}O_{1344}]$
Rock Island Dam, Washington, U.S.A.

REFINED COMPOSITION: $|Na_{9.68}K_{50.51}Ca_{26.75}Ba_{1.06}(H_2O)_{452}|\ [Si_{520.12}Al_{151.88}O_{1344}]$

CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 35.093$ Å $b = 35.093$ Å $c = 35.093$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.14$

REFERENCE: E. K. Gordon, S. Samson and W. B. Kamb,
Science **154** 1004–1007 (1966).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	3.56	24.814	12	42.1	9	4	1	25.12	3.545	48	0.7	10	10	0	36.20	2.481	12	3.1
2	0	0	5.04	17.546	6	63.6	10	2	0	25.89	3.441	24	2.1	14	2	0	36.20	2.481	24	0.8
2	1	1	6.17	14.327	24	4.4	10	2	2	26.39	3.377	24	4.5	14	3	1	36.76	2.445	48	1.2
2	2	0	7.12	12.407	12	13.7	6	6	6	26.39	3.377	8	0.9	11	9	2	36.76	2.445	48	2.3
3	1	0	7.97	11.097	24	24.7	10	3	1	26.64	3.346	48	39.2	10	9	5	36.76	2.445	48	3.8
2	2	2	8.73	10.130	8	0.6	10	4	0	27.37	3.258	24	45.2	14	5	1	38.21	2.355	48	1.7
3	2	1	9.43	9.379	48	12.3	9	6	1	27.61	3.231	48	2.6	15	1	0	38.57	2.334	24	0.5
4	0	0	10.08	8.773	6	2.5	11	1	0	28.08	3.177	24	0.5	14	5	3	38.92	2.314	48	2.4
4	1	1	10.70	8.271	24	3.3	9	5	4	28.08	3.177	48	7.5	14	6	0	39.10	2.304	24	1.7
3	3	0	10.70	8.271	12	100.0	10	5	1	28.55	3.126	48	17.2	13	7	4	39.27	2.294	48	0.7
4	2	0	11.28	7.847	24	3.3	11	2	1	28.55	3.126	48	12.8	10	10	6	39.45	2.284	24	1.1
3	3	2	11.83	7.482	24	7.6	9	6	3	28.55	3.126	48	3.1	14	6	2	39.45	2.284	48	2.1
4	2	2	12.36	7.163	24	11.1	8	8	0	28.78	3.102	12	1.3	11	11	0	39.96	2.256	12	3.0
5	1	0	12.86	6.882	24	2.8	11	3	0	29.01	3.078	24	64.1	12	8	6	40.14	2.247	48	0.5
4	3	1	12.86	6.882	48	83.2	9	7	0	29.01	3.078	24	1.7	14	7	1	40.31	2.237	48	2.8
4	4	0	14.28	6.204	12	13.7	10	5	3	29.46	3.032	48	1.4	16	0	0	41.16	2.193	6	0.7
6	0	0	15.15	5.849	6	21.8	8	6	6	29.69	3.009	24	1.0	16	1	1	41.32	2.185	24	0.6
5	3	2	15.57	5.693	48	26.2	11	4	1	29.91	2.987	48	28.1	14	6	6	42.15	2.144	24	0.8
6	1	1	15.57	5.693	24	2.3	10	6	2	30.13	2.966	48	13.0	11	10	7	42.32	2.136	48	0.5
5	4	1	16.37	5.415	48	9.6	9	6	5	30.35	2.945	48	0.8	11	11	6	42.97	2.105	24	2.1
6	2	2	16.76	5.290	24	4.1	11	5	0	30.79	2.904	24	1.4	12	12	0	43.78	2.068	12	1.1
6	3	1	17.14	5.174	48	4.0	9	7	4	30.79	2.904	48	1.6	12	11	5	43.94	2.061	48	1.9
7	1	0	17.87	4.963	24	23.7	11	5	2	31.21	2.865	48	3.6	17	1	0	43.94	2.061	24	0.8
6	3	3	18.58	4.776	24	44.4	10	6	4	31.43	2.846	48	3.9	13	11	0	43.94	2.061	24	0.6
6	4	2	18.92	4.689	48	10.2	12	3	1	31.64	2.828	48	2.1	17	2	1	44.25	2.047	48	2.4
7	3	0	19.26	4.608	24	1.9	9	8	3	31.64	2.828	48	1.5	14	7	7	44.25	2.047	24	5.0
6	5	1	19.92	4.457	48	1.9	10	7	3	32.06	2.792	48	4.8	13	11	2	44.25	2.047	48	0.6
8	0	0	20.24	4.387	6	14.0	12	4	0	32.27	2.774	24	0.9	17	3	0	44.57	2.033	24	1.0
8	1	1	20.56	4.320	24	0.5	12	4	2	32.68	2.740	48	2.7	12	12	4	45.04	2.013	24	1.6
5	5	4	20.56	4.320	24	2.0	11	6	3	32.88	2.724	48	20.5	11	11	8	45.20	2.006	24	1.4
6	4	4	20.87	4.256	24	5.8	10	8	2	33.09	2.707	48	1.7	13	11	4	45.20	2.006	48	4.7
8	2	0	20.87	4.256	24	4.4	13	2	1	33.69	2.660	48	0.7	14	10	4	45.66	1.987	48	1.3
6	5	3	21.18	4.194	48	1.3	12	4	4	33.89	2.645	24	0.9	14	11	1	46.12	1.968	48	0.8
8	2	2	21.49	4.136	24	1.0	9	9	4	34.08	2.630	24	6.7	13	12	3	46.43	1.956	48	1.3
7	5	0	21.79	4.079	24	0.9	12	5	3	34.08	2.630	48	3.3	18	0	0	46.58	1.950	6	0.6
7	4	3	21.79	4.079	48	10.6	10	8	4	34.28	2.616	48	29.7	14	11	3	46.74	1.944	48	2.3
8	4	0	22.66	3.924	24	0.9	10	9	1	34.48	2.601	48	2.1	18	2	0	46.89	1.938	24	1.3
9	1	0	22.95	3.875	24	2.7	12	6	2	34.67	2.587	48	0.7	17	6	3	47.34	1.920	48	0.8
8	3	3	22.95	3.875	24	10.2	11	7	4	34.87	2.573	48	5.4	15	10	3	47.34	1.920	48	0.7
6	5	5	23.51	3.784	24	1.2	10	9	3	35.25	2.546	48	1.2	13	13	0	47.64	1.909	12	0.8
9	3	0	24.06	3.699	24	5.7	11	8	3	35.63	2.520	48	7.0	12	11	9	48.24	1.887	48	0.6
7	5	4	24.06	3.699	48	1.1	13	4	3	35.63	2.520	48	4.1	17	7	4	48.83	1.865	48	0.6
9	3	2	24.59	3.620	48	9.6	12	6	4	35.82	2.507	48	1.3	19	1	0	49.41	1.844	24	1.5
8	4	4	24.86	3.582	24	24.4	14	0	0	35.82	2.507	6	2.2	19	3	0	49.99	1.824	24	0.8
8	5	3	25.12	3.545	48	1.5	14	1	1	36.01	2.494	24	1.3	17	9	0	49.99	1.824	24	0.8

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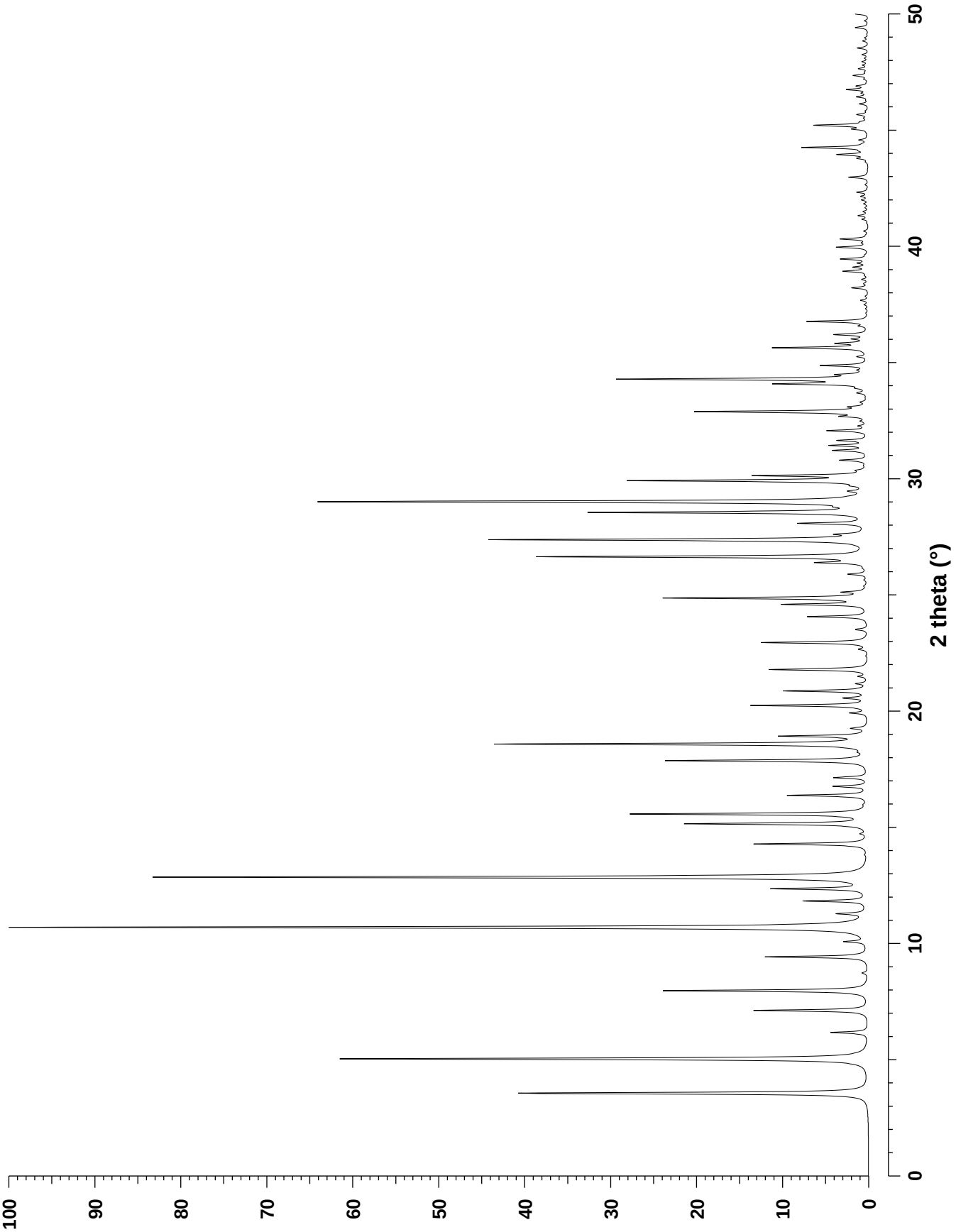

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CHEMICAL COMPOSITION: $|K_2Ca_{1.7}Na_{0.4}(H_2O)_{13.5}|\ [Si_{10.6}Al_{5.3}O_{32}]$
Casal Brunori, Rome, Italy

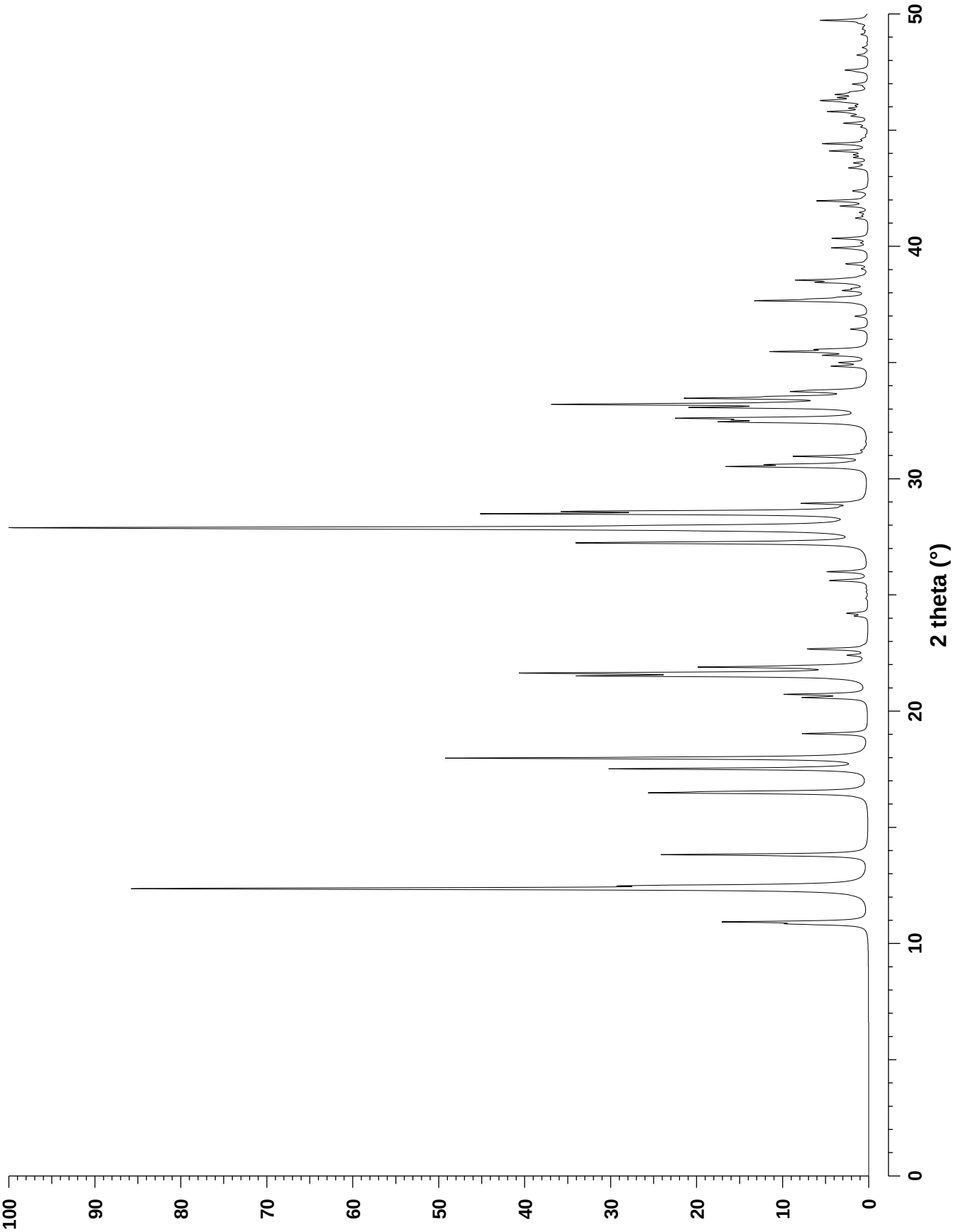
REFINED COMPOSITION: $|K_2Ca_{1.648}(H_2O)_{12}|\ [Si_{10.7}Al_{5.3}O_{32}]$

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 9.865$ Å $b = 14.300$ Å $c = 8.668$ Å
$\alpha = 90°$ $\beta = 124.20°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.057$

REFERENCE: R. Rinaldi, J. J. Pluth and J. V. Smith,
Acta Cryst. **B30** 2426–2433 (1974).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	10.84	8.159	2	10.8	1	0	2	32.44	2.760	2	22.1	-1	4	3	41.45	2.178	4	1.3
-1	0	1	10.93	8.095	2	24.3	1	4	1	32.52	2.753	4	13.3	3	4	0	41.73	2.165	4	4.8
0	0	1	12.35	7.169	2	82.5	-1	0	3	32.59	2.747	2	13.7	-3	4	3	41.95	2.154	4	9.0
0	2	0	12.38	7.150	2	64.3	-1	4	2	32.61	2.746	4	18.2	2	1	2	42.36	2.134	4	1.4
1	1	0	12.49	7.087	4	30.5	1	1	2	33.06	2.710	4	26.8	-3	5	2	42.39	2.132	4	1.6
-1	1	1	12.56	7.045	4	1.4	1	5	0	33.19	2.699	4	27.1	-3	1	4	42.47	2.128	4	0.3
0	1	1	13.82	6.409	4	37.0	-3	0	3	33.20	2.698	2	6.5	1	6	1	43.37	2.086	4	3.3
1	2	0	16.48	5.377	4	33.6	-1	1	3	33.20	2.698	4	11.0	-1	6	2	43.44	2.083	4	0.7
-1	2	1	16.54	5.359	4	18.6	-1	5	1	33.22	2.697	4	4.8	3	2	1	43.58	2.077	4	2.4
0	2	1	17.52	5.063	4	45.8	2	2	1	33.23	2.696	4	10.0	2	2	2	43.82	2.066	4	2.2
-2	0	1	17.98	4.932	2	75.3	2	4	0	33.32	2.689	4	1.7	-3	2	4	43.93	2.061	4	1.9
-2	1	1	19.03	4.663	4	11.7	-2	4	2	33.44	2.679	4	6.5	-2	6	2	44.09	2.054	4	1.7
1	0	1	20.58	4.315	2	10.6	-2	2	3	33.46	2.678	4	23.4	-2	2	4	44.10	2.053	4	5.1
-1	0	2	20.72	4.287	2	14.1	3	1	0	33.54	2.672	4	10.9	2	5	1	44.40	2.040	4	2.9
1	1	1	21.51	4.131	4	44.8	0	5	1	33.74	2.656	4	8.1	4	0	0	44.41	2.040	2	5.3
1	3	0	21.59	4.116	4	11.8	-3	3	2	33.74	2.656	4	2.4	-2	5	3	44.59	2.032	4	0.7
-1	3	1	21.63	4.107	4	6.8	-3	1	3	33.80	2.652	4	6.4	-4	4	2	44.64	2.030	4	0.5
-1	1	2	21.64	4.106	4	46.8	1	2	2	34.84	2.575	4	6.2	1	0	3	45.13	2.009	2	1.0
-2	2	1	21.89	4.060	4	27.1	-1	2	3	34.99	2.565	4	4.6	-1	0	4	45.29	2.002	2	4.3
-2	0	2	21.96	4.048	2	5.4	3	2	0	35.31	2.542	4	6.8	1	1	3	45.60	1.989	4	2.5
0	3	1	22.40	3.969	4	3.2	0	4	2	35.46	2.531	4	16.1	0	6	2	45.71	1.985	4	1.1
2	1	0	22.67	3.923	4	10.7	-3	2	3	35.56	2.525	4	7.3	1	7	0	45.79	1.982	4	6.5
1	2	1	24.09	3.695	4	2.1	-4	0	2	36.43	2.466	2	3.1	3	3	1	45.94	1.975	4	2.7
-1	2	2	24.21	3.677	4	3.6	-4	1	2	36.99	2.430	4	2.3	3	5	0	46.05	1.971	4	1.4
0	0	2	24.84	3.585	2	0.3	0	0	3	37.64	2.390	2	0.5	2	3	2	46.18	1.966	4	1.8
0	1	2	25.62	3.477	4	6.8	-3	4	1	37.65	2.389	4	14.3	0	7	1	46.21	1.965	4	0.4
-2	3	1	26.00	3.428	4	7.2	1	3	2	37.66	2.388	4	4.5	-3	5	3	46.25	1.963	4	3.7
1	4	0	27.23	3.274	4	40.0	-3	4	2	37.73	2.384	4	5.2	-3	3	4	46.28	1.962	4	1.5
-1	4	1	27.27	3.270	4	21.5	1	5	1	37.73	2.384	4	0.7	4	2	0	46.28	1.962	4	3.3
-3	0	1	27.78	3.211	2	13.5	-1	5	2	37.81	2.379	4	3.0	-5	0	2	46.40	1.957	2	3.9
0	2	2	27.84	3.204	4	59.5	3	3	0	38.09	2.362	4	3.9	-5	0	3	46.52	1.952	2	4.6
0	4	1	27.89	3.199	4	100.0	0	1	3	38.18	2.357	4	1.9	-4	4	3	46.58	1.950	4	1.5
-3	0	2	27.89	3.199	2	17.9	-3	3	3	38.33	2.348	4	0.4	-4	2	4	46.64	1.947	4	2.1
1	3	1	27.89	3.199	4	7.9	2	5	0	38.44	2.342	4	7.6	-5	1	2	46.86	1.939	4	0.4
-1	3	2	27.99	3.188	4	17.7	-2	5	2	38.54	2.336	4	11.4	-5	1	3	46.97	1.934	4	2.4
-3	1	1	28.49	3.133	4	62.1	-4	2	2	38.62	2.331	4	1.6	-3	6	1	47.51	1.914	4	1.3
-3	1	2	28.59	3.122	4	45.5	-4	0	3	38.71	2.326	2	0.7	-3	6	2	47.58	1.911	4	3.8
2	3	0	28.80	3.099	4	1.4	-4	1	1	39.03	2.307	4	1.0	-5	2	2	48.22	1.887	4	2.0
-2	3	2	28.94	3.085	4	10.5	-4	1	3	39.24	2.296	4	3.9	4	3	0	48.55	1.875	4	1.1
-3	2	1	30.52	2.929	4	22.9	0	6	1	39.86	2.262	4	0.7	3	4	1	49.11	1.855	4	1.2
-3	2	2	30.61	2.920	4	14.5	2	4	1	39.93	2.257	4	6.3	1	3	3	49.22	1.851	4	0.4
2	0	1	30.71	2.911	2	0.8	-2	4	3	40.14	2.247	4	0.9	1	7	1	49.35	1.846	4	0.6
-2	4	1	30.89	2.895	4	1.2	0	5	2	40.34	2.236	4	6.5	-3	4	4	49.43	1.844	4	0.4
-2	0	3	30.96	2.888	2	12.7	-4	3	2	41.21	2.190	4	2.2	-2	4	4	49.59	1.838	4	1.1
0	3	2	31.22	2.865	4	0.8	1	4	2	41.33	2.185	4	0.7	0	5	3	49.72	1.834	4	8.5

Phillipsite PHI



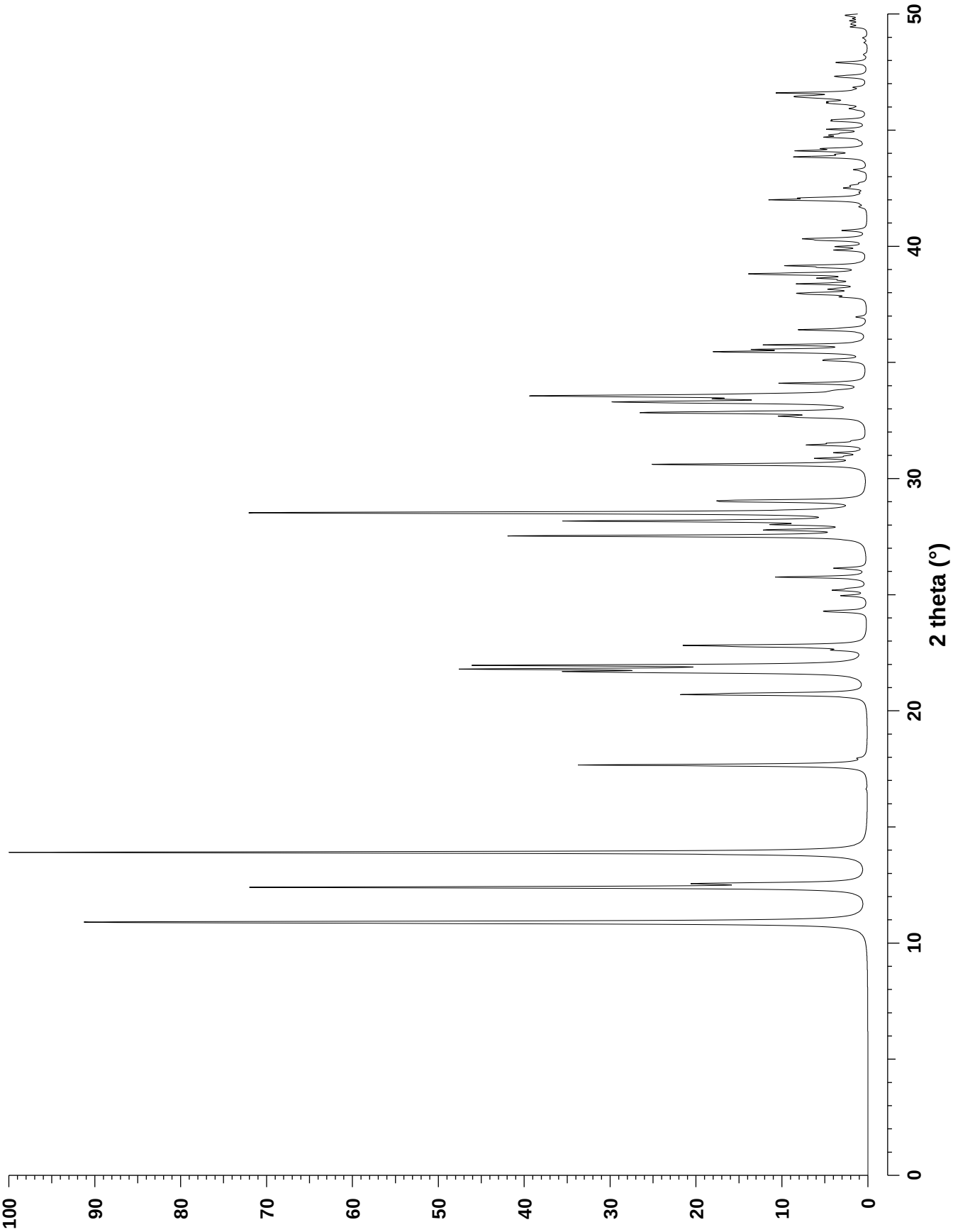
CHEMICAL COMPOSITION: $|Ba_2Ca_{0.5}(H_2O)_{12}|\ [Si_{12}Al_4O_{32}]$
Andreasberg, Hartz, Germany

REFINED COMPOSITION: $|Ba_2Ca_{0.6}(H_2O)_{12}|\ [Si_{12}Al_4O_{32}]$

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 9.879$ Å $b = 14.139$ Å $c = 8.693$ Å
$\alpha = 90°$ $\beta = 124.81°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.039$

REFERENCE: R. Rinaldi, J. J. Pluth and J. V. Smith,
Acta Cryst. **B30** 2426–2433 (1974).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
-1	0	1	10.87	8.136	2	51.2	1	0	2	32.68	2.740	2	6.7	3	4	0	42.07	2.148	4	5.2
1	0	0	10.91	8.111	2	62.2	-1	4	2	32.82	2.729	4	17.1	-2	0	4	42.10	2.146	2	1.3
0	0	1	12.40	7.137	2	70.8	1	4	1	32.86	2.726	4	14.6	-2	6	1	42.50	2.127	4	2.2
-1	1	1	12.55	7.052	4	12.0	-1	1	3	33.25	2.695	4	11.7	0	3	3	42.57	2.124	4	0.6
1	1	0	12.58	7.036	4	5.8	1	1	2	33.30	2.690	4	22.6	-3	5	1	42.63	2.121	4	0.7
0	1	1	13.90	6.372	4	100.0	-2	2	3	33.42	2.681	4	10.3	2	1	2	42.72	2.117	4	0.7
0	2	1	17.66	5.023	4	33.7	2	2	1	33.51	2.674	4	11.5	-4	3	1	43.29	2.090	4	1.5
-2	0	1	17.96	4.939	2	0.7	-1	5	1	33.55	2.671	4	14.0	-1	6	2	43.83	2.066	4	3.6
-1	0	2	20.69	4.292	2	18.6	1	5	0	33.56	2.670	4	14.3	1	6	1	43.85	2.064	4	5.0
1	0	1	20.75	4.282	2	10.0	-2	4	2	33.59	2.668	4	7.0	3	2	1	43.95	2.060	4	2.1
-1	1	2	21.64	4.107	4	14.1	2	4	0	33.63	2.665	4	1.3	-2	2	4	44.10	2.054	4	7.5
1	1	1	21.69	4.098	4	23.6	-3	1	3	33.65	2.663	4	4.2	2	2	2	44.20	2.049	4	4.3
-1	3	1	21.79	4.078	4	29.2	-3	3	2	33.78	2.654	4	0.8	4	0	0	44.69	2.028	2	4.2
1	3	0	21.81	4.075	4	14.5	-3	3	1	33.81	2.651	4	0.8	-4	4	2	44.76	2.025	4	1.2
-2	2	1	21.95	4.049	4	42.4	0	5	1	34.10	2.629	4	9.9	-2	5	3	44.79	2.024	4	2.5
0	3	1	22.61	3.933	4	2.6	-1	2	3	35.07	2.559	4	3.6	2	5	1	44.86	2.021	4	1.9
-2	1	2	22.75	3.909	4	8.6	1	2	2	35.12	2.555	4	3.0	-4	1	4	45.03	2.013	4	4.4
2	1	0	22.81	3.898	4	18.6	-3	2	3	35.45	2.532	4	16.2	-1	0	4	45.38	1.998	2	3.1
-1	2	2	24.26	3.669	4	2.9	3	2	0	35.55	2.525	4	10.8	1	0	3	45.44	1.996	2	3.1
1	2	1	24.30	3.662	4	3.5	0	4	2	35.75	2.511	4	11.4	1	1	3	45.92	1.976	4	1.5
0	0	2	24.95	3.569	2	2.9	-4	0	2	36.38	2.470	2	2.0	1	5	2	46.12	1.968	4	1.6
0	4	0	25.19	3.535	2	3.6	-2	3	3	36.40	2.468	4	6.1	0	6	2	46.16	1.966	4	2.5
-2	2	2	25.26	3.526	4	1.4	2	3	1	36.48	2.463	4	1.4	-3	3	4	46.22	1.964	4	2.9
0	1	2	25.75	3.460	4	10.6	-4	1	2	36.95	2.433	4	1.3	-1	7	1	46.31	1.960	4	0.9
-2	3	1	26.13	3.410	4	3.8	0	0	3	37.81	2.379	2	2.3	3	3	1	46.35	1.959	4	0.8
-1	4	1	27.51	3.242	4	16.4	-1	3	3	37.93	2.372	4	4.1	-5	0	3	46.37	1.958	2	1.3
1	4	0	27.53	3.240	4	27.6	1	3	2	37.98	2.369	4	6.1	-3	5	3	46.39	1.957	4	1.0
-3	0	2	27.78	3.211	2	9.8	1	5	1	38.14	2.360	4	2.9	-5	0	2	46.42	1.956	2	3.9
-3	0	1	27.82	3.206	2	1.0	0	6	0	38.19	2.357	2	1.5	-4	2	4	46.46	1.955	4	3.1
0	2	2	28.01	3.186	4	8.0	0	1	3	38.37	2.346	4	1.3	3	5	0	46.47	1.954	4	1.8
-1	3	2	28.12	3.173	4	2.6	3	3	0	38.38	2.345	4	6.4	4	2	0	46.59	1.949	4	6.7
0	4	1	28.17	3.168	4	32.2	-4	0	3	38.53	2.336	2	1.8	2	3	2	46.60	1.949	4	1.9
-3	1	2	28.51	3.131	4	42.8	-4	2	2	38.62	2.332	4	4.0	-4	4	3	46.60	1.949	4	1.3
-3	1	1	28.54	3.127	4	38.9	-2	5	2	38.78	2.322	4	6.6	-5	1	3	46.84	1.939	4	1.2
-2	3	2	29.00	3.079	4	11.2	2	5	0	38.82	2.320	4	9.7	-1	2	4	47.27	1.923	4	1.9
2	3	0	29.05	3.074	4	12.0	-4	1	3	39.08	2.305	4	3.6	1	2	3	47.32	1.921	4	3.0
-3	2	2	30.58	2.924	4	6.8	-4	1	1	39.16	2.301	4	8.7	-3	6	2	47.88	1.900	4	1.6
-3	2	1	30.61	2.920	4	20.5	-1	6	1	39.82	2.263	4	0.9	-3	6	1	47.91	1.899	4	2.5
-2	0	3	30.86	2.897	2	5.2	1	6	0	39.83	2.263	4	2.8	-3	4	4	49.44	1.843	4	1.8
2	0	1	30.96	2.888	2	1.4	0	2	3	39.98	2.255	4	3.4	-1	3	4	49.54	1.840	4	1.0
-2	4	1	31.11	2.875	4	3.4	-2	4	3	40.25	2.241	4	4.0	1	3	3	49.60	1.838	4	0.9
0	3	2	31.44	2.845	4	6.3	0	6	1	40.30	2.238	4	1.1	-2	4	4	49.70	1.834	4	1.6
-2	1	3	31.52	2.838	4	3.2	2	4	1	40.32	2.237	4	5.6	2	4	2	49.80	1.831	4	1.2
2	1	1	31.62	2.830	4	1.0	-4	2	3	40.67	2.218	4	2.8	-5	0	4	49.92	1.827	2	1.2
-1	0	3	32.62	2.745	2	4.5	-3	4	3	41.99	2.152	4	10.2	2	6	1	49.95	1.826	4	1.4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2 theta (°)
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100

RHO Rho, Hydrated

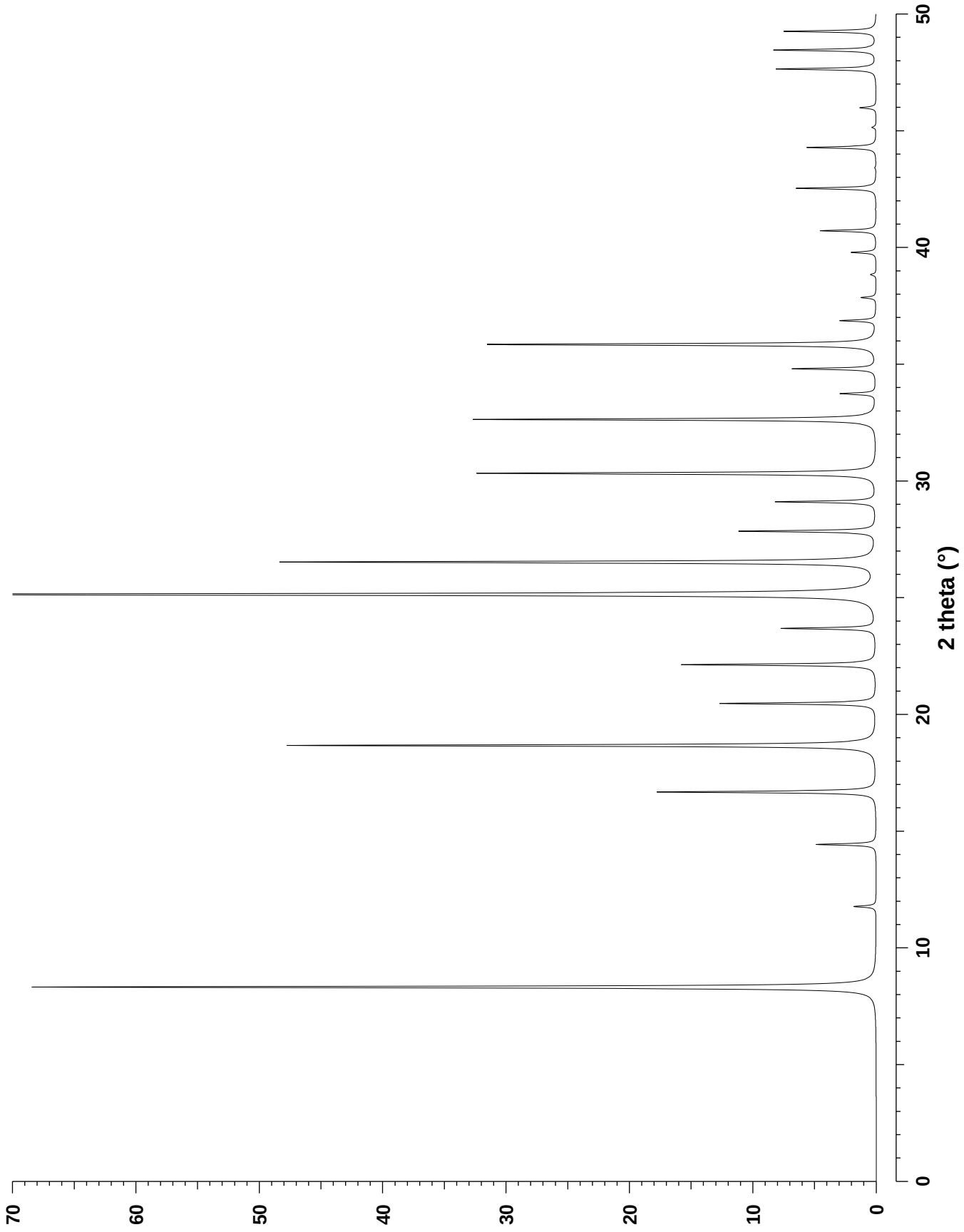
CHEMICAL COMPOSITION: $|Na_3Cs_3(H_2O)_{73}|\ [Si_{36}Al_{12}O_{96}]$

REFINED COMPOSITION: $|Na_{2.88}Cs_{3.12}(H_2O)_{73.27}|\ [Si_{35.95}Al_{12.05}O_{96}]$

CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 15.031$ Å $b = 15.031$ Å $c = 15.031$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.18$, $R_F = 0.134$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
in *Proceedings of the 6th International Zeolite Conference, Reno 1983*,
Ed. by D. H. Olson and A. Bisio (Butterworth: Guildford) 812–822 (1984).

h	k	l	2θ	d	M	I_{rel}
1	1	0	8.32	10.629	12	70.2
2	0	0	11.77	7.516	6	1.9
2	1	1	14.43	6.136	24	5.0
2	2	0	16.68	5.314	12	18.2
3	1	0	18.67	4.753	24	49.0
2	2	2	20.47	4.339	8	13.0
3	2	1	22.13	4.017	48	16.2
4	0	0	23.68	3.758	6	7.8
3	3	0	25.14	3.543	12	2.6
4	1	1	25.14	3.543	24	100.0
4	2	0	26.52	3.361	24	49.5
3	3	2	27.84	3.205	24	11.4
4	2	2	29.10	3.068	24	8.4
4	3	1	30.32	2.948	48	7.1
5	1	0	30.32	2.948	24	26.1
5	2	1	32.63	2.744	48	33.5
4	4	0	33.73	2.657	12	3.0
4	3	3	34.80	2.578	24	3.5
5	3	0	34.80	2.578	24	3.5
6	0	0	35.84	2.505	6	0.2
4	4	2	35.84	2.505	24	32.1
5	3	2	36.86	2.438	48	2.9
6	1	1	36.86	2.438	24	0.1
6	2	0	37.85	2.377	24	1.3
5	4	1	38.83	2.319	48	0.5
6	2	2	39.78	2.266	24	2.1
6	3	1	40.71	2.216	48	4.7
7	1	0	42.53	2.126	24	2.9
5	5	0	42.53	2.126	12	3.8
6	4	0	43.41	2.084	24	0.1
7	2	1	44.28	2.045	48	0.3
5	5	2	44.28	2.045	24	5.5
6	4	2	45.14	2.009	48	0.3
7	3	0	45.98	1.974	24	1.4
7	3	2	47.64	1.909	48	1.5
6	5	1	47.64	1.909	48	6.8
8	0	0	48.45	1.879	6	8.5
7	4	1	49.25	1.850	48	2.5
8	1	1	49.25	1.850	24	1.1
5	5	4	49.25	1.850	24	4.0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2 theta (°)
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RHO Pahasapaite

CHEMICAL COMPOSITION: $|Li_{11.6}Na_{0.192}K_{1.2}Ca_{5.5}(H_2O)_{38}\square_{13.5}|\ [Be_{24}P_{24}O_{96}]$
$\square$ = cation vacancy.
Custer, S. Dakota, U.S.A.

REFINED COMPOSITION: $|Li_{11.6}Na_{0.192}K_{1.2}Ca_{5.5}(H_2O)_{38}|\ [Be_{24}P_{24}O_{96}]$

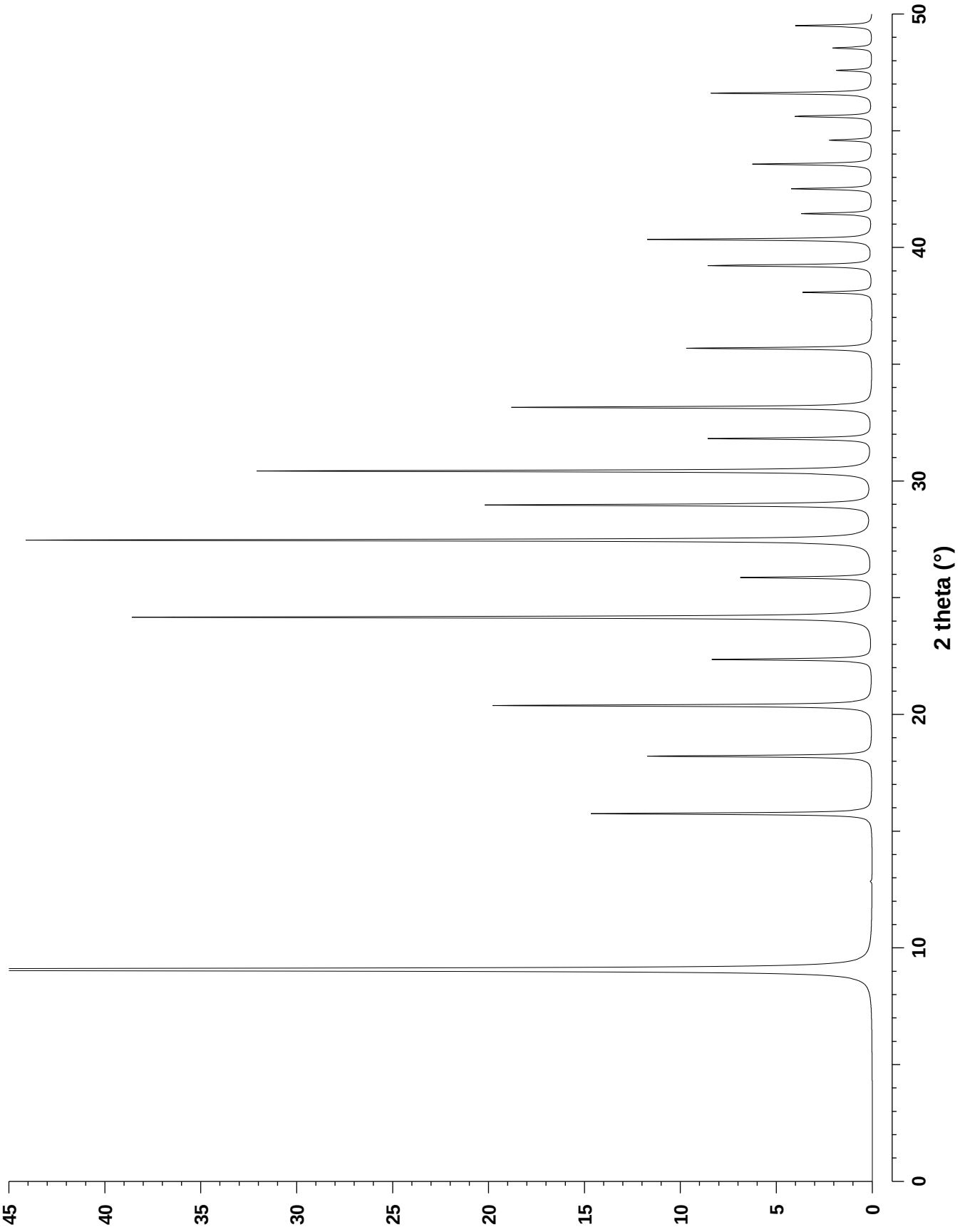
CRYSTAL DATA: $I23$ (No. 197)
$a = 13.781$ Å $b = 13.781$ Å $c = 13.781$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.035$

REFERENCE: R. C. Rouse, D. R. Peacor and S. Merlino, *American Mineralogist* **74** 1195–1202 (1989).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.07	9.745	12	100.0	4	1	3	33.15	2.703	24	5.2	6	2	2	43.56	2.078	24	6.2
2	1	1	15.75	5.626	24	14.7	4	3	1	33.15	2.703	24	3.4	6	1	3	44.59	2.032	24	2.1
2	2	0	18.21	4.872	12	11.7	5	0	1	33.15	2.703	12	9.9	6	3	1	44.59	2.032	24	0.1
3	1	0	20.38	4.358	12	19.0	5	2	1	35.68	2.516	24	5.5	4	4	4	45.61	1.989	8	4.0
3	0	1	20.38	4.358	12	0.7	5	1	2	35.68	2.516	24	4.2	5	3	4	46.60	1.949	24	1.6
2	2	2	22.35	3.978	8	8.3	4	3	3	38.07	2.363	24	1.2	5	5	0	46.60	1.949	12	3.8
3	1	2	24.16	3.683	24	31.3	5	3	0	38.07	2.363	12	2.3	7	1	0	46.60	1.949	12	1.1
3	2	1	24.16	3.683	24	7.3	6	0	0	39.22	2.297	6	7.4	7	0	1	46.60	1.949	12	1.3
4	0	0	25.86	3.445	6	6.8	4	4	2	39.22	2.297	24	1.1	5	4	3	46.60	1.949	24	0.7
4	1	1	27.46	3.248	24	43.7	5	3	2	40.34	2.236	24	0.4	6	0	4	47.58	1.911	12	1.8
3	3	0	27.46	3.248	12	0.4	6	1	1	40.34	2.236	24	6.1	6	3	3	48.54	1.875	24	0.7
4	2	0	28.97	3.082	12	0.4	5	2	3	40.34	2.236	24	5.3	7	1	2	48.54	1.875	24	0.3
4	0	2	28.97	3.082	12	19.7	6	0	2	41.44	2.179	12	0.6	7	2	1	48.54	1.875	24	0.7
3	3	2	30.42	2.938	24	32.0	6	2	0	41.44	2.179	12	3.1	5	5	2	48.54	1.875	24	0.3
4	2	2	31.81	2.813	24	8.5	5	1	4	42.51	2.126	24	0.9	6	2	4	49.49	1.842	24	3.9
5	1	0	33.15	2.703	12	0.3	5	4	1	42.51	2.126	24	3.3	6	4	2	49.49	1.842	24	0.1

Pahasapaite

RHO



RHO Rho, Deuterated Berylloarsenate

CHEMICAL COMPOSITION: $|Rb_{24}(D_2O)_{3.2}|\ [Be_{24}As_{24}O_{96}]$

REFINED COMPOSITION: $|Rb_{24}(D_2O)_{3.6}|\ [Be_{24}As_{24}O_{96}]$

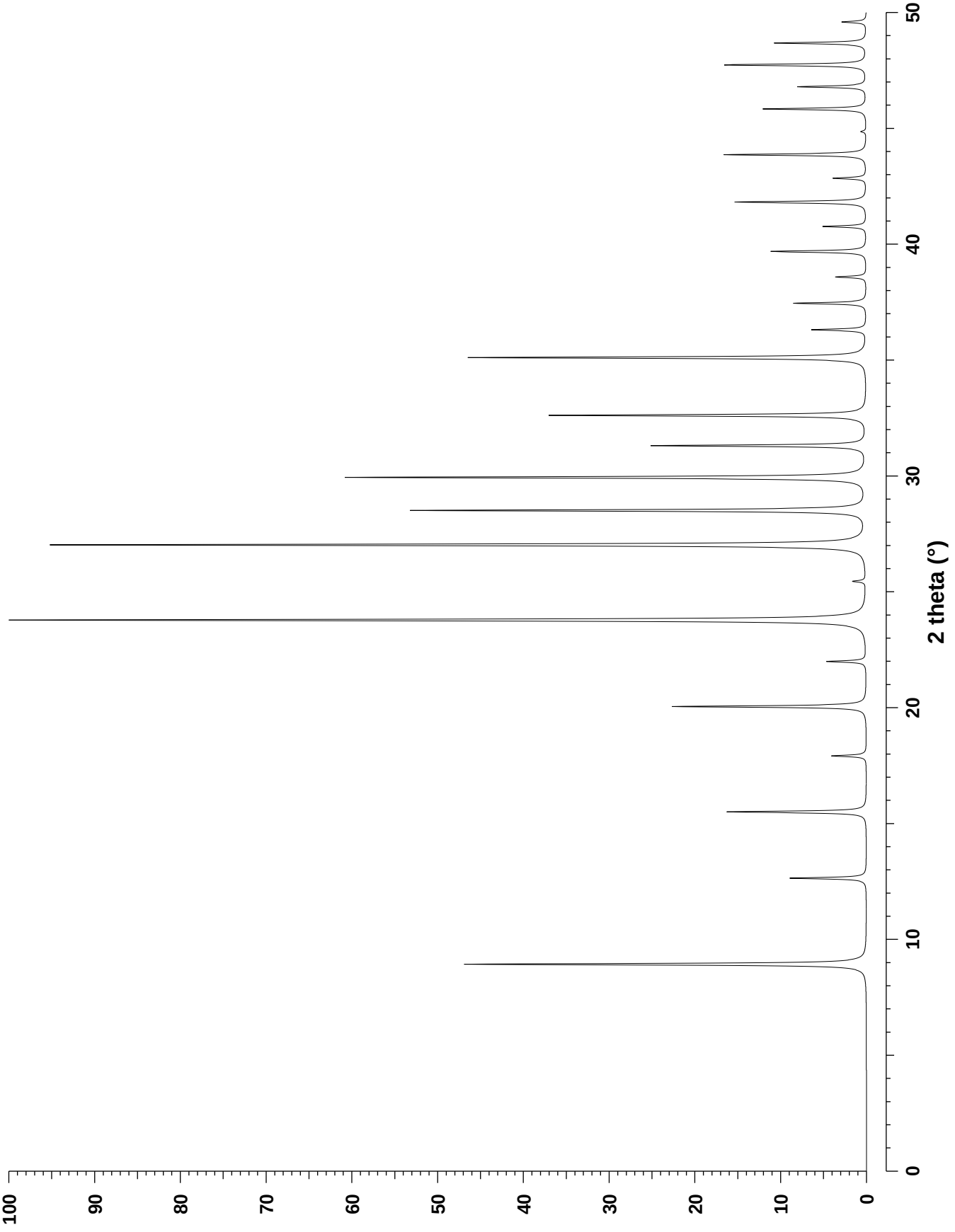
CRYSTAL DATA: $I23$ (No. 197)
$a = 14.001$ Å $b = 14.001$ Å $c = 14.001$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
neutron $R_{wp} = 0.041$, X-ray $R_{wp} = 0.145$

REFERENCE: J. B. Parise, D. R. Corbin, T. E. Gier, R. L. Harlow, L. Abrams and R. B. Von Dreele, *Zeolites* **12** 360–368 (1992).
And J. B. Parise, Private communication (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.93	9.900	12	50.6	5	0	1	32.61	2.746	12	10.3	6	3	1	43.86	2.064	24	14.9
2	0	0	12.64	7.001	6	9.6	5	1	0	32.61	2.746	12	0.5	6	1	3	43.86	2.064	24	3.0
2	1	1	15.50	5.716	24	17.6	5	1	2	35.10	2.556	24	31.7	4	4	4	44.85	2.021	8	0.7
2	2	0	17.92	4.950	12	4.4	5	2	1	35.10	2.556	24	18.4	5	4	3	45.83	1.980	24	4.6
3	1	0	20.05	4.428	12	1.6	4	4	0	36.30	2.475	12	6.9	7	1	0	45.83	1.980	12	0.2
3	0	1	20.05	4.428	12	22.9	5	0	3	37.45	2.401	12	4.7	7	0	1	45.83	1.980	12	0.3
2	2	2	21.99	4.042	8	5.0	4	3	3	37.45	2.401	24	3.5	5	3	4	45.83	1.980	24	5.8
3	2	1	23.78	3.742	24	84.6	5	3	0	37.45	2.401	12	0.9	5	5	0	45.83	1.980	12	2.0
3	1	2	23.78	3.742	24	23.3	6	0	0	38.58	2.334	6	2.0	6	0	4	46.79	1.942	12	7.6
4	0	0	25.45	3.500	6	1.7	4	4	2	38.58	2.334	24	1.8	6	4	0	46.79	1.942	12	1.1
4	1	1	27.02	3.300	24	100.0	6	1	1	39.68	2.271	24	4.6	6	3	3	47.73	1.905	24	3.4
3	3	0	27.02	3.300	12	2.6	5	3	2	39.68	2.271	24	0.5	7	1	2	47.73	1.905	24	5.9
4	2	0	28.51	3.131	12	4.0	5	2	3	39.68	2.271	24	6.9	5	5	2	47.73	1.905	24	1.0
4	0	2	28.51	3.131	12	53.3	6	2	0	40.76	2.214	12	5.3	7	2	1	47.73	1.905	24	7.5
3	3	2	29.93	2.985	24	65.5	6	0	2	40.76	2.214	12	0.2	6	4	2	48.67	1.871	24	8.7
4	2	2	31.30	2.858	24	27.0	5	1	4	41.81	2.160	24	7.6	6	2	4	48.67	1.871	24	2.9
4	3	1	32.61	2.746	24	22.7	5	4	1	41.81	2.160	24	8.9	7	3	0	49.58	1.838	12	0.8
4	1	3	32.61	2.746	24	6.3	6	2	2	42.84	2.111	24	4.2	7	0	3	49.58	1.838	12	2.3

Rho, Deuterated Berylloarsenate

RHO



Roggianite

CHEMICAL COMPOSITION: $|Ca_{16}(H_2O)_{<2.5}|\ [(Be(OH)_2)_8Si_{32}Al_{16}O_{104}]$
Pizzo Marcio, Val Vigezzo, Italy

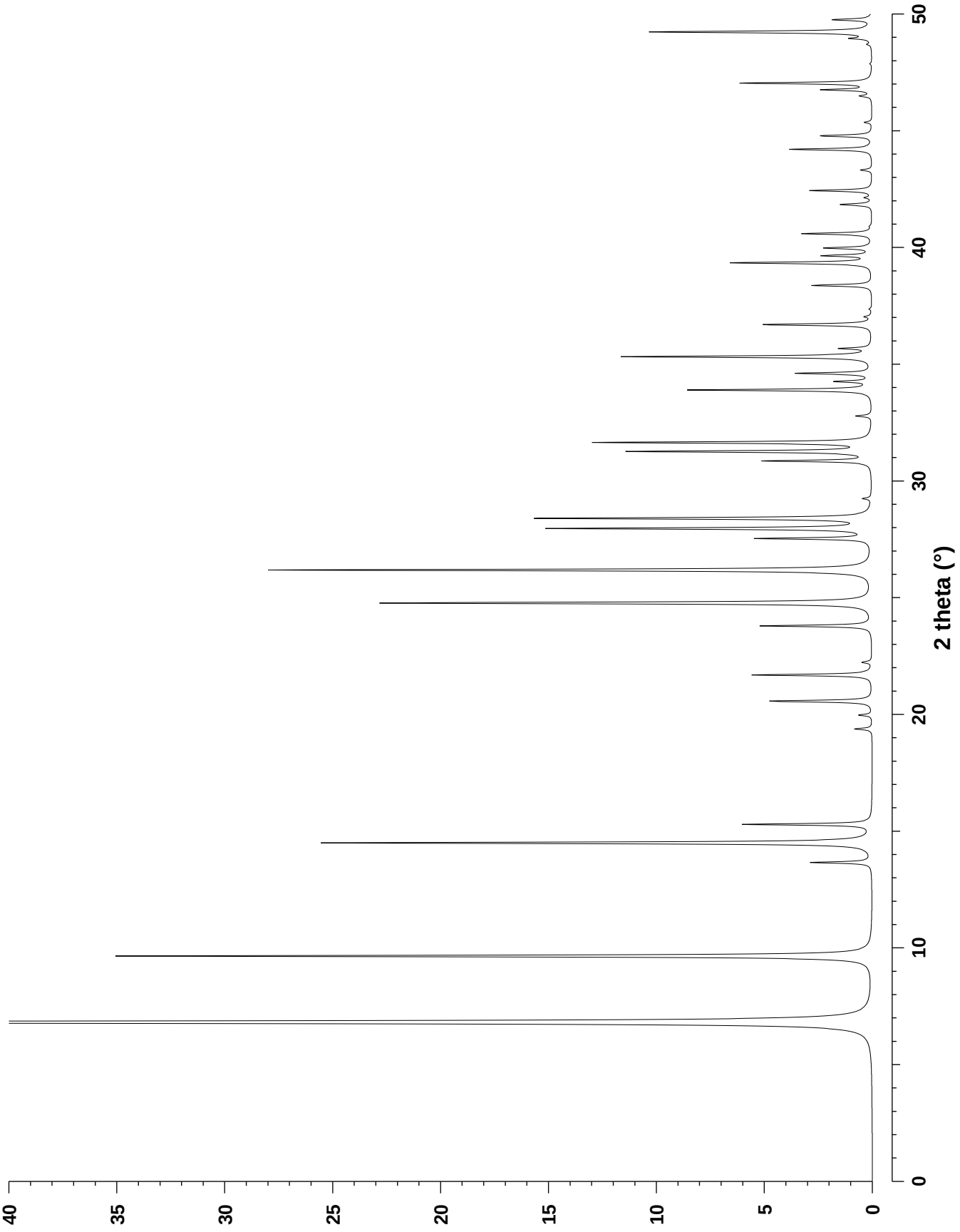
REFINED COMPOSITION: $|Ca_{16}(H_2O)_{18.72}|\ [(Be(OH)_2)_8Si_{32}Al_{16}O_{104}]$

CRYSTAL DATA: $I\,4/m\,cm$ (No. 140)
$a = 18.33$ Å $b = 18.33$ Å $c = 9.16$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{\rm obs} = 0.034$

REFERENCE: G. Giuseppetti, F. Mazzi, C. Tadini and E. Galli,
Neues Jahrb. Mineral. Monatsh. **7** 307–314 (1991).

h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$
1	1	0	6.82	12.961	4	100.0	2	1	3	31.26	2.861	16	6.3	6	6	0	41.82	2.160	4	0.8
2	0	0	9.65	9.165	4	35.0	5	1	2	31.64	2.828	16	12.8	2	2	4	41.84	2.159	8	0.8
2	2	0	13.66	6.481	4	2.8	5	4	1	32.78	2.732	16	0.7	6	1	3	42.13	2.145	16	0.3
2	1	1	14.50	6.109	16	25.5	4	4	2	33.89	2.645	8	8.5	7	3	2	42.43	2.131	16	2.6
3	1	0	15.29	5.796	8	6.0	6	3	1	34.24	2.618	16	0.7	3	1	4	42.44	2.130	16	0.3
4	0	0	19.37	4.582	4	0.6	3	2	3	34.26	2.618	16	1.0	8	3	1	43.31	2.089	16	0.5
0	0	2	19.38	4.580	2	0.2	7	1	0	34.60	2.592	8	0.5	8	4	0	44.19	2.049	8	0.6
3	2	1	19.97	4.445	16	0.6	5	5	0	34.60	2.592	4	2.5	8	0	2	44.20	2.049	8	3.1
3	3	0	20.56	4.320	4	1.8	5	3	2	34.61	2.592	16	0.5	4	0	4	44.21	2.048	8	0.2
1	1	2	20.57	4.318	8	3.0	6	4	0	35.31	2.542	8	0.2	9	1	0	44.77	2.024	8	2.0
4	2	0	21.68	4.099	8	0.6	6	0	2	35.32	2.541	8	11.4	3	3	4	44.79	2.023	8	0.5
2	0	2	21.69	4.097	8	5.0	4	1	3	35.67	2.517	16	1.4	8	2	2	45.35	2.000	16	0.3
4	1	1	22.23	4.000	16	0.4	6	2	2	36.69	2.449	16	5.0	6	6	2	46.48	1.954	8	0.5
2	2	2	23.79	3.740	8	5.2	7	2	1	37.03	2.428	16	0.3	7	6	1	46.75	1.943	16	1.9
5	1	0	24.77	3.595	8	1.1	7	3	0	37.36	2.407	8	0.1	9	2	1	46.75	1.943	16	0.3
3	1	2	24.77	3.594	16	21.7	4	3	3	38.37	2.346	16	2.8	9	3	0	47.03	1.932	8	5.5
4	3	1	26.18	3.404	16	28.0	8	0	0	39.32	2.291	4	2.2	7	5	2	47.03	1.932	16	0.1
4	0	2	27.53	3.239	8	5.3	0	0	4	39.34	2.290	2	4.8	5	1	4	47.05	1.931	16	0.6
5	2	1	27.96	3.191	16	14.9	6	5	1	39.64	2.273	16	1.5	4	4	4	48.69	1.870	8	0.2
5	3	0	28.39	3.144	8	9.7	5	2	3	39.65	2.273	16	0.7	6	5	3	48.95	1.861	16	0.9
3	3	2	28.40	3.143	8	6.2	5	5	2	39.96	2.256	8	0.8	7	7	0	49.21	1.852	4	3.2
4	2	2	29.24	3.054	16	0.4	1	1	4	39.98	2.255	8	1.5	5	3	4	49.23	1.851	16	7.7
6	2	0	30.85	2.898	8	5.0	8	2	0	40.58	2.223	8	3.1	8	6	0	49.74	1.833	8	1.0
6	1	1	31.25	2.863	16	5.2	2	0	4	40.61	2.222	8	0.3	6	0	4	49.76	1.832	8	0.9

Roggianite -RON



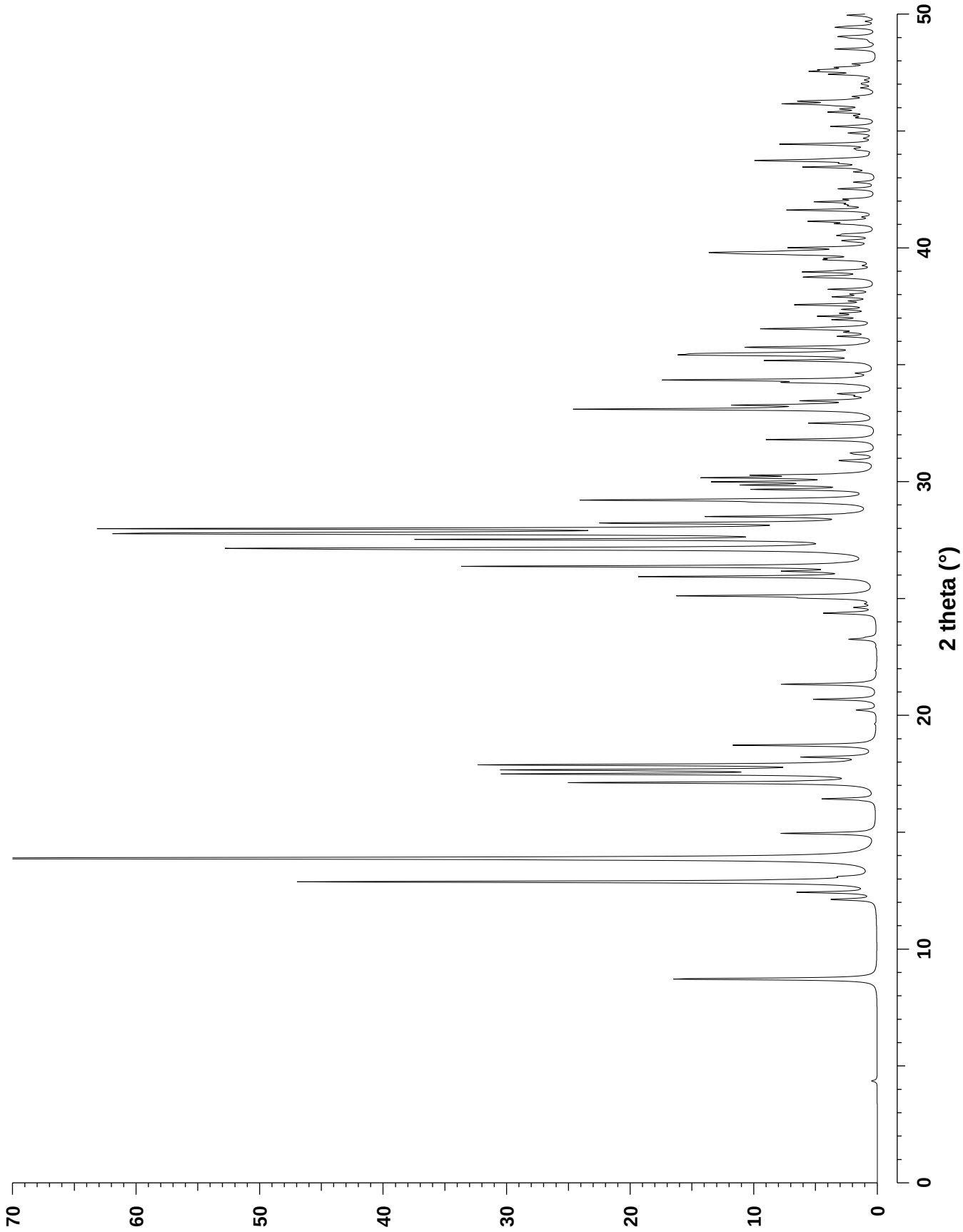
CHEMICAL COMPOSITION: $|K_4Na_{12}(H_2O)_{18}|\ [Si_{28}Zn_8O_{72}]$

REFINED COMPOSITION: $|K_4Na_{12}(H_2O)_{20.7}|\ [Si_{28}Zn_8O_{72}]$

CRYSTAL DATA: $C1m1$ (No. 8) unique axis **b**, cell choice 1
$a = 7.238$ Å $b = 40.56$ Å $c = 7.308$ Å
$\alpha = 90°$ $\beta = 91.8°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.238$, $R_{wp} = 0.164$, $R_I = 0.090$

REFERENCE: C. Röhrig and H. Gies,
Angew. Chem., Int. ed. **34** 63–65 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	4	0	8.72	10.140	2	16.5	2	6	1	30.90	2.894	4	2.2	3	3	1	40.31	2.238	4	1.9
0	0	1	12.12	7.304	2	3.5	1	13	0	31.22	2.865	4	1.6	3	7	0	40.52	2.226	4	2.5
1	1	0	12.43	7.122	4	6.0	1	7	2	31.79	2.814	4	8.9	-3	5	1	40.58	2.223	4	1.8
0	2	1	12.88	6.872	4	46.7	-2	8	1	32.49	2.756	4	5.4	1	5	3	41.02	2.200	4	2.7
0	6	0	13.10	6.760	2	1.4	2	8	1	33.09	2.707	4	23.6	0	8	3	41.13	2.195	4	4.2
1	3	0	13.88	6.379	4	100.0	2	10	0	33.18	2.700	4	2.3	-1	17	1	41.61	2.170	4	7.1
0	4	1	14.95	5.927	4	7.6	0	14	1	33.27	2.693	4	10.0	-1	7	3	41.79	2.162	4	1.4
1	5	0	16.42	5.399	4	4.3	-1	13	1	33.45	2.678	4	5.3	1	17	1	41.86	2.158	4	1.4
-1	1	1	17.12	5.180	4	24.4	1	13	1	33.75	2.656	4	2.7	0	18	1	41.96	2.153	4	4.4
0	8	0	17.49	5.070	2	28.4	1	9	2	34.23	2.620	4	5.7	-3	7	1	42.08	2.147	4	1.8
1	1	1	17.66	5.022	4	27.9	-2	0	2	34.34	2.611	2	16.6	3	9	0	42.52	2.126	4	2.6
0	6	1	17.88	4.961	4	31.0	-2	10	1	35.17	2.552	4	8.5	3	7	1	42.80	2.113	4	1.8
-1	3	1	18.21	4.872	4	5.4	0	16	0	35.41	2.535	2	10.9	-1	15	2	43.24	2.092	4	1.5
1	3	1	18.72	4.740	4	11.5	1	15	0	35.44	2.533	4	2.4	0	16	2	43.45	2.083	4	5.6
-1	5	1	20.22	4.391	4	1.7	2	0	2	35.47	2.531	2	7.8	2	16	0	43.60	2.076	4	1.6
1	5	1	20.68	4.294	4	5.1	-2	4	2	35.50	2.529	4	2.5	1	15	2	43.71	2.071	4	4.5
0	8	1	21.33	4.165	4	7.8	2	10	1	35.73	2.513	4	6.4	-1	9	3	43.74	2.070	4	6.0
1	9	0	23.25	3.825	4	2.2	2	2	2	35.76	2.511	4	5.2	-2	12	2	43.81	2.066	4	1.7
0	0	2	24.37	3.652	2	4.2	0	12	2	36.21	2.481	4	2.8	-3	1	2	44.42	2.040	4	2.9
2	0	0	24.61	3.617	2	1.6	2	12	0	36.38	2.470	4	1.8	-2	2	3	44.42	2.039	4	3.5
2	2	0	25.01	3.561	4	4.0	-1	11	2	36.53	2.460	4	8.7	1	9	3	44.44	2.039	4	1.7
0	10	1	25.11	3.546	4	15.5	2	4	2	36.60	2.455	4	1.9	3	11	0	44.91	2.018	4	1.3
0	4	2	25.93	3.436	4	18.7	0	0	3	36.92	2.435	2	3.0	-2	16	1	45.19	2.006	4	3.5
2	4	0	26.16	3.407	4	5.3	1	11	2	37.07	2.425	4	4.2	2	0	3	45.56	1.991	2	1.3
0	12	0	26.37	3.380	2	32.9	0	2	3	37.19	2.417	4	2.3	2	16	1	45.65	1.987	4	1.3
-1	1	2	27.09	3.291	4	24.8	3	1	0	37.36	2.407	4	2.3	2	2	3	45.79	1.982	4	1.9
1	11	0	27.14	3.285	4	37.8	0	16	1	37.56	2.395	4	6.3	-3	5	2	45.82	1.980	4	1.3
-2	0	1	27.16	3.283	2	5.4	1	15	1	37.72	2.385	4	1.7	0	12	3	45.94	1.976	4	1.7
-2	2	1	27.52	3.241	4	34.4	3	3	0	37.90	2.374	4	3.2	-1	11	3	46.08	1.970	4	1.6
0	6	2	27.76	3.213	4	38.5	0	4	3	38.01	2.368	4	1.5	1	19	1	46.15	1.967	4	6.4
1	1	2	27.79	3.210	4	17.2	-2	12	1	38.22	2.355	4	3.7	3	3	2	46.25	1.963	4	2.8
-1	3	2	27.81	3.208	4	14.8	2	12	1	38.74	2.324	4	4.7	-2	6	3	46.28	1.962	4	3.4
2	0	1	27.86	3.202	2	6.6	-2	8	2	38.79	2.322	4	2.2	0	20	1	46.47	1.954	4	1.4
2	6	0	27.98	3.189	4	58.7	3	5	0	38.96	2.312	4	5.3	0	18	2	47.41	1.918	4	3.1
2	2	1	28.22	3.163	4	19.7	-3	1	1	39.03	2.308	4	1.7	2	18	0	47.54	1.913	4	4.3
1	3	2	28.50	3.132	4	12.3	1	1	3	39.48	2.282	4	3.2	2	6	3	47.61	1.910	4	3.0
-2	4	1	28.58	3.123	4	1.9	-3	3	1	39.55	2.279	4	2.7	2	14	2	47.72	1.906	4	2.5
0	12	1	29.11	3.068	4	5.8	0	14	2	39.71	2.270	4	3.2	-2	8	3	47.86	1.900	4	1.6
-1	5	2	29.20	3.059	4	21.2	-1	13	2	39.74	2.268	4	4.6	3	7	2	48.50	1.877	4	3.4
2	4	1	29.25	3.053	4	4.0	1	17	0	39.78	2.266	4	4.2	-3	9	2	48.97	1.860	4	1.4
-1	11	1	29.66	3.012	4	9.2	3	1	1	39.79	2.265	4	2.0	-2	18	1	49.03	1.858	4	1.3
1	5	2	29.85	2.993	4	9.2	2	8	2	39.81	2.264	4	5.1	-3	13	1	49.04	1.857	4	1.5
1	11	1	29.98	2.980	4	11.6	2	14	0	39.87	2.261	4	3.3	1	13	3	49.42	1.844	4	2.5
0	8	2	30.16	2.963	4	12.4	1	3	3	40.00	2.254	4	4.9	2	18	1	49.46	1.843	4	1.5
-2	6	1	30.27	2.953	4	8.4	0	18	0	40.01	2.253	2	1.4	0	0	4	49.94	1.826	2	2.4


0
10
20
30
40
50
2 theta (°)
0
10
20
30
40
50
60
70

CHEMICAL COMPOSITION: $|(C_7H_{13}N)_2|\ [Si_{24}O_{48}]$
$C_7H_{13}N$ = (±)-exo-2-aminobicyclo[2.2.1]heptane

REFINED COMPOSITION: $|C_{17.6}|\ [Si_{24}O_{48}]$

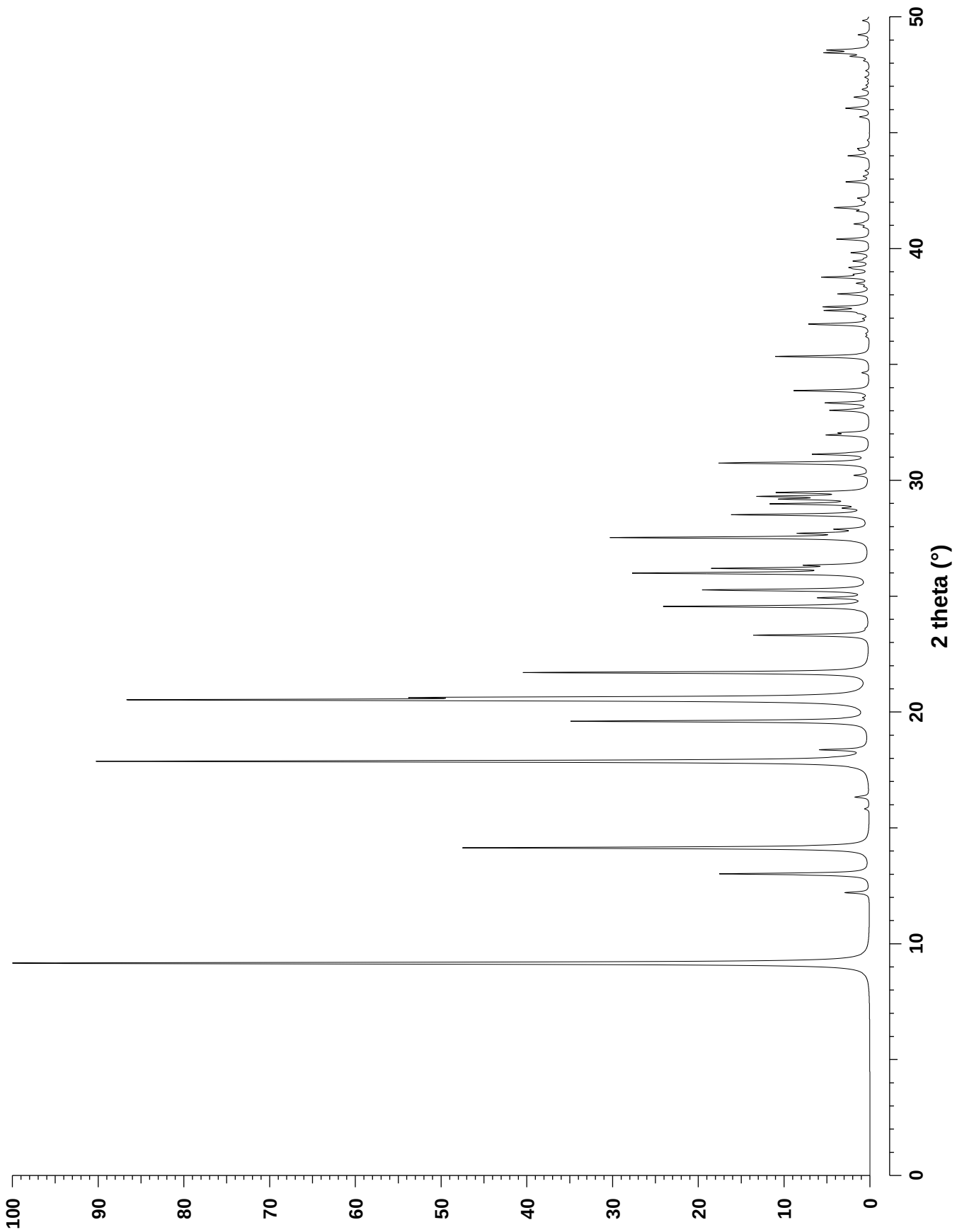
CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.018$ Å $b = 13.612$ Å $c = 7.418$ Å
$\alpha = 90°$ $\beta = 102.12°$ $\gamma = 90°$
X-ray single crystal refinement, $R_1 = 0.099$

REFERENCE: B. Marler, A. Grünewald-Lüke and H. Gies,
Microporous and Mesoporous Materials **26** 49–59 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.16	9.658	4	100.0	-1	3	2	31.17	2.869	4	0.8	-1	5	2	41.15	2.193	4	0.3
0	0	1	12.20	7.253	2	2.8	-4	0	2	31.95	2.801	2	4.6	-1	3	3	41.61	2.170	4	1.2
2	0	0	12.92	6.853	2	0.4	3	3	1	32.04	2.793	4	2.9	6	2	0	41.71	2.166	4	0.4
0	2	0	13.01	6.806	2	17.4	2	4	1	32.92	2.721	4	0.3	-4	4	2	41.76	2.163	4	3.9
-1	1	1	14.14	6.261	4	47.5	2	2	2	33.01	2.713	4	4.4	3	5	1	41.84	2.159	4	0.1
-2	0	1	15.82	5.603	2	0.6	-5	1	1	33.08	2.708	4	0.4	-5	3	2	41.93	2.154	4	0.2
1	1	1	16.33	5.427	4	1.7	1	3	2	33.33	2.688	4	4.9	4	2	2	42.05	2.149	4	0.5
0	2	1	17.87	4.963	4	90.2	5	1	0	33.34	2.687	4	0.2	-6	0	2	42.09	2.147	2	0.3
2	2	0	18.37	4.829	4	5.3	1	5	0	33.56	2.670	4	0.5	2	0	3	42.17	2.143	2	1.3
2	0	1	19.60	4.529	2	34.6	4	2	1	33.86	2.647	4	8.8	1	5	2	42.87	2.109	4	2.8
3	1	0	20.51	4.331	4	29.7	-4	2	2	34.63	2.591	4	0.9	-4	2	3	43.11	2.098	4	0.7
-2	2	1	20.53	4.326	4	56.0	-1	5	1	35.34	2.540	4	11.0	-3	3	3	43.35	2.087	4	0.5
1	3	0	20.62	4.307	4	40.8	0	4	2	36.20	2.481	4	0.4	6	0	1	43.99	2.058	2	2.5
-3	1	1	21.70	4.095	4	40.3	1	5	1	36.32	2.473	4	0.3	1	3	3	44.15	2.051	4	0.2
-1	3	1	23.31	3.816	4	13.5	-2	4	2	36.70	2.449	4	0.6	-6	2	2	44.24	2.047	4	0.9
2	2	1	23.60	3.770	4	0.2	-2	0	3	36.73	2.447	2	6.7	2	2	3	44.31	2.044	4	1.2
0	0	2	24.55	3.626	2	23.9	-1	1	3	36.97	2.431	4	0.5	2	6	1	44.67	2.028	4	0.3
-1	1	2	24.92	3.573	4	5.5	0	0	3	37.19	2.418	2	0.8	-2	4	3	45.67	1.987	4	1.2
-2	0	2	25.26	3.526	2	19.3	4	4	0	37.24	2.415	4	0.1	0	4	3	46.05	1.971	4	2.8
3	1	1	25.98	3.430	4	13.5	-5	1	2	37.32	2.409	4	4.9	3	1	3	46.52	1.952	4	1.8
4	0	0	26.00	3.426	2	15.1	-4	4	1	37.48	2.400	4	5.1	-5	5	1	46.85	1.939	4	0.5
0	4	0	26.19	3.403	2	16.8	5	1	1	38.03	2.366	4	3.7	7	1	0	46.88	1.938	4	0.4
-4	0	1	26.33	3.385	2	6.0	-5	3	1	38.13	2.360	4	0.2	5	5	0	47.04	1.932	4	0.4
1	1	2	27.52	3.241	4	29.9	5	3	0	38.36	2.346	4	0.5	1	7	0	47.21	1.925	4	0.2
3	3	0	27.71	3.219	4	6.9	3	5	0	38.49	2.339	4	1.4	-6	4	1	47.38	1.919	4	0.5
0	2	2	27.88	3.200	4	3.4	-6	0	1	38.76	2.323	2	5.4	-2	6	2	47.67	1.908	4	0.4
-2	2	2	28.51	3.131	4	15.9	-3	1	3	38.88	2.316	4	1.3	4	6	0	48.10	1.892	4	0.6
-3	1	2	28.79	3.101	4	2.2	-2	2	3	39.12	2.302	4	1.3	4	4	2	48.27	1.885	4	0.5
0	4	1	28.98	3.081	4	10.8	-3	5	1	39.18	2.299	4	1.9	-4	6	1	48.29	1.884	4	1.5
4	2	0	29.18	3.060	4	8.8	6	0	0	39.45	2.284	2	1.8	-7	1	2	48.44	1.879	4	4.8
2	4	0	29.30	3.048	4	11.5	0	2	3	39.56	2.278	4	0.4	-1	7	1	48.56	1.875	4	4.5
-4	2	1	29.47	3.031	4	10.1	4	0	2	39.81	2.264	2	2.1	-5	3	3	49.00	1.859	4	0.2
2	0	2	30.21	2.959	2	1.7	2	4	2	40.40	2.233	4	3.9	-2	0	4	49.21	1.852	2	1.1
-2	4	1	30.74	2.909	4	17.5	-4	0	3	40.92	2.205	2	0.6	-4	4	3	49.23	1.851	4	0.2
4	0	1	31.12	2.874	2	6.2	-6	2	1	41.05	2.198	4	1.7	-1	5	3	49.83	1.830	4	0.8

RUB-3

RTE



RTH RUB-13

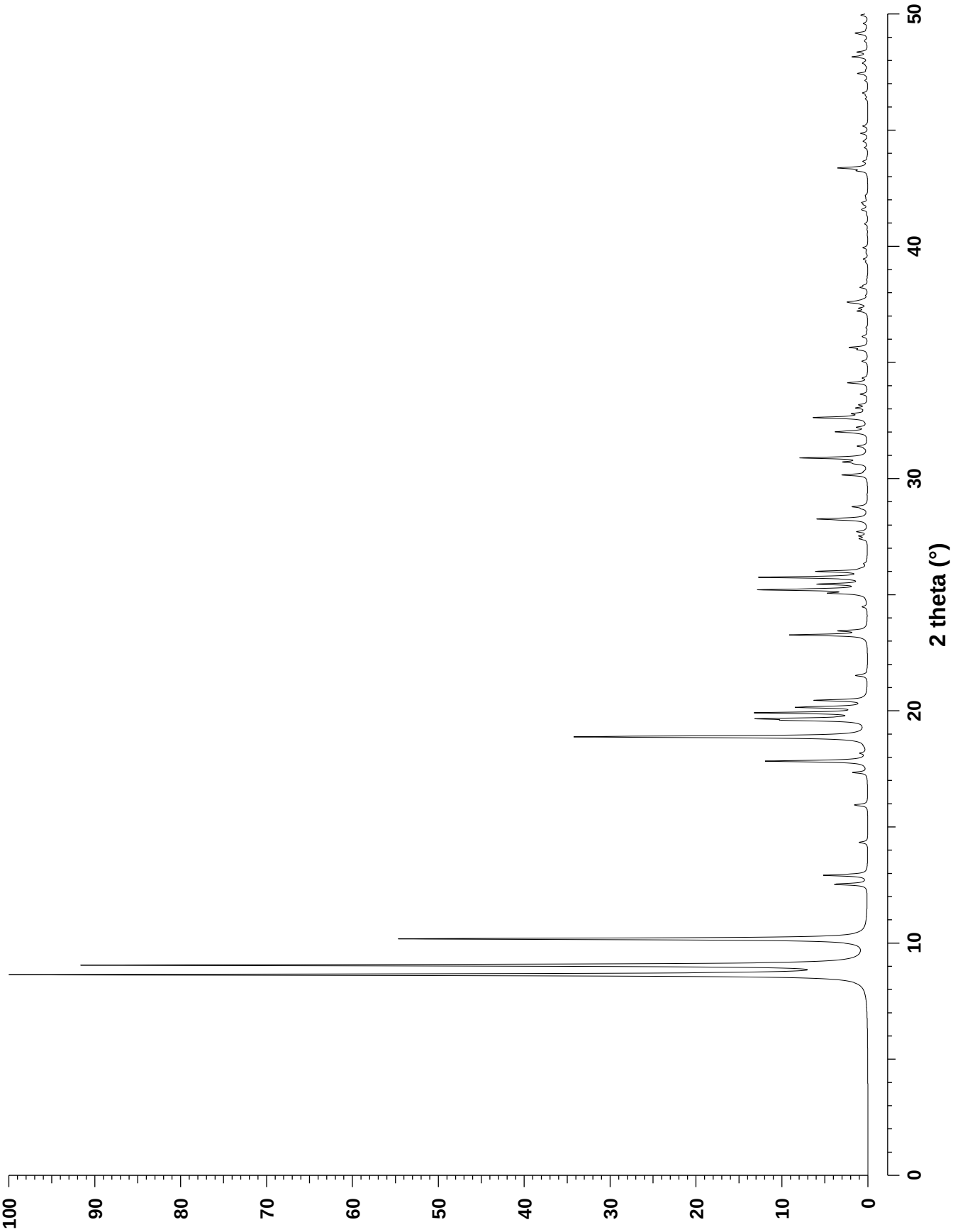
CHEMICAL COMPOSITION: $|(C_{10}H_{21}N)_{1.7}|\ [Si_{30.4}B_{1.6}O_{64}]$
$(C_{10}H_{21}N)^+$ = 1,2,2,6,6,-pentamethylpiperidine

REFINED COMPOSITION: $[Si_{31}O_{64}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.659$ Å $b = 20.461$ Å $c = 9.831$ Å
$\alpha = 90°$ $\beta = 96.58°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.06$

REFERENCE: S. Vortmann, B. Marler, H. Gies and P. Daniels,
Microporous Materials **4** 111–121 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	8.64	10.231	2	100.0	-2	0	3	31.39	2.850	2	1.1	2	8	1	41.55	2.173	4	0.4
0	0	1	9.05	9.766	2	91.5	-3	1	2	31.94	2.802	4	0.4	4	4	0	41.58	2.172	4	0.4
1	1	0	10.18	8.688	4	55.0	1	7	0	32.01	2.796	4	2.0	-1	9	1	41.62	2.170	4	0.2
0	2	1	12.53	7.064	4	3.8	0	6	2	32.01	2.796	4	1.7	3	5	2	41.79	2.161	4	0.4
-1	1	1	12.92	6.854	4	5.2	2	6	0	32.20	2.780	4	1.1	3	7	0	41.87	2.158	4	0.6
1	1	1	14.33	6.180	4	1.0	0	4	3	32.60	2.746	4	1.5	3	1	3	42.04	2.149	4	0.1
1	3	0	15.94	5.559	4	1.6	-2	2	3	32.62	2.745	4	5.0	1	9	1	42.12	2.145	4	0.2
0	4	0	17.34	5.115	2	1.7	2	4	2	32.70	2.738	4	0.4	-3	7	1	42.19	2.142	4	0.2
-1	3	1	17.83	4.975	4	12.0	1	3	3	32.79	2.731	4	1.5	-2	8	2	43.24	2.092	4	1.0
0	0	2	18.17	4.883	2	0.7	-2	6	1	32.91	2.721	4	0.2	1	7	3	43.36	2.087	4	2.7
2	0	0	18.49	4.798	2	0.1	-1	7	1	33.03	2.712	4	1.2	-2	4	4	43.38	2.086	4	0.8
1	3	1	18.88	4.699	4	34.4	3	3	1	33.17	2.701	4	0.9	4	4	1	43.62	2.075	4	0.1
0	4	1	19.59	4.531	4	7.0	1	7	1	33.63	2.665	4	0.9	3	7	1	43.65	2.073	4	0.4
-2	0	1	19.66	4.516	2	11.1	2	6	1	34.12	2.628	4	2.4	-3	1	4	44.24	2.047	4	0.3
-1	1	2	19.91	4.459	4	12.7	-3	3	2	34.32	2.613	4	0.6	-1	9	2	44.51	2.035	4	0.5
0	2	2	20.15	4.407	4	8.0	2	0	3	35.04	2.561	2	0.7	-3	7	2	44.58	2.033	4	0.2
2	2	0	20.45	4.344	4	6.1	3	1	2	35.54	2.526	4	1.0	4	2	2	44.85	2.021	4	0.8
-2	2	1	21.51	4.131	4	1.3	3	5	0	35.63	2.520	4	0.4	1	5	4	45.16	2.008	4	0.1
2	0	1	21.55	4.123	2	0.3	-1	5	3	35.64	2.519	4	1.7	-4	2	3	45.18	2.007	4	0.4
2	2	1	23.26	3.824	4	9.1	-2	4	3	36.08	2.490	4	0.2	-4	6	1	46.34	1.959	4	0.3
-1	3	2	23.44	3.796	4	3.1	-2	6	2	36.11	2.488	4	0.5	0	0	5	46.49	1.953	2	0.2
-2	0	2	24.47	3.637	2	0.6	2	2	3	36.16	2.484	4	0.1	-1	1	5	46.59	1.949	4	0.6
-1	5	1	24.97	3.567	4	0.1	0	8	1	36.31	2.474	4	0.1	2	4	4	47.13	1.928	4	0.3
1	3	2	25.06	3.554	4	3.8	-1	7	2	36.49	2.462	4	0.2	-5	1	1	47.43	1.917	4	1.2
0	4	2	25.21	3.532	4	12.5	-1	1	4	37.20	2.417	4	1.2	5	1	0	47.59	1.911	4	0.1
2	4	0	25.45	3.499	4	5.4	1	5	3	37.32	2.409	4	0.8	-2	8	3	47.78	1.903	4	0.2
1	5	1	25.74	3.461	4	12.5	-3	1	3	37.35	2.408	4	0.1	-4	4	3	47.87	1.900	4	0.5
-2	2	2	26.00	3.427	4	5.8	4	0	0	37.49	2.399	2	0.3	-2	6	4	47.93	1.898	4	0.2
0	6	0	26.13	3.410	2	0.2	-4	0	1	37.57	2.394	2	1.3	4	6	1	48.15	1.890	4	1.8
-2	4	1	26.33	3.385	4	0.3	1	7	2	37.60	2.392	4	1.3	0	10	2	48.22	1.887	4	0.1
0	0	3	27.40	3.255	2	0.9	3	5	1	37.66	2.388	4	0.4	-1	3	5	48.35	1.882	4	1.0
2	0	2	27.52	3.242	2	0.9	3	3	2	37.72	2.385	4	0.2	2	10	0	48.36	1.882	4	0.2
0	6	1	27.71	3.220	4	1.2	0	2	4	37.88	2.375	4	0.2	-3	7	3	48.80	1.866	4	0.2
3	1	0	28.24	3.160	4	3.7	0	6	3	38.22	2.355	4	0.8	1	1	5	48.84	1.865	4	0.2
-1	1	3	28.26	3.158	4	2.7	2	6	2	38.31	2.349	4	0.4	-2	10	1	48.87	1.864	4	0.2
-3	1	1	28.69	3.112	4	0.5	4	2	0	38.55	2.335	4	0.1	-2	2	5	49.12	1.855	4	0.5
0	2	3	28.78	3.102	4	1.7	-1	3	4	39.31	2.292	4	0.2	3	9	0	49.17	1.853	4	0.7
-2	4	2	30.15	2.964	4	3.0	-3	3	3	39.44	2.285	4	0.4	-5	3	1	49.17	1.853	4	0.3
1	1	3	30.30	2.950	4	0.3	4	0	1	39.70	2.270	2	0.2	-1	9	3	49.18	1.853	4	0.1
1	5	2	30.63	2.918	4	1.0	0	8	2	39.78	2.266	4	0.1	-5	1	2	49.18	1.852	4	0.1
3	1	1	30.71	2.912	4	2.4	-4	0	2	39.93	2.258	2	0.3	5	3	0	49.33	1.847	4	0.1
3	3	0	30.88	2.896	4	7.5	2	8	0	39.94	2.257	4	0.2	-3	5	4	49.58	1.838	4	0.5
-1	3	3	30.90	2.894	4	0.4	0	4	4	40.96	2.203	4	0.4	1	11	0	49.94	1.826	4	0.8
-3	3	1	31.29	2.858	4	0.2	1	3	4	41.36	2.183	4	0.1							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RUT RUB-10, SiO_2 Framework

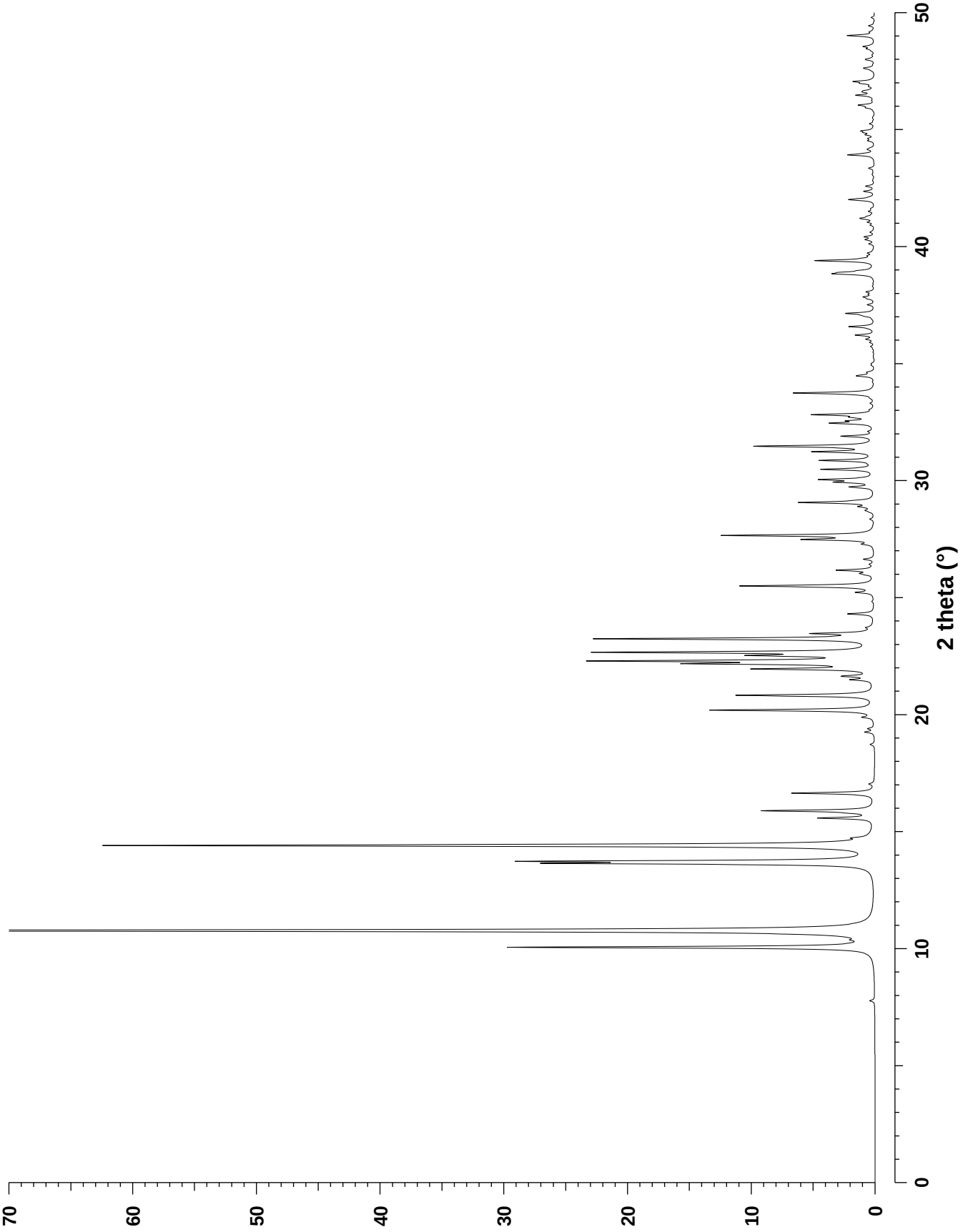
CHEMICAL COMPOSITION: $[Si_{32}B_4O_{72}]$

REFINED COMPOSITION: $[Si_{36}O_{72}]$

CRYSTAL DATA: $P1\,2_1/a\,1$ (No. 14) unique axis **b**, cell choice 3
$a = 13.112$ Å $b = 12.903$ Å $c = 12.407$ Å
$\alpha = 90°$ $\beta = 113.50°$ $\gamma = 90°$
DLS refinement.

REFERENCE: H. Gies and J. Rius,
Z. Kristallogr. **210** 475–480 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	1	7.77	11.378	2	0.4	2	2	2	29.06	3.073	4	6.0	0	0	5	39.60	2.276	2	0.3
1	1	0	10.06	8.797	4	29.4	-3	3	1	29.15	3.064	4	0.8	4	1	2	39.72	2.269	4	0.5
0	1	1	10.37	8.534	4	0.6	4	0	0	29.72	3.006	2	1.9	2	0	4	40.11	2.248	2	0.4
-1	1	1	10.77	8.215	4	100.0	-3	3	2	29.93	2.985	4	2.8	-5	3	2	40.29	2.238	4	0.3
-2	0	1	13.64	6.491	2	22.7	-1	3	3	30.04	2.975	4	3.8	1	5	2	40.30	2.238	4	0.4
0	2	0	13.73	6.451	2	25.1	-1	1	4	30.07	2.972	4	0.6	-2	4	4	40.41	2.232	4	0.8
1	1	1	14.41	6.146	4	62.3	3	3	0	30.48	2.932	4	4.0	-3	5	1	40.61	2.221	4	0.3
2	0	0	14.73	6.012	2	0.9	-4	2	1	30.86	2.898	4	4.3	-5	3	1	40.91	2.206	4	0.3
0	0	2	15.58	5.689	2	4.3	-3	1	4	31.23	2.864	4	4.7	4	4	0	41.04	2.199	4	0.5
0	2	1	15.79	5.612	4	0.9	0	0	4	31.45	2.844	2	4.5	3	2	3	41.19	2.191	4	0.3
-1	1	2	15.89	5.576	4	9.0	2	4	0	31.47	2.842	4	5.7	-3	5	2	41.20	2.191	4	0.8
-2	0	2	16.64	5.326	2	6.7	0	4	2	31.89	2.806	4	2.6	-5	3	3	41.28	2.187	4	0.4
0	1	2	17.03	5.205	4	0.4	-2	2	4	32.10	2.788	4	0.4	-4	2	5	41.50	2.176	4	0.4
1	2	1	18.72	4.741	4	0.4	-1	2	4	32.43	2.761	4	0.3	5	1	1	41.97	2.153	4	0.3
2	0	1	19.25	4.610	2	0.8	-2	4	2	32.45	2.759	4	3.1	0	6	0	42.01	2.151	2	1.8
-2	2	1	19.40	4.576	4	0.5	2	0	3	32.55	2.751	2	1.7	0	4	4	42.36	2.133	4	0.7
-1	2	2	19.89	4.464	4	0.8	-3	3	3	32.70	2.738	4	1.3	-6	0	1	42.57	2.124	2	0.5
2	2	0	20.19	4.398	4	13.3	-4	2	3	32.81	2.729	4	4.9	-3	5	3	43.34	2.088	4	0.5
0	2	2	20.82	4.267	4	11.1	2	1	3	33.30	2.690	4	0.3	1	1	5	43.91	2.062	4	2.0
-3	1	1	21.49	4.135	4	1.7	-4	0	4	33.65	2.663	2	0.3	-2	0	6	43.97	2.059	2	0.5
-2	2	2	21.64	4.107	4	2.2	3	3	1	33.72	2.658	4	0.8	-6	2	3	44.14	2.051	4	0.3
1	3	0	21.95	4.050	4	9.2	4	0	1	33.74	2.657	2	5.9	-3	1	6	44.52	2.035	4	0.4
-2	0	3	22.17	4.009	2	13.0	0	2	4	34.46	2.603	4	1.1	-1	6	2	44.61	2.031	4	0.3
-1	3	1	22.29	3.988	4	21.4	1	3	3	34.50	2.600	4	0.6	1	5	3	44.77	2.024	4	0.6
-3	1	2	22.52	3.947	4	8.0	-4	3	2	34.62	2.591	4	0.3	-4	5	2	44.87	2.020	4	0.6
-1	1	3	22.66	3.924	4	21.9	3	2	2	35.00	2.564	4	0.2	-6	2	1	44.94	2.017	4	0.9
3	1	0	23.24	3.828	4	22.4	1	1	4	35.90	2.501	4	0.3	6	0	0	45.25	2.004	2	0.2
0	0	3	23.46	3.793	2	4.5	-5	1	3	36.04	2.492	4	0.6	-1	1	6	45.92	1.976	4	0.5
2	2	1	23.72	3.751	4	0.4	-2	0	5	36.21	2.481	2	1.5	-6	2	4	45.98	1.974	4	0.2
1	3	1	24.30	3.663	4	2.1	0	4	3	36.57	2.457	4	1.8	-1	5	4	46.04	1.971	4	1.2
-1	3	2	25.22	3.531	4	1.3	4	2	1	36.58	2.456	4	0.2	3	1	4	46.46	1.954	4	1.5
2	0	2	25.49	3.495	2	10.7	-5	2	2	37.01	2.429	4	0.4	2	6	1	46.60	1.949	4	0.7
-3	2	2	25.54	3.488	4	0.5	-3	3	4	37.06	2.426	4	0.5	5	3	1	46.65	1.947	4	0.5
0	3	2	25.97	3.431	4	0.4	1	5	1	37.14	2.421	4	2.2	1	6	2	46.83	1.940	4	0.3
-3	1	3	26.03	3.424	4	0.8	-3	1	5	37.51	2.398	4	0.4	-6	0	5	46.97	1.934	2	0.8
-2	2	3	26.17	3.405	4	2.8	-1	5	2	37.77	2.382	4	0.4	5	1	2	47.05	1.931	4	1.6
2	1	2	26.42	3.373	4	0.3	-1	1	5	37.84	2.378	4	0.8	4	2	3	47.61	1.910	4	0.5
-2	3	2	26.64	3.346	4	0.9	2	4	2	37.96	2.370	4	0.3	-5	3	5	47.63	1.909	4	0.2
0	2	3	27.28	3.270	4	0.7	5	1	0	38.06	2.364	4	0.5	3	5	2	47.99	1.896	4	0.5
-4	0	2	27.48	3.246	2	4.6	-5	1	4	38.83	2.319	4	2.7	1	3	5	48.44	1.879	4	0.5
-4	0	1	27.50	3.243	2	0.9	-2	2	5	38.89	2.316	4	2.0	4	4	2	48.54	1.875	4	0.8
0	4	0	27.65	3.226	2	12.1	-4	0	5	38.97	2.311	2	0.8	-3	3	6	49.01	1.859	4	2.1
-4	1	2	28.35	3.148	4	0.3	-4	4	2	39.38	2.288	4	0.9	-6	2	5	49.17	1.853	4	0.3
1	3	2	28.72	3.108	4	0.5	-4	4	1	39.40	2.287	4	4.0	-7	1	2	49.43	1.844	4	0.4
-2	0	4	28.88	3.092	2	1.0	-3	2	5	39.48	2.282	4	0.3	2	6	2	49.78	1.832	4	0.3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STA-1, Magnesium Aluminophosphate

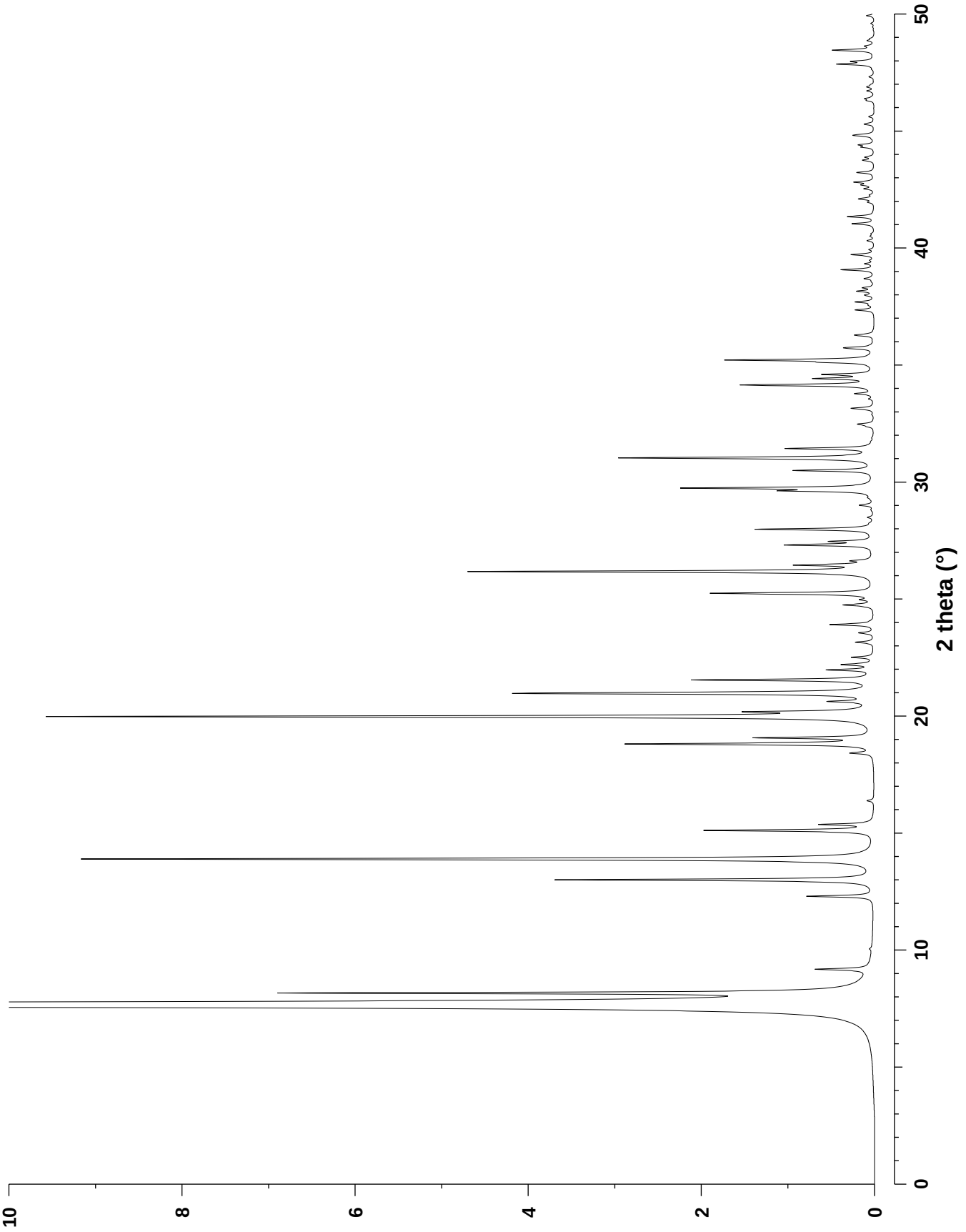
CHEMICAL COMPOSITION: $|((CH_2)_7(C_7H_{13}N)_2)_{2.74}(H_2O)_{6.16}|\ [Mg_{5.04}Al_{22.96}P_{28}O_{112}]$
$((CH_2)_7(C_7H_{13}N)_2)^+$ = diquinuclidinium template

REFINED COMPOSITION: $[P_{28}Al_{28}O_{112}]$

CRYSTAL DATA: $P\bar{4}n2$ (No. 118)
$a = 13.620$ Å $b = 13.620$ Å $c = 21.649$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.059$, $R_w = 0.076$; At $T = 200$K.

REFERENCE: G. W. Noble, P. A. Wright, P. Lightfoot, R. E. Morris, K. J. Hudson, Å. Kvick and H. Graafsma, *Angew. Chem., Int. ed.* **36** 81–83 (1997).

h	k	l	2θ	d	M	I_{rel}
1	0	1	7.67	11.528	8	100.0
0	0	2	8.17	10.825	2	6.3
1	1	0	9.18	9.631	4	0.6
1	1	2	12.30	7.195	8	0.8
2	0	0	13.00	6.810	4	3.7
1	0	3	13.89	6.377	8	9.2
2	1	1	15.11	5.863	16	1.9
2	0	2	15.37	5.764	8	0.6
2	2	0	18.42	4.815	4	0.2
1	1	4	18.81	4.718	8	2.8
2	1	3	19.07	4.655	16	1.3
3	0	1	19.98	4.443	8	9.5
2	2	2	20.18	4.400	8	1.1
3	1	0	20.62	4.307	8	0.4
2	0	4	20.97	4.237	8	4.0
3	1	1	21.03	4.224	16	0.5
1	0	5	21.54	4.126	8	2.1
2	1	4	21.97	4.046	16	0.5
2	2	3	22.19	4.005	8	0.2
3	1	2	22.21	4.002	16	0.2
1	1	5	22.51	3.949	8	0.2
3	0	3	23.15	3.843	8	0.2
3	2	0	23.55	3.778	8	0.2
3	2	1	23.91	3.721	16	0.5
2	2	4	24.75	3.598	8	0.3
3	2	2	24.97	3.567	16	0.1
2	1	5	25.24	3.529	16	1.9
4	0	0	26.17	3.405	4	4.7
3	1	4	26.45	3.370	16	0.8
3	2	3	26.63	3.347	16	0.2
4	1	1	27.31	3.266	16	1.0
4	0	2	27.46	3.248	8	0.5
2	0	6	27.98	3.188	8	1.4
3	3	2	29.01	3.078	8	0.2
1	0	7	29.62	3.016	8	0.9
4	1	3	29.74	3.004	16	2.1
4	2	2	30.49	2.932	16	0.9
4	0	4	31.03	2.882	8	2.9
3	2	5	31.43	2.846	16	1.0
2	1	7	32.47	2.758	16	0.2
4	3	1	33.15	2.703	16	0.2
4	2	4	33.77	2.654	16	0.2
4	1	5	34.14	2.626	16	1.5
1	1	8	34.42	2.605	8	0.6
5	1	2	34.59	2.593	16	0.6
3	0	7	35.11	2.556	8	0.4
4	3	3	35.21	2.548	16	0.2
5	0	3	35.21	2.548	8	1.4
2	0	8	35.70	2.515	8	0.1
5	2	1	35.74	2.512	16	0.3
4	0	6	36.27	2.476	8	0.2
4	4	0	37.35	2.408	4	0.2
5	2	3	37.69	2.387	16	0.2
2	2	8	38.15	2.359	8	0.2
4	4	2	38.30	2.350	8	0.1
4	2	6	38.69	2.327	16	0.1
5	0	5	39.07	2.306	8	0.2
4	3	5	39.07	2.306	16	0.2
6	0	0	39.71	2.270	4	0.3
4	4	4	41.03	2.200	8	0.3
5	2	5	41.34	2.184	16	0.3
5	1	6	42.09	2.147	16	0.1
3	0	9	42.53	2.126	8	0.1
1	1	10	42.81	2.112	8	0.2
6	0	4	43.22	2.093	8	0.2
3	3	8	43.75	2.069	8	0.1
5	0	7	44.31	2.044	8	0.1
5	4	3	44.40	2.040	16	0.2
4	2	8	44.80	2.023	16	0.2
4	4	6	45.28	2.003	8	0.1
5	1	8	47.85	1.901	16	0.4
7	1	2	47.97	1.896	16	0.2
7	0	3	48.45	1.879	8	0.5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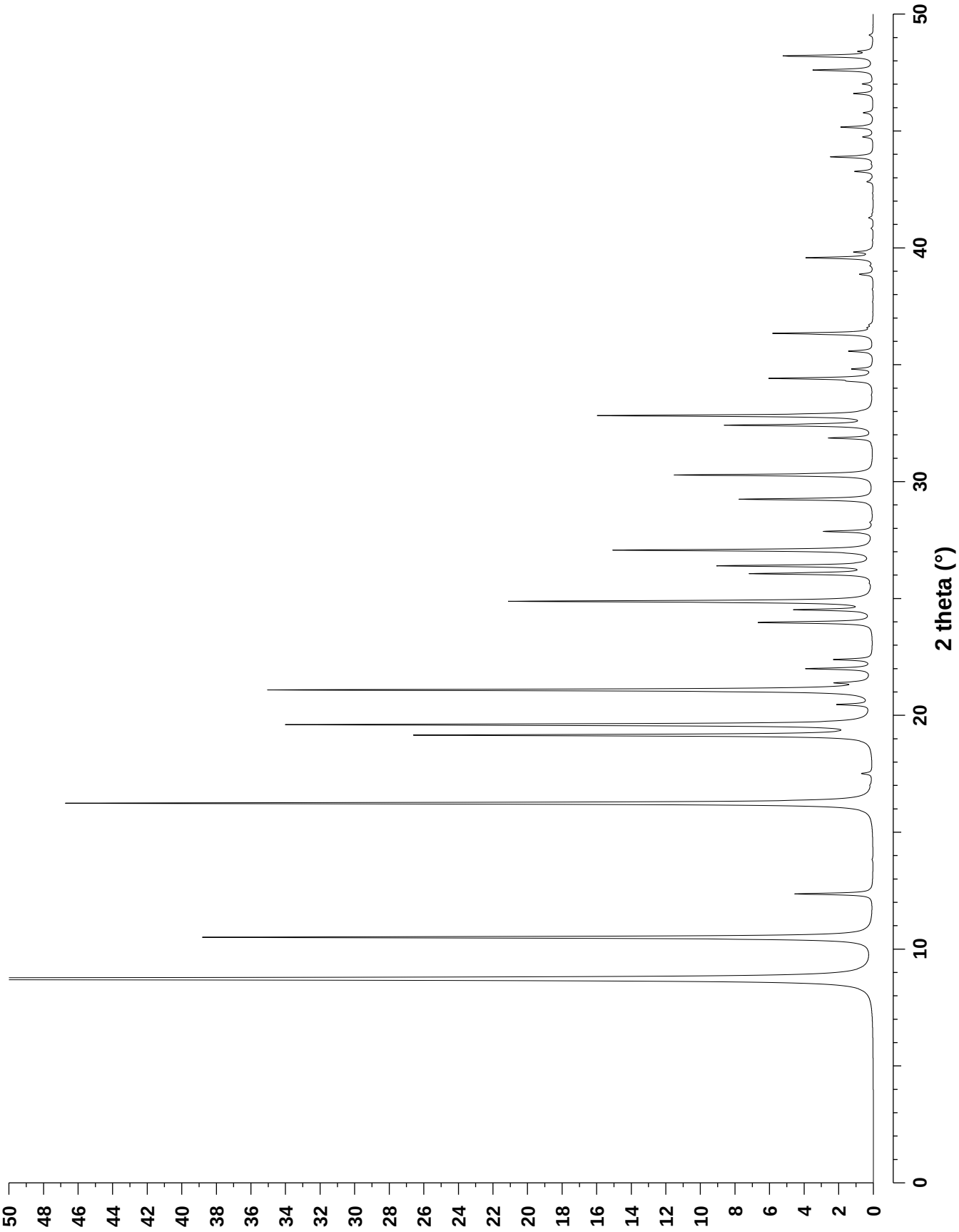
CHEMICAL COMPOSITION: $|(C_{14}H_{34}N_4)^{2+}_{1.5}(H_2O)_{2.5}|\ [Mg_3Al_{13}P_{16}O_{64}]$
$C_{14}H_{32}N_4$ = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane

REFINED COMPOSITION: $|C_{19.44}N_{5.04}|\ [Mg_{2.4}Al_{13.6}P_{16}O_{64}]$

CRYSTAL DATA: $P\,4/m\,nc$ (No. 128)
$a = 14.322$ Å $b = 14.322$ Å $c = 10.424$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray synchrotron single crystal refinement, $R_F = 0.094$, $wR_2 = 0.313$

REFERENCE: V. Patinec, P. A. Wright, P. Lightfoot, R. A. Aitken and P. A. Cox, *J. Chem. Soc., Dalton Trans.* **22** 3909–3911 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.73	10.127	4	100.0	3	2	2	28.25	3.159	16	0.1	5	0	3	40.83	2.210	8	0.1
1	0	1	10.50	8.428	8	38.8	2	1	3	29.24	3.054	16	7.7	5	4	1	41.28	2.187	16	0.3
2	0	0	12.36	7.161	4	4.5	4	0	2	30.28	2.951	8	11.5	5	2	3	42.82	2.112	16	0.4
2	1	1	16.24	5.457	16	46.7	5	1	0	31.86	2.809	8	2.5	4	0	4	42.92	2.107	8	0.1
2	2	0	17.51	5.064	4	0.6	4	3	1	32.41	2.762	16	2.4	6	3	1	43.26	2.092	16	1.1
1	1	2	19.15	4.634	8	26.3	5	0	1	32.41	2.762	8	6.1	1	0	5	43.88	2.063	8	0.6
3	1	0	19.60	4.529	8	33.8	3	1	3	32.48	2.757	16	0.2	3	3	4	43.89	2.063	8	1.9
3	0	1	20.46	4.340	8	1.9	4	2	2	32.82	2.729	16	15.9	7	1	0	44.74	2.025	8	0.5
2	0	2	21.08	4.214	8	35.0	5	1	1	33.03	2.712	16	0.1	7	0	1	45.16	2.008	8	1.9
3	1	1	21.39	4.154	16	1.7	3	2	3	34.29	2.615	16	0.9	2	1	5	45.77	1.982	16	0.6
2	1	2	21.99	4.043	16	3.8	0	0	4	34.41	2.606	2	5.9	6	1	3	46.59	1.949	16	1.1
3	2	0	22.38	3.972	8	2.2	5	2	1	34.81	2.577	16	1.2	7	2	1	47.00	1.933	16	0.6
3	2	1	23.97	3.712	16	6.6	1	1	4	35.57	2.524	8	1.4	3	0	5	47.59	1.911	8	0.9
2	2	2	24.51	3.632	8	4.3	5	1	2	36.33	2.473	16	5.8	5	1	4	47.60	1.910	16	2.7
4	0	0	24.87	3.580	4	21.0	4	1	3	36.58	2.457	16	0.1	5	5	2	48.20	1.888	8	3.3
3	1	2	26.06	3.419	16	7.0	2	0	4	36.70	2.449	8	0.2	7	1	2	48.20	1.888	16	1.8
1	0	3	26.39	3.377	8	5.6	2	2	4	38.86	2.317	8	0.8	5	4	3	48.40	1.881	16	0.6
3	3	0	26.40	3.376	4	3.5	6	1	1	39.23	2.297	16	0.1	7	3	0	48.40	1.881	8	0.1
4	1	1	27.06	3.295	16	15.0	4	4	2	39.57	2.277	8	3.9	6	4	2	49.09	1.856	16	0.2
4	2	0	27.86	3.202	8	2.8	6	2	0	39.81	2.265	8	1.0							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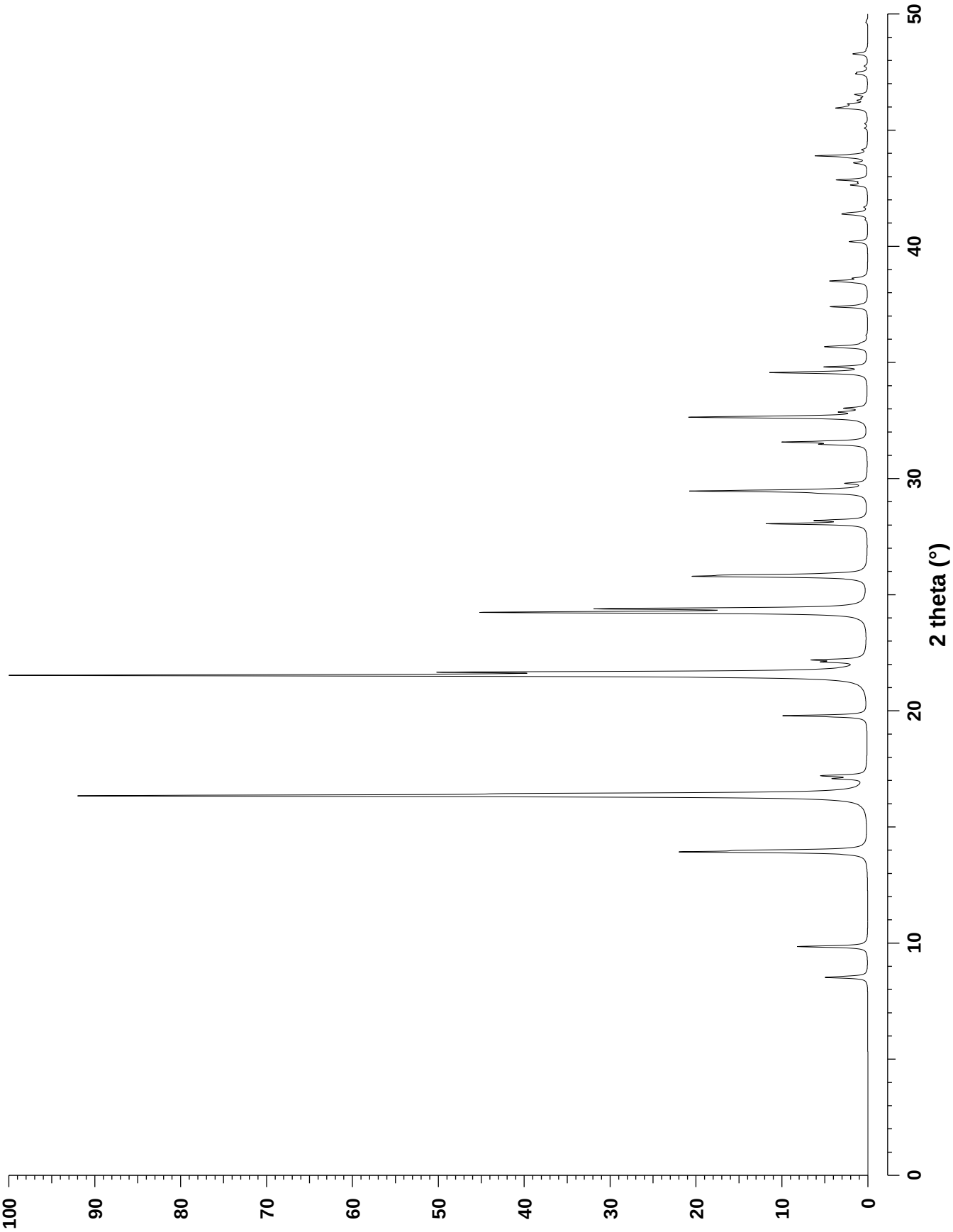
CHEMICAL COMPOSITION: $|((CH_2)_4(C_7H_{13}N)_2)_3(H_2O)_{22.5}|\ [Mg_{5.4}Al_{30.6}P_{36}O_{144}]$
$((CH_2)_4(C_7H_{13}N)_2)^+$ = diquinuclidinium template

REFINED COMPOSITION: $|(C_{22}H_{50}N_2)_3|\ [Al_{36}P_{36}O_{144}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 12.726$ Å $b = 12.726$ Å $c = 30.939$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement at 200 K. $R_F = 0.0757$

REFERENCE: G. W. Noble, P. A. Wright and Å. Kvick,
J. Chem. Soc., Dalton Trans. 4485–4490 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	8.52	10.382	6	5.4	1	2	8	31.57	2.834	6	7.0	2	3	8	42.73	2.116	6	0.5
0	0	3	8.57	10.313	2	1.2	3	-2	8	31.57	2.834	6	4.0	0	3	12	42.85	2.110	6	2.3
0	1	2	9.85	8.976	6	9.7	4	0	1	32.63	2.744	6	21.2	3	0	12	42.85	2.110	6	1.9
1	1	0	13.92	6.363	6	22.8	3	1	5	32.67	2.741	6	1.7	6	-3	3	43.56	2.078	6	0.4
1	0	4	13.99	6.331	6	12.4	4	-1	5	32.67	2.741	6	4.6	3	3	3	43.56	2.078	6	0.4
0	2	1	16.34	5.425	6	100.0	0	1	11	32.86	2.725	6	3.0	5	0	5	43.59	2.076	6	1.2
2	-1	3	16.37	5.415	6	2.2	0	4	2	33.02	2.713	6	2.8	4	-1	11	43.74	2.070	6	0.1
1	1	3	16.37	5.415	6	2.4	2	2	6	33.08	2.708	6	0.1	2	1	13	43.81	2.066	6	1.3
0	1	5	16.43	5.396	6	31.9	4	0	4	34.56	2.596	6	13.3	3	-1	13	43.81	2.066	6	0.3
2	0	2	17.08	5.191	6	3.9	0	0	12	34.80	2.578	2	5.7	0	0	15	43.89	2.063	2	6.8
0	0	6	17.20	5.156	2	5.8	5	-2	1	35.63	2.520	6	1.6	2	0	14	44.15	2.051	6	0.7
0	2	4	19.78	4.488	6	11.5	0	4	5	35.67	2.517	6	4.4	6	-4	4	45.08	2.011	6	0.1
2	1	1	21.52	4.128	6	75.3	4	-3	7	35.71	2.514	6	0.3	2	4	4	45.08	2.011	6	0.3
3	-1	1	21.52	4.128	6	35.7	1	3	7	35.71	2.514	6	1.0	2	2	12	45.27	2.003	6	0.4
2	0	5	21.59	4.115	6	12.1	0	3	9	35.77	2.510	6	0.2	6	-1	1	45.94	1.975	6	1.6
1	0	7	21.66	4.102	6	47.6	2	0	11	35.84	2.505	6	0.5	5	1	1	45.94	1.975	6	2.0
3	-2	2	22.10	4.022	6	4.5	3	-1	10	36.16	2.484	6	0.1	4	2	5	45.98	1.974	6	0.4
2	-1	6	22.19	4.006	6	6.2	1	4	0	37.39	2.405	6	3.2	6	-2	5	45.98	1.974	6	0.2
0	3	0	24.23	3.674	6	44.5	4	1	0	37.39	2.405	6	1.4	0	5	7	46.01	1.973	6	1.2
2	1	4	24.27	3.668	6	8.0	3	2	4	37.42	2.403	6	0.2	5	-1	9	46.06	1.971	6	0.7
3	-1	4	24.27	3.668	6	5.2	5	-2	4	37.42	2.403	6	0.5	4	1	9	46.06	1.971	6	0.2
0	1	8	24.39	3.649	6	33.6	4	-1	8	37.50	2.398	6	0.3	1	4	9	46.06	1.971	6	0.1
3	0	3	25.74	3.461	6	0.8	2	3	5	38.46	2.341	6	0.4	0	4	11	46.12	1.968	6	2.1
3	-2	5	25.78	3.456	6	2.1	5	-3	5	38.46	2.341	6	1.4	1	1	15	46.27	1.962	6	0.6
1	2	5	25.78	3.456	6	17.3	4	0	7	38.50	2.338	6	4.1	2	-1	15	46.27	1.962	6	0.2
0	2	7	25.84	3.448	6	13.4	3	-2	11	38.62	2.331	6	0.7	6	-3	6	46.28	1.962	6	0.3
0	0	9	25.92	3.438	2	1.5	1	2	11	38.62	2.331	6	0.9	5	-2	10	46.38	1.958	6	0.2
2	2	0	28.05	3.181	6	13.4	1	0	13	38.71	2.326	6	0.1	3	2	10	46.38	1.958	6	0.4
2	0	8	28.19	3.166	6	6.3	0	4	8	40.19	2.244	6	2.6	1	2	14	46.52	1.952	6	0.8
4	-3	1	29.36	3.042	6	0.3	3	2	7	41.13	2.195	6	0.2	3	-2	14	46.52	1.952	6	0.9
1	3	1	29.36	3.042	6	3.0	0	2	13	41.32	2.185	6	0.3	6	-1	4	47.41	1.918	6	0.4
4	-2	3	29.38	3.040	6	0.2	5	0	2	41.38	2.182	6	2.8	5	1	4	47.41	1.918	6	0.9
3	-1	7	29.46	3.031	6	12.1	1	4	6	41.43	2.180	6	0.5	5	0	8	47.48	1.915	6	1.2
2	1	7	29.46	3.031	6	11.4	4	1	6	41.43	2.180	6	0.2	1	0	16	47.75	1.905	6	0.4
2	-1	9	29.53	3.024	6	0.3	5	-4	6	41.43	2.180	6	0.5	1	5	5	48.27	1.885	6	1.6
1	1	9	29.53	3.024	6	1.4	5	-1	6	41.43	2.180	6	0.3	6	-5	5	48.27	1.885	6	0.3
3	1	2	29.79	2.999	6	0.1	0	1	14	41.68	2.167	6	0.5	2	4	7	48.31	1.884	6	0.2
4	-1	2	29.79	2.999	6	2.6	3	3	0	42.63	2.121	6	2.0	1	3	13	48.48	1.878	6	0.2
4	-3	4	31.47	2.843	6	1.4	0	5	4	42.65	2.120	6	0.2	0	6	0	49.63	1.837	6	0.3
1	3	4	31.47	2.843	6	3.8	5	-3	8	42.73	2.116	6	0.1	6	-2	8	49.72	1.834	6	0.1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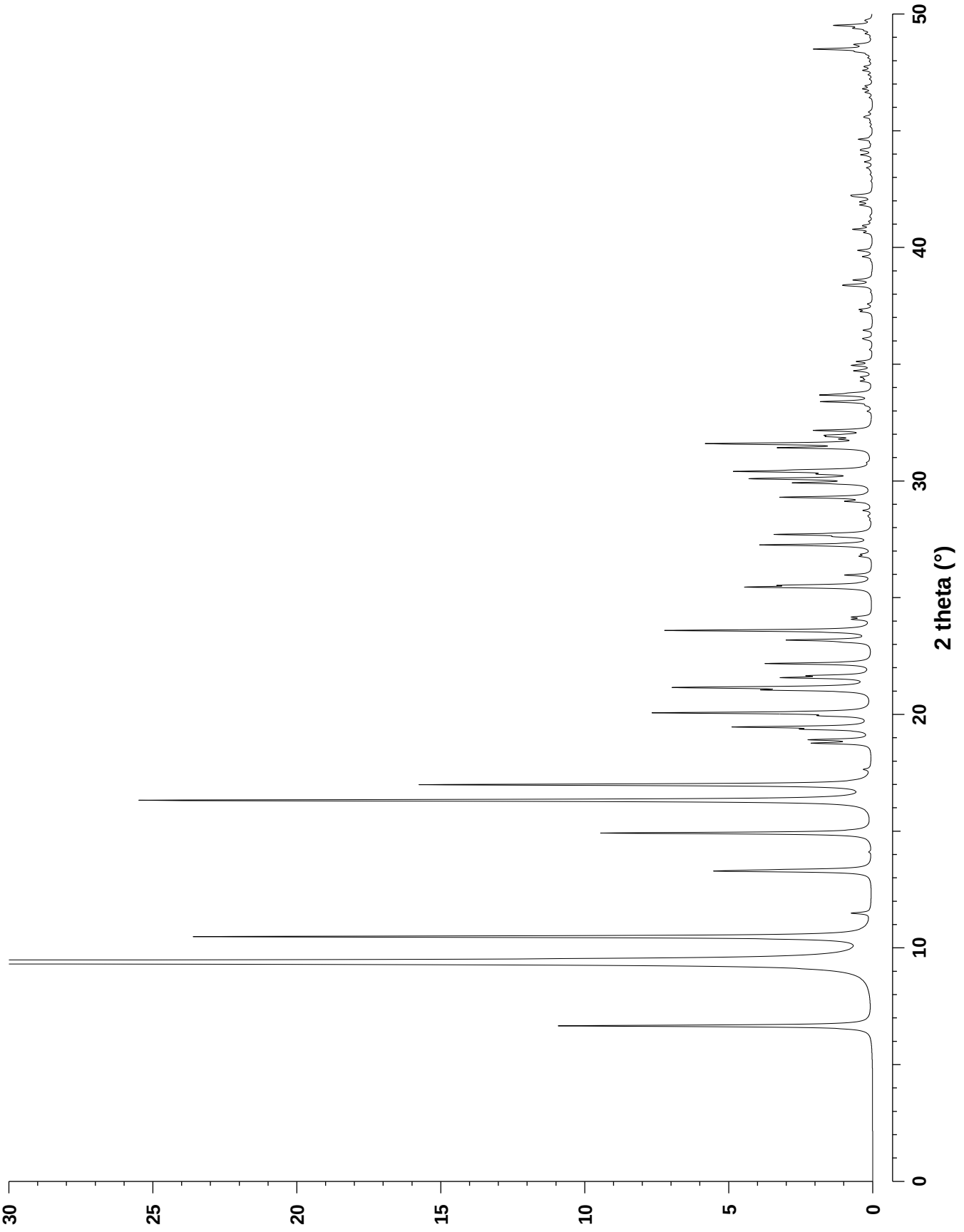
CHEMICAL COMPOSITION: $|(C_{18}H_{42}N_6)_{1.96}(H_2O)_7|$ $[Mg_{4.8}Al_{19.2}P_{24}O_{96}]$
$C_{18}H_{42}N_6$=1,4,7,10,13,16-hexamethyl-1,4,7,10,13,16-hexaazacyclooctadecane

REFINED COMPOSITION: $[Mg_{4.8}Al_{19.2}P_{24}O_{96}]$

CRYSTAL DATA: $P\,4/n$ (No. 85) origin at centre $\overline{1}$
$a = 18.7732$ Å $b = 18.7732$ Å $c = 9.4537$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray synchrotron single crystal refinement, $R_p = 0.0539$, $wR_{wp} = 0.1422$

REFERENCE: P. A. Wright, M. J. Maple, A. M. Z. Slawin, V. Patinec, R. A. Aitken, S. Welsh and P. A. Cox, *J. Chem. Soc., Dalton Trans.* 1243–1248 (2000).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	6.66	13.275	4	11.9	3	3	2	27.61	3.230	8	1.0	3	6	2	37.34	2.408	8	0.2
0	0	1	9.35	9.454	2	38.2	3	5	0	27.71	3.220	4	1.8	8	0	0	38.36	2.347	4	0.6
2	0	0	9.42	9.387	4	100.0	5	3	0	27.71	3.220	4	1.8	1	0	4	38.39	2.345	8	0.7
1	0	1	10.48	8.444	8	25.6	1	0	3	28.73	3.108	8	0.3	7	0	2	38.60	2.333	8	0.7
1	1	1	11.49	7.701	8	0.7	1	1	3	29.12	3.066	8	0.9	1	2	4	39.61	2.275	8	0.2
2	0	1	13.29	6.661	8	5.0	3	5	1	29.30	3.048	8	1.9	8	1	1	39.87	2.261	8	0.3
2	2	0	13.34	6.637	4	2.6	5	3	1	29.30	3.048	8	1.5	1	8	1	39.87	2.261	8	0.2
1	3	0	14.92	5.937	4	5.8	2	0	3	29.91	2.987	8	2.8	6	0	3	40.63	2.220	8	0.3
3	1	0	14.92	5.937	4	4.5	6	0	1	30.08	2.970	8	2.8	2	8	1	40.77	2.213	8	0.2
2	2	1	16.32	5.432	8	27.8	2	6	0	30.11	2.968	4	0.9	8	2	1	40.77	2.213	8	0.2
3	0	1	16.99	5.218	8	17.1	6	2	0	30.11	2.968	4	1.3	6	6	0	40.78	2.212	4	0.3
1	3	1	17.64	5.028	8	0.2	2	1	3	30.29	2.950	8	0.4	1	6	3	40.93	2.205	8	0.2
0	0	2	18.77	4.727	2	2.1	1	2	3	30.29	2.950	8	0.9	6	2	3	41.81	2.161	8	0.2
4	0	0	18.91	4.693	4	2.2	5	0	2	30.40	2.940	8	2.8	2	6	3	41.81	2.161	8	0.3
1	0	2	19.36	4.584	8	2.0	4	3	2	30.40	2.940	8	0.9	6	6	1	41.94	2.154	8	0.3
2	3	1	19.46	4.561	8	2.3	3	4	2	30.40	2.940	8	0.8	6	5	2	42.18	2.143	8	0.2
3	2	1	19.46	4.561	8	2.7	6	1	1	30.47	2.934	8	0.6	5	6	2	42.18	2.143	8	0.3
1	1	2	19.94	4.453	8	1.3	1	6	1	30.47	2.934	8	1.2	3	8	1	42.23	2.140	8	0.2
3	3	0	20.07	4.425	4	8.2	2	2	3	31.42	2.847	8	3.3	8	3	1	42.23	2.140	8	0.4
2	0	2	21.04	4.222	8	3.2	2	6	1	31.59	2.832	8	2.8	3	3	4	43.41	2.085	8	0.2
4	0	1	21.13	4.204	8	2.8	6	2	1	31.59	2.832	8	3.3	2	4	4	43.96	2.059	8	0.2
4	2	0	21.16	4.198	4	0.6	3	0	3	31.79	2.815	8	0.8	4	2	4	43.96	2.059	8	0.3
2	4	0	21.16	4.198	4	4.7	5	2	2	31.90	2.806	8	0.3	2	8	2	44.15	2.051	8	0.2
1	2	2	21.57	4.119	8	3.1	2	5	2	31.90	2.806	8	0.9	4	8	1	44.20	2.049	8	0.2
1	4	1	21.66	4.102	8	1.5	4	5	1	31.96	2.800	8	0.4	5	5	3	44.63	2.030	8	0.2
4	1	1	21.66	4.102	8	0.4	5	4	1	31.96	2.800	8	0.9	7	1	3	44.63	2.030	8	0.2
3	3	1	22.18	4.008	8	4.0	1	3	3	32.16	2.783	8	1.1	1	7	3	44.63	2.030	8	0.2
2	2	2	23.10	3.850	8	0.6	3	1	3	32.16	2.783	8	1.0	3	7	3	46.79	1.942	8	0.2
2	4	1	23.18	3.837	8	2.7	4	4	2	32.98	2.716	8	0.2	6	5	3	47.58	1.911	8	0.2
4	2	1	23.18	3.837	8	0.4	6	3	1	33.39	2.683	8	1.1	5	6	3	47.58	1.911	8	0.2
3	0	2	23.59	3.772	8	7.9	3	6	1	33.39	2.683	8	0.8	3	5	4	47.74	1.905	8	0.2
3	1	2	24.07	3.698	8	0.5	3	5	2	33.68	2.661	8	0.9	1	0	5	48.38	1.881	8	0.3
1	5	0	24.17	3.682	4	0.4	5	3	2	33.68	2.661	8	0.9	10	0	0	48.49	1.877	4	1.6
5	1	0	24.17	3.682	4	0.3	5	5	0	33.76	2.655	4	0.5	6	8	0	48.49	1.877	4	0.2
2	3	2	25.45	3.500	8	1.8	4	0	3	34.27	2.616	8	0.4	1	6	4	48.51	1.876	8	0.4
3	2	2	25.45	3.500	8	2.5	6	0	2	34.37	2.609	8	0.2	1	1	5	48.64	1.872	8	0.2
3	4	1	25.53	3.490	8	0.3	4	6	0	34.45	2.603	4	0.3	6	7	2	48.69	1.870	8	0.2
4	3	1	25.53	3.490	8	0.6	1	6	2	34.71	2.584	8	0.2	7	6	2	48.69	1.870	8	0.2
5	0	1	25.53	3.490	8	1.8	6	1	2	34.71	2.584	8	0.4	2	0	5	49.15	1.854	8	0.2
5	1	1	25.97	3.431	8	0.4	3	3	3	34.95	2.567	8	0.8	2	8	3	49.38	1.845	8	0.3
1	5	1	25.97	3.431	8	0.6	5	5	1	35.11	2.556	8	0.3	8	6	1	49.50	1.841	8	0.2
4	0	2	26.77	3.330	8	0.4	7	2	1	36.10	2.488	8	0.2	6	8	1	49.50	1.841	8	0.4
4	4	0	26.86	3.319	4	0.3	3	7	0	36.45	2.465	4	0.3	10	0	1	49.50	1.841	8	0.4
2	5	1	27.26	3.271	8	2.2	5	0	3	37.25	2.414	8	0.3	10	2	0	49.51	1.841	4	0.2
5	2	1	27.26	3.271	8	2.0	6	3	2	37.34	2.408	8	0.3	2	10	0	49.51	1.841	4	0.2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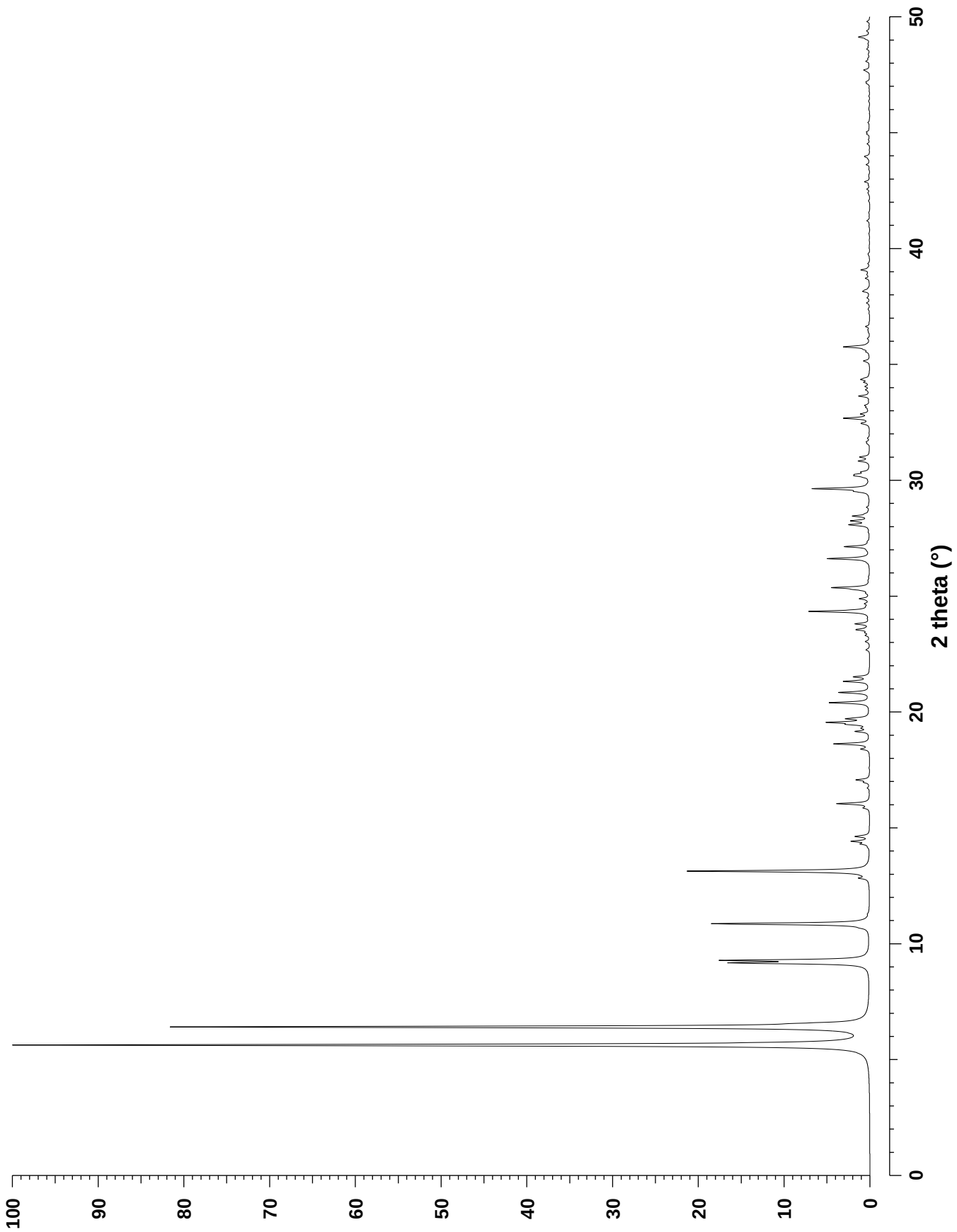
CHEMICAL COMPOSITION: $|(H_3N(CH_2)_9NH_3)^{2+}_{16}|\ [Al_{32}Co_{32}P_{64}O_{256}]$
$H_2N(CH_2)_9NH_2$ = 1,9 diaminononane

REFINED COMPOSITION: $|C_{32}N_{16}|\ [Al_{32}Co_{32}P_{64}O_{256}]$

CRYSTAL DATA: $P\,4/n\,nc$ (No. 126) origin at centre $\overline{1}$
$a = 19.0654$ Å $b = 19.0654$ Å $c = 27.594$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_F = 0.098$, $R_w = 0.26$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	5.63	15.686	8	100.0	3	0	7	26.61	3.350	8	4.9	1	0	11	36.11	2.487	8	0.2
0	0	2	6.41	13.797	2	81.3	5	2	3	26.99	3.304	16	0.1	6	4	4	36.39	2.469	16	0.1
1	1	0	6.56	13.481	4	3.8	5	1	4	27.13	3.287	16	2.9	7	3	2	36.48	2.463	16	0.2
1	1	2	9.17	9.642	8	14.7	4	1	6	27.35	3.261	16	0.2	6	1	7	36.63	2.453	16	0.5
2	0	0	9.28	9.533	4	15.9	5	3	2	28.04	3.182	16	0.5	2	1	11	37.37	2.407	16	0.1
1	0	3	10.68	8.284	8	0.4	6	0	0	28.08	3.178	4	2.1	5	0	9	37.64	2.389	8	0.4
2	1	1	10.86	8.146	16	18.5	3	2	7	28.24	3.160	16	2.1	5	4	7	37.87	2.376	16	0.3
0	0	4	12.83	6.898	2	1.0	4	3	5	28.45	3.137	16	0.7	6	5	3	38.14	2.359	16	0.7
2	2	0	13.13	6.741	4	21.4	5	0	5	28.45	3.137	8	1.2	8	1	1	38.20	2.356	16	0.3
2	1	3	14.16	6.253	16	0.1	4	2	6	28.55	3.126	16	0.3	5	5	6	38.71	2.326	8	0.5
3	0	1	14.30	6.193	8	0.9	6	0	2	28.83	3.097	8	0.3	5	2	9	38.86	2.318	16	0.1
1	1	4	14.42	6.141	8	2.1	4	4	4	29.50	3.028	8	0.1	8	2	0	38.95	2.312	8	0.1
2	2	2	14.63	6.056	8	1.7	1	0	9	29.51	3.027	8	1.1	6	3	7	39.07	2.305	16	1.0
2	0	4	15.86	5.589	8	0.6	6	2	0	29.63	3.015	8	6.6	8	1	3	39.34	2.290	16	0.1
3	1	2	16.04	5.525	16	3.9	6	1	3	30.12	2.967	16	0.3	6	1	9	41.19	2.192	16	0.3
1	0	5	16.72	5.301	8	0.3	5	4	1	30.19	2.960	16	1.3	3	1	12	42.05	2.149	16	0.1
3	0	3	16.96	5.229	8	0.6	5	3	4	30.25	2.955	16	1.3	8	4	0	42.40	2.132	8	0.2
3	2	1	17.07	5.193	16	1.6	6	2	2	30.35	2.945	16	0.8	7	1	8	42.56	2.124	16	0.3
2	2	4	18.40	4.821	8	0.9	5	1	6	30.82	2.901	16	1.3	8	0	6	42.73	2.116	8	0.1
4	0	0	18.62	4.766	4	4.2	6	0	4	30.98	2.886	8	0.2	1	0	13	42.87	2.110	8	0.3
2	1	5	19.16	4.633	16	1.6	2	1	9	31.00	2.885	16	1.0	5	3	10	42.88	2.109	16	0.2
0	0	6	19.30	4.599	2	0.7	5	4	3	31.58	2.833	16	0.2	6	5	7	43.61	2.075	16	0.4
4	1	1	19.46	4.560	16	2.0	6	3	1	31.65	2.827	16	0.3	2	1	13	43.96	2.060	16	0.5
3	1	4	19.55	4.540	16	4.6	5	3	5	31.81	2.813	16	0.2	6	2	10	44.51	2.035	16	0.3
4	0	2	19.71	4.505	8	2.5	0	0	10	32.45	2.759	2	0.9	8	1	7	44.69	2.028	16	0.1
1	1	6	20.40	4.353	8	4.7	4	3	7	32.67	2.741	16	0.5	7	6	3	44.93	2.018	16	0.3
4	2	0	20.84	4.263	8	3.6	5	0	7	32.67	2.741	8	2.5	9	1	4	45.02	2.014	16	0.2
3	0	5	21.32	4.167	8	3.0	6	1	5	32.86	2.725	16	1.0	3	0	13	45.03	2.013	8	0.1
4	1	3	21.51	4.131	16	1.8	7	0	1	33.05	2.710	8	0.1	7	5	6	45.43	1.997	16	0.2
4	0	4	22.68	3.921	8	0.4	1	1	10	33.14	2.703	8	0.3	6	1	11	46.36	1.959	16	0.1
1	0	7	23.04	3.860	8	0.5	5	5	0	33.23	2.696	4	0.3	5	5	10	47.12	1.928	8	0.2
3	2	5	23.30	3.818	16	0.4	7	1	0	33.23	2.696	8	0.3	7	7	0	47.19	1.926	4	0.4
2	2	6	23.42	3.799	8	0.4	5	3	6	33.63	2.665	16	1.3	6	4	10	47.63	1.909	16	0.2
5	0	1	23.55	3.777	8	1.4	6	4	0	33.90	2.644	8	0.4	10	0	0	47.70	1.907	4	0.6
3	3	4	23.63	3.765	8	0.1	5	2	7	34.04	2.634	16	0.4	10	1	1	48.07	1.893	16	0.4
5	1	0	23.80	3.739	8	1.7	5	4	5	34.22	2.620	16	0.6	9	3	5	48.19	1.888	16	0.1
5	1	1	24.02	3.705	16	0.1	7	0	3	34.34	2.612	8	0.9	3	1	14	48.60	1.873	16	0.3
3	1	6	24.34	3.657	16	7.1	7	2	1	34.40	2.607	16	0.4	10	2	0	48.71	1.870	8	0.1
4	2	4	24.55	3.627	16	0.2	4	3	8	35.08	2.558	16	0.1	10	2	1	48.82	1.865	16	0.1
5	1	2	24.67	3.609	16	0.5	2	2	10	35.14	2.554	8	0.7	10	1	3	49.03	1.858	16	0.3
2	1	7	24.88	3.578	16	1.2	6	3	5	35.53	2.527	16	0.3	7	7	4	49.11	1.855	8	0.9
4	1	5	25.12	3.544	16	0.3	7	2	3	35.64	2.519	16	0.4	5	0	13	49.12	1.855	8	0.1
5	0	3	25.28	3.522	8	1.2	5	5	4	35.75	2.511	8	1.9	7	3	10	49.14	1.854	16	0.3
5	2	1	25.36	3.512	16	4.2	7	1	4	35.75	2.511	16	0.9	7	0	11	49.39	1.845	8	0.3
3	2	6	25.67	3.470	16	0.1	3	1	10	35.79	2.509	16	0.4	7	6	7	49.79	1.831	16	0.3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2 theta (°)

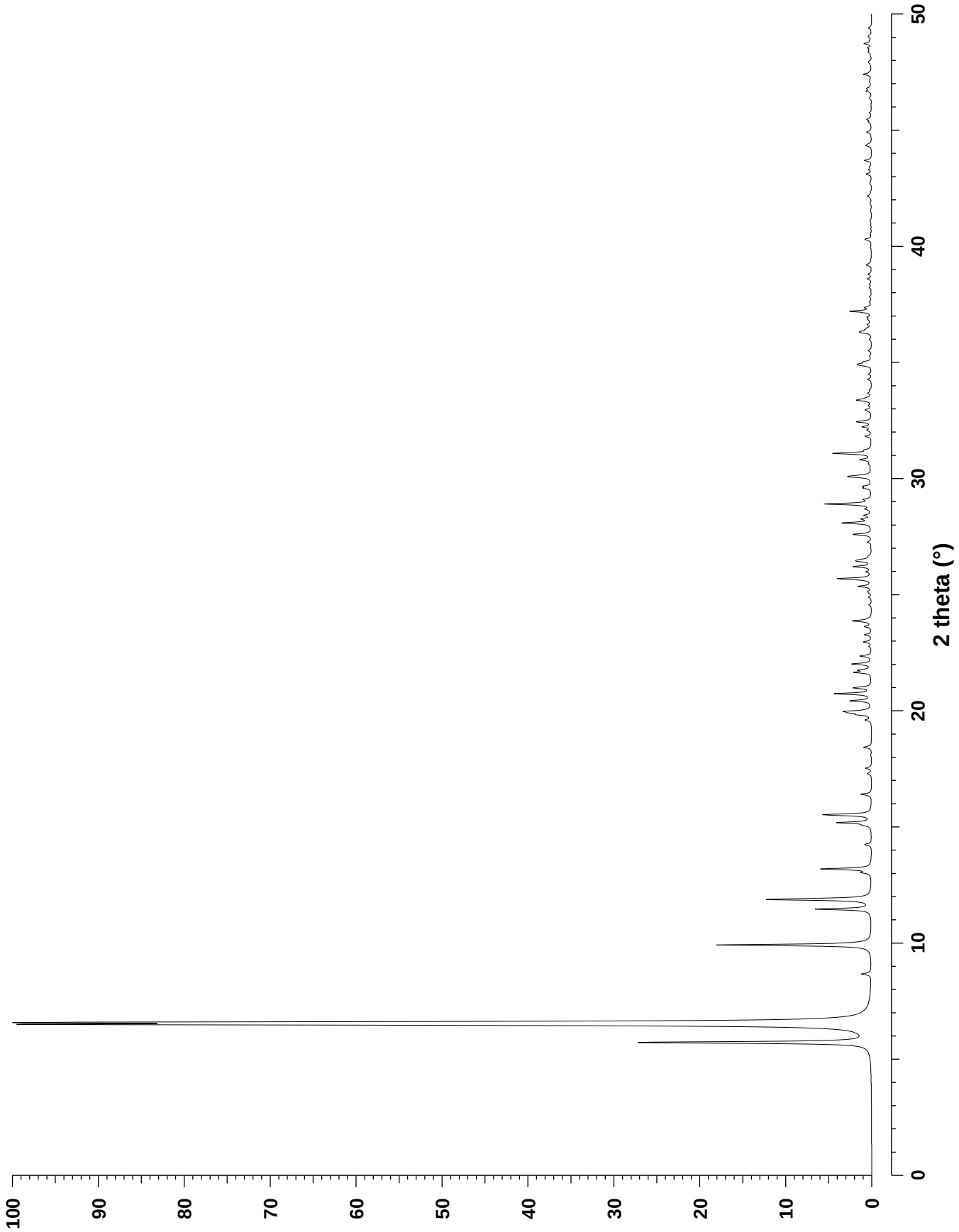
CHEMICAL COMPOSITION: $|(H_3N(CH_2)_7NH_3)^{2+}_{12}|\ [Ga_{24}Co_{24}P_{48}O_{192}]$
$H_2N(CH_2)_7NH_2$ = 1,7 diaminoheptane

REFINED COMPOSITION: $|C_{16}N_{16}O_{12}|\ [Ga_{24}Co_{24}P_{48}O_{192}]$

CRYSTAL DATA: $P\overline{3}1c$ (No. 163)
$a = 17.8356$ Å $b = 17.8356$ Å $c = 27.1816$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_F = 0.070$, $R_w = 0.201$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.72	15.446	6	32.2	3	2	0	25.13	3.544	12	0.4	1	0	10	33.47	2.677	12	0.4
0	0	2	6.50	13.591	2	99.2	5	-2	1	25.35	3.514	12	0.8	3	1	8	33.67	2.662	12	0.3
1	0	1	6.58	13.429	12	100.0	3	2	1	25.35	3.514	12	1.0	5	1	3	33.79	2.653	12	0.2
1	0	2	8.67	10.203	12	1.4	2	0	7	25.68	3.469	12	4.7	3	2	7	34.26	2.617	12	0.4
1	1	0	9.92	8.918	6	21.7	3	2	2	25.98	3.429	12	0.6	1	1	10	34.49	2.600	6	0.3
2	0	0	11.46	7.723	6	7.7	3	0	6	26.20	3.401	12	2.4	6	0	0	34.85	2.574	6	0.6
1	1	2	11.87	7.456	6	6.2	4	1	0	26.44	3.371	12	1.5	6	-2	5	34.89	2.572	12	0.9
2	-1	2	11.87	7.456	6	6.3	3	1	5	26.49	3.365	12	0.9	5	1	4	34.93	2.568	12	0.4
2	0	1	11.91	7.429	12	4.3	4	-1	5	26.49	3.365	12	0.4	6	-1	4	34.93	2.568	12	0.7
0	0	4	13.03	6.795	2	1.1	4	1	1	26.65	3.345	12	0.3	6	0	1	35.01	2.563	12	1.0
2	0	2	13.19	6.715	12	7.0	4	1	2	27.26	3.272	12	0.5	5	-1	7	35.26	2.545	12	0.2
1	0	4	14.24	6.220	12	0.9	2	1	7	27.59	3.233	12	1.7	6	0	2	35.49	2.529	12	0.2
2	0	3	15.07	5.878	12	0.8	3	-1	7	27.59	3.233	12	0.9	7	-3	1	35.51	2.528	12	0.2
2	1	0	15.18	5.838	12	4.7	4	-2	6	28.08	3.178	6	2.7	6	0	3	36.28	2.476	12	1.0
3	-1	1	15.52	5.708	12	5.1	2	2	6	28.08	3.178	6	1.0	5	2	0	36.32	2.473	12	1.0
2	1	1	15.52	5.708	12	1.7	1	1	8	28.10	3.175	6	0.4	3	1	9	36.40	2.468	12	0.4
1	1	4	16.40	5.405	6	0.4	4	1	3	28.25	3.159	12	1.2	5	-2	8	36.64	2.452	12	0.2
2	-1	4	16.40	5.405	6	1.1	5	-2	4	28.41	3.142	12	0.6	1	0	11	36.84	2.440	12	0.4
1	0	5	17.29	5.128	12	0.6	3	2	4	28.41	3.142	12	0.3	7	-2	2	36.94	2.433	12	0.4
3	0	1	17.53	5.059	12	0.8	4	-1	6	28.68	3.113	12	0.7	5	0	7	37.19	2.418	12	3.0
3	0	2	18.43	4.815	12	1.1	5	0	0	28.90	3.089	6	6.5	6	0	4	37.35	2.407	12	0.8
0	0	6	19.60	4.530	2	0.8	5	0	1	29.09	3.069	12	0.9	6	1	0	38.21	2.356	12	0.2
3	0	3	19.83	4.476	12	1.6	4	1	4	29.58	3.020	12	0.6	6	-2	7	38.59	2.333	12	0.4
2	2	0	19.91	4.459	6	2.0	5	-1	4	29.58	3.020	12	0.3	5	-2	9	39.19	2.299	12	0.4
2	0	5	19.97	4.445	12	3.2	5	0	2	29.66	3.012	12	1.0	3	2	9	39.19	2.299	12	0.2
1	0	6	20.43	4.347	12	2.9	3	3	0	30.06	2.973	6	2.2	6	0	6	40.29	2.238	12	0.7
3	1	0	20.73	4.284	12	5.1	5	-2	5	30.10	2.969	12	1.3	8	-3	3	42.15	2.144	12	0.4
3	1	1	20.99	4.232	12	1.4	3	2	5	30.10	2.969	12	0.5	8	-3	4	43.10	2.099	12	0.4
4	-1	1	20.99	4.232	12	0.9	1	0	9	30.15	2.964	12	0.5	6	1	6	43.29	2.090	12	0.2
3	0	4	21.65	4.104	12	2.2	4	2	0	30.63	2.919	12	0.3	1	0	13	43.69	2.072	12	1.0
3	1	2	21.75	4.086	12	1.0	3	3	2	30.79	2.904	6	0.5	8	-2	4	44.34	2.043	12	0.3
4	-1	2	21.75	4.086	12	0.7	6	-2	1	30.81	2.902	12	0.7	4	-2	12	44.88	2.019	6	0.3
2	-1	6	22.01	4.039	6	0.4	4	-1	7	31.08	2.877	12	3.6	2	0	13	44.91	2.018	12	0.5
1	1	6	22.01	4.039	6	2.3	3	1	7	31.08	2.877	12	1.8	4	4	6	45.34	2.000	6	0.3
2	1	5	22.35	3.979	12	1.6	4	1	5	31.22	2.865	12	0.5	7	1	3	45.45	1.996	12	0.4
2	0	6	22.76	3.908	12	0.3	2	0	9	31.81	2.813	12	0.8	6	3	0	46.67	1.946	12	0.7
4	-1	3	22.96	3.873	12	1.0	3	2	6	32.07	2.791	12	0.2	0	0	14	46.79	1.942	2	0.4
4	0	1	23.27	3.823	12	1.0	5	-2	6	32.07	2.791	12	0.3	7	0	7	47.39	1.918	12	1.1
1	0	7	23.62	3.766	12	1.0	6	-2	3	32.22	2.778	12	1.2	5	4	4	47.90	1.899	12	0.3
2	2	4	23.87	3.728	6	1.8	6	-1	1	32.44	2.760	12	2.0	2	-1	14	47.95	1.897	6	0.2
4	-2	4	23.87	3.728	6	0.8	0	0	10	32.95	2.718	2	0.8	7	2	1	48.35	1.883	12	0.2
4	0	2	23.96	3.714	12	0.3	5	-1	6	33.13	2.704	12	0.3	6	2	7	48.54	1.876	12	0.3
3	1	4	24.56	3.624	12	0.3	5	0	5	33.36	2.686	12	1.8	6	0	10	48.72	1.869	12	0.9
3	-1	6	24.88	3.579	12	0.2	6	-2	4	33.41	2.682	12	0.3	9	-4	5	49.01	1.859	12	0.2
4	0	3	25.07	3.552	12	0.2	4	2	4	33.41	2.682	12	0.3	6	-1	11	49.39	1.845	12	0.3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SBT UCSB–10GaZn

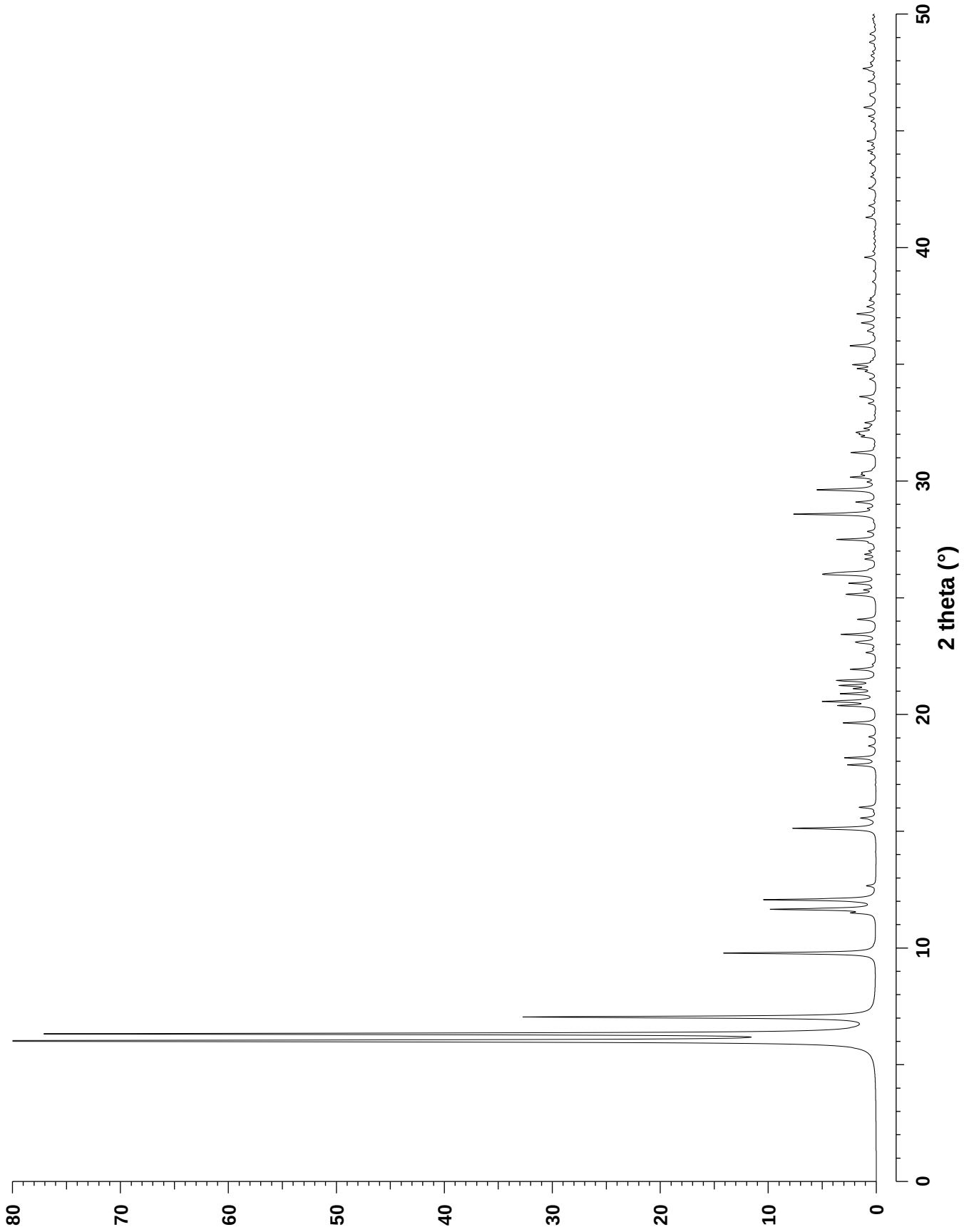
CHEMICAL COMPOSITION: $|(H_3N(CH_2)_3O((CH_2)_2O)_2(CH_2)_3NH_3)^{2+}_{18}|\ [Ga_{36}Zn_{36}P_{72}O_{288}]$
$H_2N(CH_2)_3O((CH_2)_2O)_2(CH_2)_3NH_2$ = 4,7,10-trioxa-1,13-tridecanediamine

REFINED COMPOSITION: $|C_{30}N_{24}|\ [Ga_{36}Zn_{36}P_{72}O_{288}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 18.0804$ Å $b = 18.0804$ Å $c = 41.9511$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_F = 0.045$, $R_w = 0.140$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	6.02	14.670	6	100.0	3	0	9	25.62	3.477	6	1.1	1	0	16	34.69	2.586	6	0.7
0	0	3	6.32	13.984	2	76.3	2	0	11	25.99	3.429	6	3.3	4	2	8	34.81	2.577	6	0.5
0	1	2	7.04	12.548	6	32.8	3	-1	10	26.03	3.422	6	0.8	6	-2	8	34.81	2.577	6	1.1
1	1	0	9.78	9.040	6	14.3	2	1	10	26.03	3.422	6	1.4	6	0	3	34.98	2.565	6	0.4
0	2	1	11.50	7.696	6	1.8	1	4	0	26.08	3.417	6	1.4	0	6	3	34.98	2.565	6	1.7
2	-1	3	11.66	7.592	6	5.0	4	1	0	26.08	3.417	6	0.8	7	-4	2	35.12	2.555	6	0.3
1	1	3	11.66	7.592	6	4.7	5	-2	4	26.22	3.398	6	0.2	0	5	10	35.78	2.510	6	1.7
0	1	5	11.97	7.395	6	0.4	3	1	8	26.65	3.345	6	0.9	5	2	0	35.81	2.507	6	0.2
2	0	2	12.07	7.335	6	10.4	1	4	3	26.86	3.319	6	0.6	2	5	0	35.81	2.507	6	0.8
0	0	6	12.66	6.992	2	0.9	5	-3	5	27.00	3.302	6	0.4	7	-5	3	36.40	2.468	6	0.3
3	-1	1	15.12	5.860	6	4.4	1	1	12	27.35	3.261	6	0.3	3	1	14	36.43	2.466	6	0.3
2	1	1	15.12	5.860	6	3.5	4	-2	9	27.49	3.245	6	2.8	6	0	6	36.76	2.445	6	1.0
1	2	2	15.56	5.696	6	0.6	2	2	9	27.49	3.245	6	0.9	5	0	11	37.15	2.420	6	1.7
3	-2	2	15.56	5.696	6	0.8	3	-2	11	27.83	3.206	6	0.4	3	2	13	37.46	2.401	6	0.3
2	-1	6	16.02	5.531	6	0.8	1	2	11	27.83	3.206	6	0.3	5	-2	13	37.46	2.401	6	0.5
1	1	6	16.02	5.531	6	0.7	0	5	1	28.58	3.123	6	7.7	7	-6	1	37.73	2.384	6	0.3
0	1	8	17.84	4.972	6	2.6	5	0	2	28.82	3.097	6	0.6	1	6	1	37.73	2.384	6	0.3
3	0	3	18.14	4.890	6	2.9	1	4	6	29.09	3.070	6	1.2	4	-2	15	37.83	2.378	6	0.3
0	2	7	18.65	4.759	6	0.7	5	-4	6	29.09	3.070	6	0.3	6	0	9	39.58	2.277	6	0.4
0	0	9	19.04	4.661	2	0.7	5	-1	6	29.09	3.070	6	0.3	0	6	9	39.58	2.277	6	0.4
2	2	0	19.64	4.520	6	3.1	4	-3	10	29.61	3.017	6	3.8	1	0	19	41.29	2.186	6	0.9
2	0	8	20.38	4.357	6	3.4	1	3	10	29.61	3.017	6	0.5	8	-3	5	41.79	2.161	6	0.4
4	-3	1	20.56	4.320	6	0.5	3	3	0	29.64	3.013	6	1.9	0	2	19	42.54	2.125	6	0.6
1	3	1	20.56	4.320	6	4.3	0	2	13	29.95	2.984	6	0.7	8	-6	5	43.03	2.102	6	0.3
4	-1	2	20.89	4.253	6	3.1	5	-3	8	30.16	2.964	6	1.6	8	-5	7	43.17	2.096	6	0.3
2	1	7	21.10	4.211	6	1.7	2	3	8	30.16	2.964	6	0.6	0	1	20	43.53	2.079	6	0.3
3	0	6	21.24	4.183	6	0.3	6	-4	1	30.28	2.952	6	0.9	1	6	10	43.61	2.075	6	0.4
0	3	6	21.24	4.183	6	2.8	3	3	3	30.34	2.946	6	0.3	4	-2	18	43.70	2.071	6	0.3
2	-1	9	21.45	4.143	6	0.3	0	1	14	30.37	2.943	6	0.7	5	3	8	44.01	2.057	6	0.3
1	1	9	21.45	4.143	6	3.3	4	-1	11	31.21	2.866	6	0.5	1	7	3	44.14	2.052	6	0.3
1	0	10	21.93	4.052	6	2.4	3	1	11	31.21	2.866	6	1.8	2	3	17	44.54	2.034	6	0.3
1	2	8	22.65	3.925	6	0.8	6	-1	1	31.89	2.806	6	1.0	4	4	9	44.55	2.034	6	0.5
4	0	1	22.82	3.898	6	0.2	2	0	14	31.98	2.799	6	0.4	0	0	21	45.40	1.998	2	0.4
3	1	5	23.06	3.857	6	0.4	0	0	15	32.00	2.797	2	0.7	7	1	6	45.62	1.988	6	0.5
4	-1	5	23.06	3.857	6	0.5	6	-2	5	32.07	2.791	6	1.1	7	0	10	45.98	1.974	6	0.4
0	4	2	23.11	3.848	6	1.5	4	2	5	32.07	2.791	6	0.2	3	6	0	46.01	1.973	6	0.5
2	2	6	23.43	3.796	6	2.2	6	-5	2	32.11	2.787	6	0.3	0	7	11	47.10	1.929	6	0.6
4	-2	6	23.43	3.796	6	1.1	1	5	2	32.11	2.787	6	0.3	2	7	1	47.58	1.911	6	0.4
0	2	10	24.07	3.698	6	1.7	0	5	7	32.25	2.776	6	1.0	6	0	15	47.66	1.908	6	0.5
0	4	5	25.10	3.547	6	0.7	5	-1	9	32.49	2.756	6	0.8	0	6	15	47.66	1.908	6	0.6
5	-3	2	25.15	3.541	6	0.8	5	0	8	33.32	2.689	6	0.7	5	4	7	47.84	1.901	6	0.2
2	3	2	25.15	3.541	6	1.7	1	5	5	33.61	2.666	6	0.9	1	5	17	49.12	1.855	6	0.3
4	-3	7	25.33	3.517	6	0.4	6	-5	5	33.61	2.666	6	0.6	0	2	22	49.18	1.853	6	0.3
1	3	7	25.33	3.517	6	0.6	0	6	0	34.36	2.610	6	0.6	8	1	1	49.80	1.831	6	0.3
0	3	9	25.62	3.477	6	1.4	4	-3	13	34.63	2.590	6	0.3	1	8	2	49.95	1.826	6	0.2


0
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20
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40
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2 theta (°)
0
10
20
30
40
50
60
70
80

SFE SSZ–48, Calcined

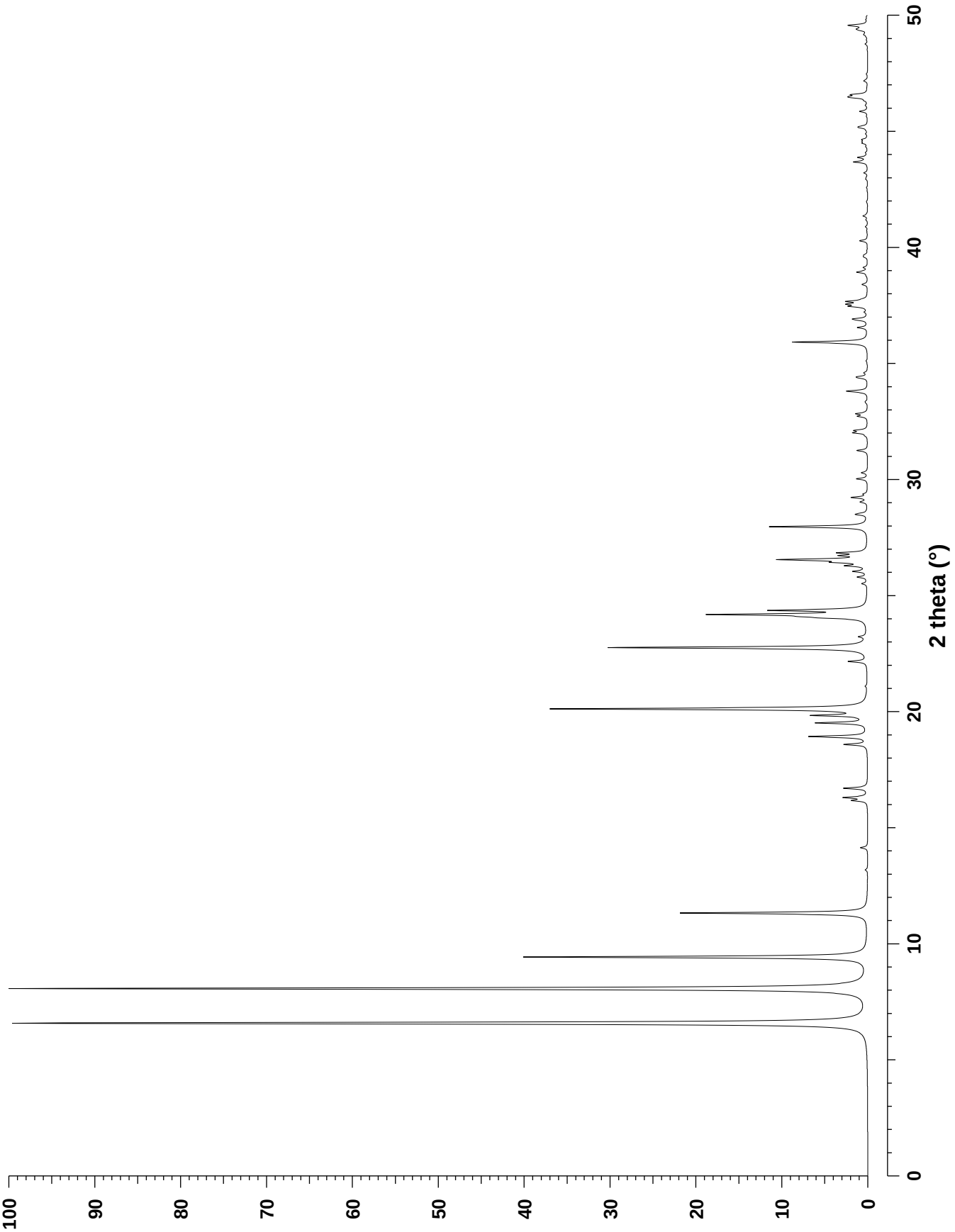
CHEMICAL COMPOSITION: $[Si_{14}O_{28}]$

REFINED COMPOSITION: $[Si_{14}O_{28}]$

CRYSTAL DATA: $P2_1$ (No. 4) unique axis **b**
$a = 11.1527$ Å $b = 5.002$ Å $c = 13.667$ Å
$\alpha = 90°$ $\beta = 100.633°$ $\gamma = 90°$
Electron diffraction, and X-ray powder, $R_w = 0.0971$, $R_p = 0.0887$

REFERENCE: P. Wagner, O. Terasaki, S. Ritsch, J. G. Nery, S. I. Zones, M. E. Davis and K. Hiraga, *J. Phys. Chem. B* **103** 8245–8250 (1999).

h	k	l	2θ	d	M	I_{rel}
0	0	1	6.58	13.432	2	99.6
1	0	0	8.07	10.961	2	100.0
-1	0	1	9.43	9.383	2	40.0
1	0	1	11.32	7.815	2	21.8
0	0	2	13.18	6.716	2	0.3
-1	0	2	14.14	6.265	2	0.8
2	0	0	16.17	5.481	2	1.7
-2	0	1	16.30	5.438	2	2.7
1	0	2	16.70	5.307	2	2.8
2	0	1	18.58	4.776	2	2.7
-2	0	2	18.92	4.691	2	5.4
0	1	1	18.93	4.688	4	1.5
1	1	0	19.51	4.551	4	5.8
0	0	3	19.83	4.477	2	5.9
-1	0	3	19.99	4.442	2	0.2
-1	1	1	20.12	4.414	4	36.9
1	1	1	21.09	4.213	4	0.2
0	1	2	22.16	4.012	4	2.2
-1	1	2	22.75	3.909	4	24.5
2	0	2	22.76	3.908	2	6.0
-2	0	3	23.22	3.831	2	0.8
-3	0	1	24.03	3.703	2	3.2
2	1	0	24.09	3.695	4	4.2
-2	1	1	24.18	3.681	4	17.4
3	0	0	24.36	3.654	2	10.7
1	1	2	24.45	3.640	4	0.2
-3	0	2	25.51	3.491	2	0.6
2	1	1	25.79	3.454	4	1.1
-2	1	2	26.04	3.422	4	1.6
-1	0	4	26.28	3.391	2	2.2
3	0	1	26.43	3.372	2	3.1
0	0	4	26.54	3.358	2	10.0
0	1	3	26.72	3.336	4	2.6
-1	1	3	26.84	3.321	4	3.2
2	0	3	27.96	3.191	2	11.5
-2	0	4	28.49	3.132	2	1.2
-3	0	3	28.54	3.128	2	0.5
1	1	3	29.03	3.076	4	0.8
1	0	4	29.22	3.057	2	1.9
-2	1	3	29.37	3.041	4	0.4
-3	1	1	30.02	2.976	4	1.3
3	1	0	30.29	2.950	4	0.7
-3	1	2	31.24	2.863	4	1.3
-1	1	4	31.88	2.807	4	0.2
3	1	1	32.01	2.796	4	1.5
0	1	4	32.10	2.788	4	1.0
-4	0	1	32.11	2.788	2	0.4
-3	0	4	32.72	2.737	2	1.1
-1	0	5	32.83	2.728	2	1.3
2	1	3	33.30	2.690	4	0.1
0	0	5	33.35	2.686	2	0.2
-2	1	4	33.76	2.655	4	0.3
2	0	4	33.78	2.654	2	0.2
-3	1	3	33.80	2.652	4	2.1
-2	0	5	34.36	2.610	2	0.3
1	1	4	34.38	2.608	4	0.5
3	0	3	34.42	2.605	2	0.9
4	0	1	34.59	2.593	2	0.4
-4	0	3	35.10	2.557	2	0.2
1	0	5	35.85	2.505	2	0.3
0	2	0	35.91	2.501	2	8.7
0	2	1	36.54	2.459	4	1.2
1	2	0	36.86	2.438	4	0.8
-4	1	1	36.91	2.435	4	1.5
-1	2	1	37.20	2.417	4	0.3
4	1	0	37.42	2.403	4	0.2
-3	1	4	37.46	2.401	4	1.8
-1	1	5	37.55	2.395	4	2.0
-4	1	2	37.66	2.389	4	2.1
-3	0	5	37.72	2.385	2	0.2
1	2	1	37.77	2.382	4	0.3
2	1	4	38.40	2.344	4	0.6
-1	2	2	38.77	2.323	4	0.1
-2	1	5	38.92	2.314	4	1.2
3	1	3	38.98	2.311	4	0.2
4	1	1	39.13	2.302	4	0.5
-1	0	6	39.57	2.277	2	0.2
-4	1	3	39.59	2.277	4	0.1
2	2	0	39.61	2.275	4	0.2
3	0	4	39.66	2.272	2	0.1
-2	2	1	39.67	2.272	4	0.2
1	1	5	40.27	2.240	4	0.5
0	0	6	40.28	2.239	2	0.5
-5	0	2	40.88	2.208	2	0.1
-2	2	2	40.89	2.207	4	0.2
5	0	0	41.18	2.192	2	0.2
0	2	3	41.35	2.183	4	0.5
-3	1	5	41.97	2.152	4	0.1
-4	1	4	42.57	2.124	4	0.1
2	2	2	42.93	2.107	4	0.2
5	0	1	43.01	2.103	2	0.1
-2	2	3	43.20	2.094	4	0.4
-1	1	6	43.67	2.073	4	1.5
-3	2	1	43.67	2.073	4	0.1
3	1	4	43.75	2.069	4	0.2
3	2	0	43.87	2.064	4	1.1
2	1	5	44.07	2.055	4	0.2
0	1	6	44.33	2.043	4	0.2
-5	1	1	44.48	2.037	4	0.5
-3	2	2	44.56	2.033	4	0.5
-2	1	6	44.64	2.030	4	0.6
-5	1	2	44.88	2.020	4	0.2
3	2	1	45.14	2.009	4	0.2
5	1	0	45.16	2.008	4	0.6
0	2	4	45.20	2.006	4	0.7
5	0	2	45.85	1.979	2	0.9
2	2	3	46.11	1.968	4	0.2
-5	1	3	46.32	1.960	4	0.3
-4	1	5	46.44	1.955	4	0.8
-2	2	4	46.46	1.954	4	0.6
-3	2	3	46.49	1.953	4	1.2
1	1	6	46.56	1.950	4	0.3
2	0	6	46.57	1.950	2	1.4
-3	1	6	47.16	1.927	4	0.4
-2	0	7	47.21	1.925	2	0.1
-4	0	6	47.46	1.916	2	0.1
-5	1	4	48.75	1.868	4	0.3
-4	2	1	48.93	1.862	4	0.1
-6	0	1	49.07	1.857	2	0.1
3	1	5	49.15	1.854	4	0.3
-6	0	2	49.21	1.851	2	0.1
4	2	0	49.33	1.847	4	0.3
-3	2	4	49.36	1.846	4	0.4
-3	0	7	49.40	1.845	2	0.7
-1	2	5	49.44	1.844	4	0.3
-4	2	2	49.52	1.841	4	0.5
5	1	2	49.53	1.840	4	0.2
5	0	3	49.56	1.839	2	1.8
0	2	5	49.81	1.831	4	0.1
6	0	0	49.92	1.827	2	0.1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90
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2 theta (°)

SFF SSZ-44, Calcined

CHEMICAL COMPOSITION: $[Si_{32}O_{64}]$

REFINED COMPOSITION: $[Si_{32}O_{64}]$

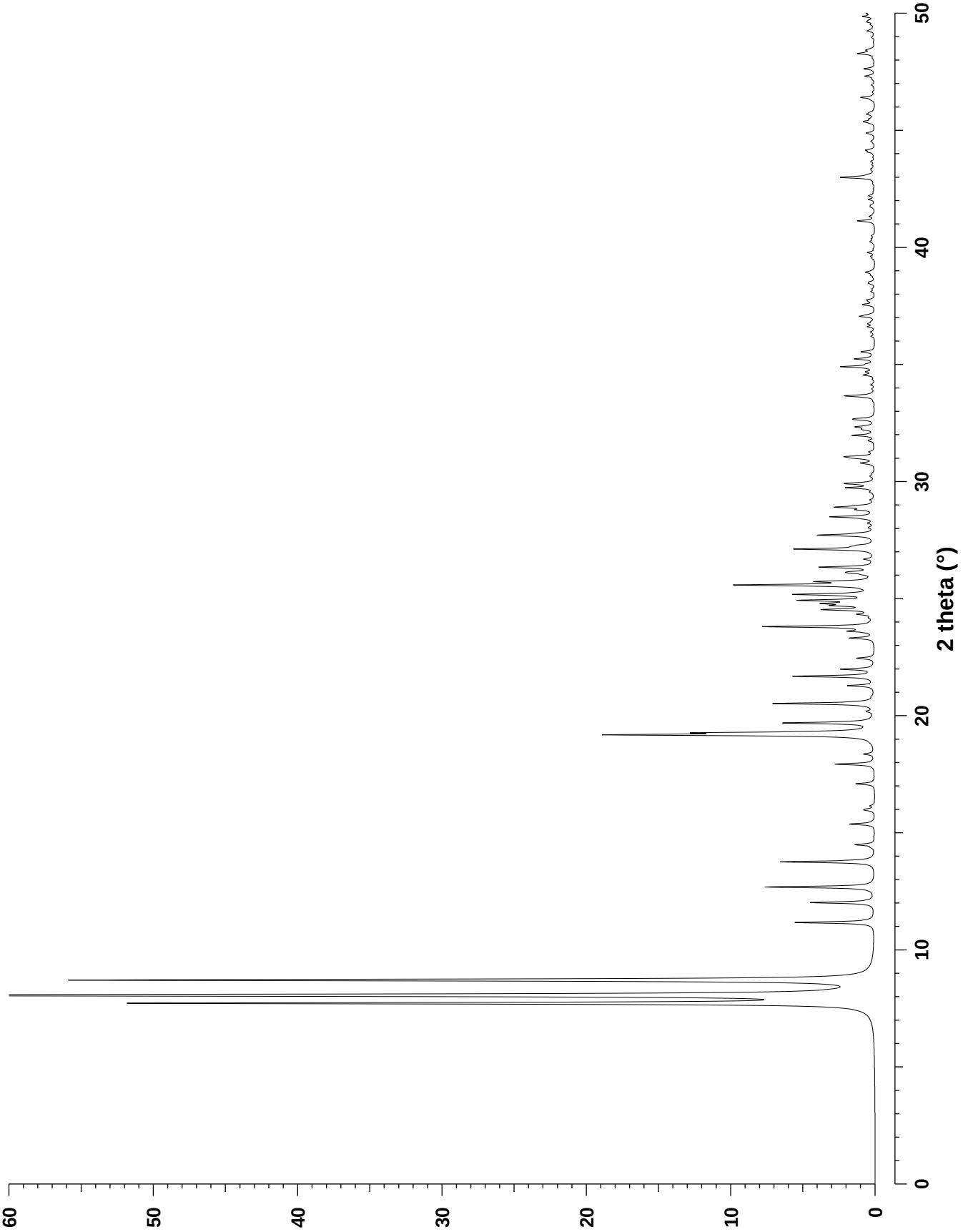
CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 11.4853$ Å $b = 21.9458$ Å $c = 7.3881$ Å
$\alpha = 90.0°$ $\beta = 94.702°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0892$, $R_{wp} = 0.1058$

REFERENCE: P. Wagner, S. I. Zones, M. E. Davis and R. C. Medrud, *Angew. Chem., Int. ed.* **38** 1269–1272 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.72	11.447	2	50.8	3	3	0	26.34	3.383	4	0.8	4	3	1	36.73	2.447	4	0.4
0	2	0	8.06	10.973	2	100.0	1	1	2	26.34	3.383	4	3.0	-1	1	3	37.05	2.426	4	1.0
1	1	0	8.71	10.149	4	55.9	-3	2	1	26.68	3.341	4	0.7	3	7	0	37.11	2.422	4	0.4
1	2	0	11.17	7.921	4	5.6	0	3	2	27.11	3.289	4	5.5	0	2	3	37.55	2.395	4	0.8
0	0	1	12.02	7.363	2	4.5	0	6	1	27.22	3.276	4	0.8	0	7	2	37.68	2.387	4	0.3
0	1	1	12.68	6.981	4	7.7	1	2	2	27.28	3.269	4	0.7	-1	2	3	37.75	2.383	4	0.5
-1	0	1	13.76	6.437	2	6.6	-1	3	2	27.67	3.224	4	0.3	-1	7	2	38.10	2.362	4	0.2
0	2	1	14.49	6.114	4	1.4	-2	0	2	27.71	3.219	2	3.7	-4	1	2	38.45	2.341	4	0.3
1	1	1	15.37	5.764	4	1.8	-2	5	1	27.78	3.211	4	0.6	-3	7	1	38.51	2.337	4	0.3
-1	2	1	15.96	5.552	4	0.5	-2	1	2	28.02	3.185	4	0.3	2	8	1	38.81	2.320	4	0.2
2	1	0	16.00	5.538	4	0.4	-3	3	1	28.22	3.163	4	0.4	2	6	2	38.93	2.314	4	0.4
0	4	0	16.15	5.486	2	0.3	3	2	1	28.40	3.142	4	0.4	-2	2	3	39.61	2.275	4	0.3
0	3	1	17.09	5.190	4	1.3	3	4	0	28.49	3.133	4	3.0	3	7	1	39.77	2.266	4	0.5
1	4	0	17.93	4.947	4	2.8	1	3	2	28.79	3.101	4	1.0	-4	3	2	40.23	2.242	4	0.2
-1	3	1	18.36	4.833	4	0.7	2	5	1	28.90	3.089	4	2.3	-4	6	1	41.12	2.195	4	0.8
1	3	1	19.18	4.627	4	17.4	-2	2	2	28.91	3.089	4	0.2	0	10	0	41.13	2.195	2	0.4
-2	1	1	19.27	4.605	4	10.0	2	6	0	28.97	3.082	4	0.7	5	3	0	41.32	2.185	4	0.3
2	3	0	19.69	4.508	4	6.3	0	4	2	29.21	3.057	4	0.3	-3	8	1	41.80	2.161	4	0.2
0	4	1	20.18	4.399	4	0.4	1	7	0	29.54	3.024	4	0.2	2	2	3	42.04	2.149	4	0.4
-2	2	1	20.52	4.328	4	7.1	-1	4	2	29.73	3.005	4	1.9	-2	4	3	42.20	2.141	4	0.2
-1	4	1	21.28	4.176	4	1.8	2	0	2	29.91	2.987	2	2.0	3	8	1	42.98	2.104	4	1.9
1	5	0	21.68	4.098	4	5.7	1	4	2	30.78	2.905	4	0.9	0	10	1	43.01	2.103	4	0.7
2	2	1	21.98	4.043	4	2.3	-2	6	1	30.95	2.889	4	0.2	2	3	3	43.09	2.099	4	0.2
2	4	0	22.45	3.961	4	0.2	0	7	1	31.00	2.885	4	1.0	3	9	0	44.07	2.055	4	0.3
-2	3	1	22.45	3.960	4	1.0	3	5	0	31.06	2.880	4	1.8	5	3	1	44.15	2.051	4	0.6
3	0	0	23.31	3.816	2	1.7	4	0	0	31.26	2.862	2	0.3	2	4	3	44.52	2.035	4	0.2
0	5	1	23.60	3.770	4	1.5	-1	7	1	31.75	2.819	4	0.3	-5	0	2	44.88	2.020	2	0.4
3	1	0	23.67	3.759	4	0.3	2	6	1	31.97	2.799	4	1.5	4	7	1	45.35	2.000	4	0.4
2	3	1	23.80	3.738	4	7.7	-1	5	2	32.20	2.780	4	0.4	-3	4	3	45.38	1.998	4	0.4
0	0	2	24.17	3.682	2	0.2	-2	4	2	32.24	2.776	4	0.3	-5	5	1	45.48	1.994	4	0.3
0	6	0	24.33	3.658	2	1.0	4	2	0	32.33	2.769	4	1.1	1	9	2	45.68	1.986	4	0.4
0	1	2	24.52	3.631	4	3.1	0	8	0	32.64	2.743	2	1.0	1	6	3	45.75	1.983	4	0.2
-1	5	1	24.55	3.626	4	0.5	-3	5	1	32.68	2.740	4	0.9	3	9	1	46.40	1.957	4	1.0
3	2	0	24.70	3.604	4	2.3	4	3	0	33.63	2.665	4	0.4	-4	1	3	46.93	1.936	4	0.2
-1	0	2	24.79	3.592	2	2.8	-4	2	1	33.66	2.662	4	1.8	3	3	3	47.31	1.921	4	0.6
-2	4	1	24.92	3.574	4	4.9	3	5	1	34.13	2.627	4	0.2	-5	6	1	47.62	1.909	4	0.7
-1	1	2	25.12	3.545	4	0.6	4	0	1	34.54	2.596	2	0.6	1	7	3	48.26	1.886	4	0.2
1	5	1	25.18	3.537	4	5.3	-3	3	2	34.68	2.586	4	0.5	4	8	1	48.26	1.886	4	0.8
0	2	2	25.52	3.490	4	0.6	0	8	1	34.90	2.571	4	2.3	2	6	3	48.42	1.880	4	0.5
1	6	0	25.57	3.484	4	0.5	-1	6	2	35.01	2.563	4	0.4	-3	6	3	49.23	1.851	4	0.5
2	5	0	25.58	3.483	4	8.9	3	0	2	35.23	2.547	2	1.3	-1	0	4	49.50	1.841	2	0.2
-3	1	1	25.72	3.463	4	3.5	4	2	1	35.53	2.527	4	0.9	-2	11	1	49.62	1.837	4	0.5
1	0	2	26.02	3.424	2	0.4	3	2	2	36.20	2.481	4	0.3	-1	1	4	49.69	1.835	4	0.2
-1	2	2	26.10	3.413	4	1.2	-3	4	2	36.38	2.469	4	0.3	-3	9	2	49.86	1.829	4	0.6
2	4	1	26.14	3.408	4	1.0	0	0	3	36.61	2.454	2	0.4	-6	3	1	49.97	1.825	4	0.5

SSZ-44, Calcined

SFF



SGT 1-aminoadamantane Sigma-2

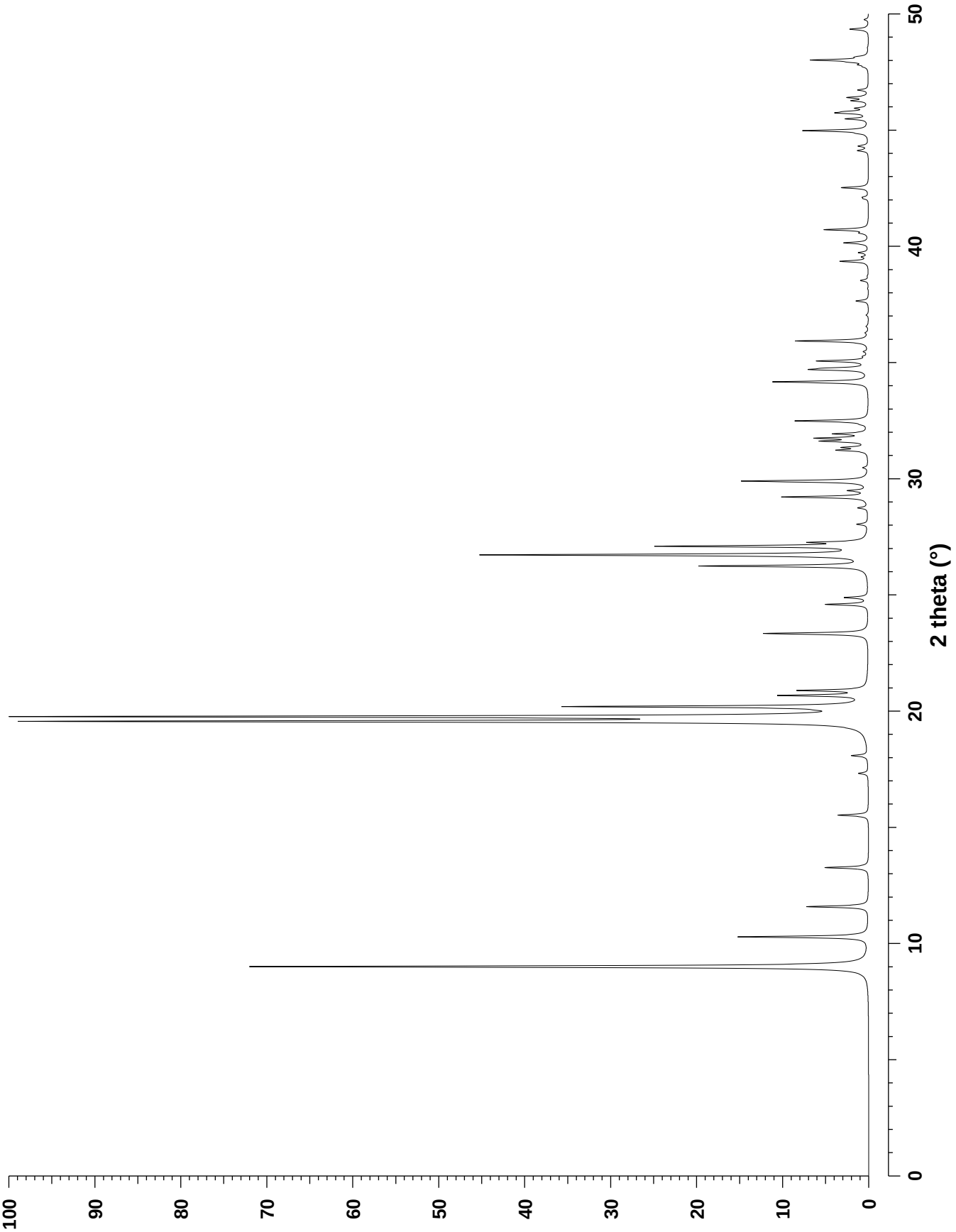
CHEMICAL COMPOSITION: $|(C_{10}H_{17}N)_4|\ [Si_{64}O_{128}]$
$C_{10}H_{17}N$ = 1-aminoadamantane

REFINED COMPOSITION: $|C_{43.84}|\ [Si_{64}O_{128}]$

CRYSTAL DATA: $I\,4_1/a\,md$ (No. 141) origin at centre $(2/m)$
$a = 10.2387$ Å $b = 10.2387$ Å $c = 34.3829$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.225$, $R_F = 0.100$

REFERENCE: L. B. McCusker,
J. Appl. Cryst. **21** 305–310 (1988).

h	k	l	2θ	d	M	I_{rel}
1	0	1	9.01	9.813	8	75.0
0	0	4	10.29	8.596	2	15.8
1	0	3	11.59	7.636	8	7.5
1	1	2	13.27	6.672	8	5.3
1	0	5	15.52	5.709	8	3.7
2	0	0	17.32	5.119	4	1.2
2	0	2	18.08	4.906	8	1.9
2	1	1	19.56	4.539	16	99.1
1	1	6	19.76	4.493	8	100.0
1	0	7	20.05	4.429	8	1.4
2	0	4	20.19	4.398	8	35.8
0	0	8	20.67	4.298	2	10.2
2	1	3	20.89	4.252	16	8.1
2	0	6	23.30	3.818	8	1.2
2	1	5	23.34	3.811	16	12.1
2	2	0	24.59	3.620	4	5.2
1	0	9	24.88	3.579	8	2.8
3	0	1	26.24	3.396	8	20.2
2	1	7	26.61	3.349	16	0.2
2	2	4	26.72	3.336	8	46.7
2	0	8	27.09	3.292	8	25.1
3	0	3	27.26	3.271	8	5.9
3	1	2	28.04	3.182	16	1.3
1	1	10	28.74	3.106	8	1.2
3	0	5	29.21	3.057	8	10.4
3	1	4	29.48	3.030	16	2.2
1	0	11	29.89	2.990	8	15.3
2	1	9	30.47	2.933	16	0.6
0	0	12	31.22	2.865	2	3.6
2	0	10	31.34	2.854	8	2.8
3	2	1	31.61	2.830	16	5.3
3	1	6	31.74	2.819	16	5.9
3	0	7	31.93	2.803	8	4.0
2	2	8	32.33	2.769	8	0.5
3	2	3	32.48	2.756	16	8.8
3	2	5	34.16	2.625	16	11.6
3	1	8	34.69	2.586	16	6.0
2	1	11	34.75	2.582	16	3.8
1	0	13	35.04	2.561	8	1.0
4	0	0	35.06	2.560	4	5.4
3	0	9	35.26	2.545	8	0.4
4	0	2	35.46	2.532	8	0.5
2	0	12	35.92	2.500	8	8.9
4	1	1	36.27	2.477	16	0.3
3	2	7	36.55	2.458	16	0.3
4	1	3	37.04	2.427	16	0.3
3	3	2	37.64	2.390	8	1.5
4	0	6	38.52	2.337	8	0.9
1	1	14	38.72	2.326	8	0.1
2	1	13	39.34	2.290	16	1.0
4	2	0	39.35	2.289	8	2.5
3	2	9	39.54	2.279	16	0.7
4	2	2	39.72	2.269	16	1.2
2	2	12	40.14	2.247	8	3.0
3	3	6	40.56	2.224	8	0.8
4	1	7	40.71	2.216	16	5.3
2	0	14	40.75	2.214	8	0.2
0	0	16	42.05	2.149	2	0.5
3	1	12	42.11	2.146	16	0.6
4	2	6	42.52	2.126	16	3.3
4	0	10	44.11	2.053	8	1.3
2	1	15	44.18	2.050	16	0.2
5	0	1	44.31	2.044	8	0.6
4	3	1	44.31	2.044	16	0.6
4	2	8	44.85	2.021	16	0.8
5	0	3	44.97	2.016	8	1.0
4	3	3	44.97	2.016	16	6.9
5	1	2	45.48	1.994	16	2.7
1	0	17	45.73	1.984	8	3.4
2	0	16	45.79	1.981	8	2.0
3	3	10	45.94	1.975	8	1.4
4	3	5	46.26	1.963	16	1.2
5	0	5	46.26	1.963	8	0.7
3	1	14	46.40	1.957	16	2.5
4	1	11	46.72	1.944	16	1.3
4	2	10	47.72	1.906	16	0.4
3	0	15	47.80	1.903	8	0.9
5	2	1	47.92	1.898	16	1.4
5	1	6	48.01	1.895	16	6.7
4	3	7	48.14	1.890	16	1.1
1	1	18	49.34	1.847	8	2.2
5	2	5	49.75	1.833	16	0.5


0
10
20
30
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2 theta (°)
100
90
80
70
60
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20
10
0

SOD Sodalite Octahydrate

CHEMICAL COMPOSITION: $|Na_6(H_2O)_8|\ [Si_6Al_6O_{24}]$

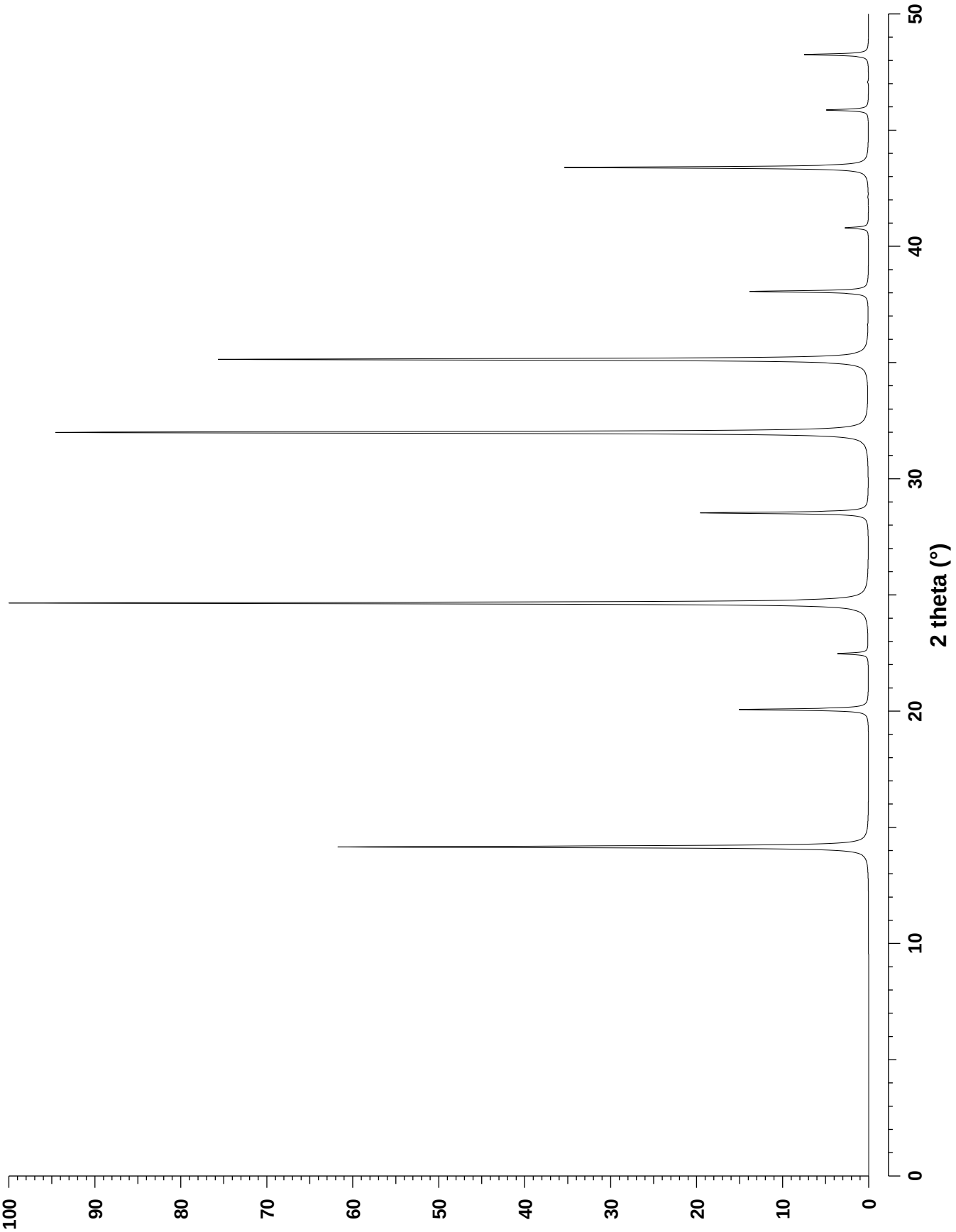
REFINED COMPOSITION: $|Na_6(H_2O)_8|\ [Si_6Al_6O_{24}]$

CRYSTAL DATA: $P\bar{4}3n$ (No. 218)
$a = 8.848$ Å $b = 8.848$ Å $c = 8.848$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.091$, $R_F = 0.047$

REFERENCE: J. Felsche, S. Luger and Ch. Baerlocher,
Zeolites **6** 367–372 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	14.16	6.256	12	61.8	3	1	0	31.99	2.798	24	94.6	4	1	1	43.39	2.085	24	19.6
2	0	0	20.07	4.424	6	15.1	2	2	2	35.13	2.554	8	75.7	4	2	0	45.86	1.978	24	4.9
2	1	0	22.47	3.957	24	3.6	3	2	1	38.05	2.365	48	13.9	4	2	1	47.06	1.931	48	0.1
2	1	1	24.65	3.612	24	100.0	4	0	0	40.79	2.212	6	2.7	3	3	2	48.24	1.886	24	7.5
2	2	0	28.53	3.128	12	19.6	3	3	0	43.39	2.085	12	15.8							

Sodalite Octahydrate SOD



SOD Bicchulite

CHEMICAL COMPOSITION: $|Ca_8(H_2O)_8|\ [Si_4Al_8O_{24}]$
Synthetic material

REFINED COMPOSITION: $|Ca_8(H_2O)_8|\ [Si_4Al_8O_{24}]$

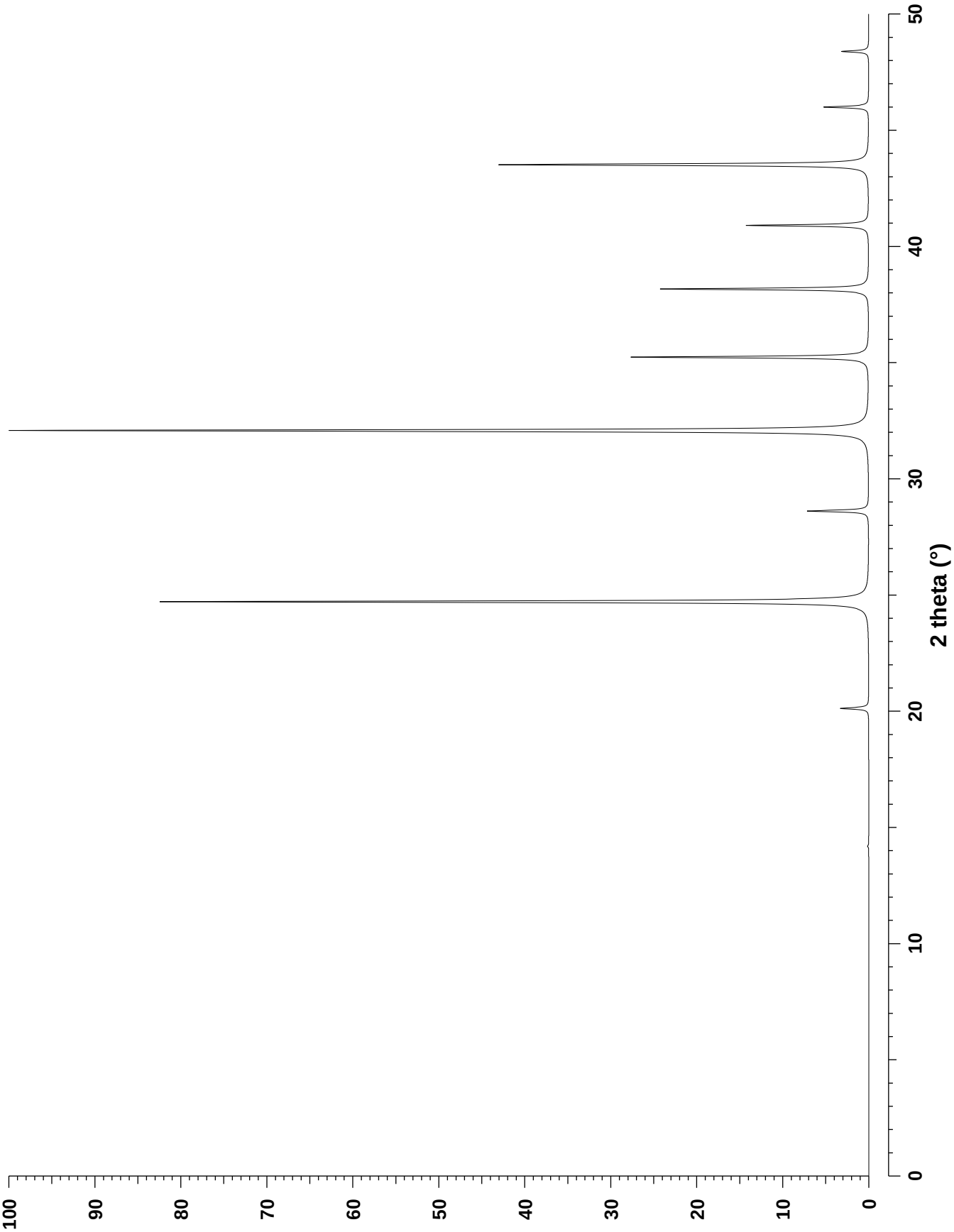
CRYSTAL DATA: $I\bar{4}3m$ (No. 217)
$a = 8.825$ Å $b = 8.825$ Å $c = 8.825$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.012$

REFERENCE: K. Sahl,
Z. Kristallogr. **152** 13–21 (1980).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	14.19	6.240	12	0.1	3	1	0	32.07	2.791	24	100.0	3	3	0	43.51	2.080	12	18.3
2	0	0	20.12	4.412	6	3.3	2	2	2	35.23	2.548	8	27.7	4	1	1	43.51	2.080	24	24.7
2	1	1	24.71	3.603	24	82.5	3	2	1	38.16	2.359	48	24.3	4	2	0	45.99	1.973	24	5.2
2	2	0	28.61	3.120	12	7.2	4	0	0	40.90	2.206	6	14.3	3	3	2	48.38	1.881	24	3.2

Bicchulite

SOD



SOD Tugtupite

CHEMICAL COMPOSITION: $|Na_8Cl_2|\ [Si_8Al_2Be_2O_{24}]$
Ilimaussaq, South Greenland

REFINED COMPOSITION: $|Na_8Cl_2|\ [Si_8Al_2Be_2O_{24}]$

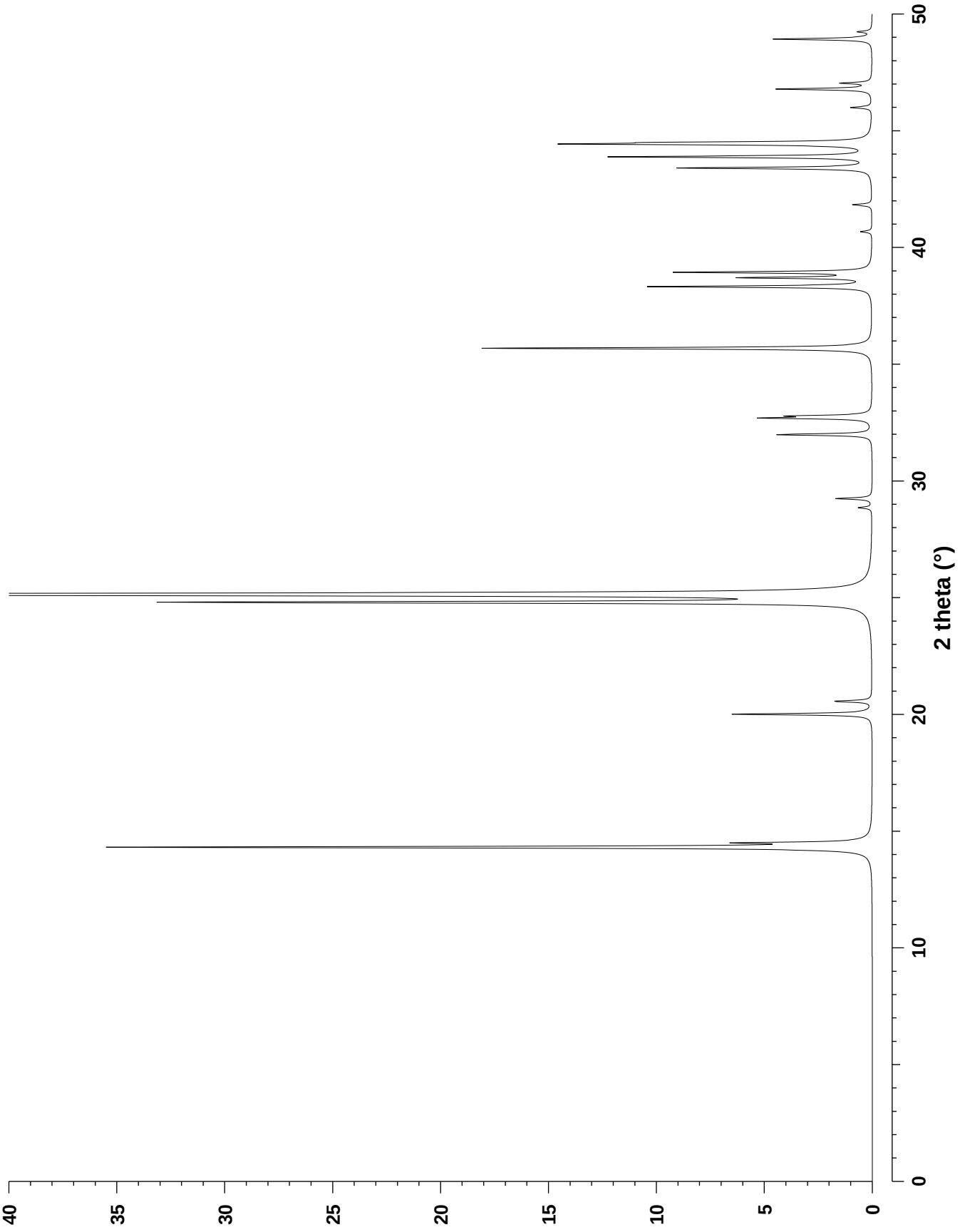
CRYSTAL DATA: $I\overline{4}$ (No. 82)
$a = 8.640$ Å $b = 8.640$ Å $c = 8.873$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.030$

REFERENCE: I. Hassan and H. D. Grundy,
Canadian Mineralogist **29** 385–390 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	14.31	6.190	8	66.0	1	3	0	32.78	2.732	4	0.3	4	1	1	44.42	2.039	8	11.2
1	1	0	14.50	6.109	4	9.6	2	2	2	35.68	2.516	8	33.8	1	4	1	44.42	2.039	8	12.5
0	0	2	20.01	4.437	2	12.1	1	2	3	38.32	2.349	8	5.6	3	3	0	44.49	2.036	4	14.0
2	0	0	20.56	4.320	4	3.2	2	1	3	38.32	2.349	8	13.7	2	0	4	45.99	1.973	8	1.8
1	1	2	24.80	3.590	8	59.5	1	3	2	38.70	2.326	8	5.9	4	0	2	46.78	1.942	8	8.3
2	1	1	25.14	3.543	8	86.2	3	1	2	38.70	2.326	8	5.2	2	4	0	47.03	1.932	4	1.3
1	2	1	25.14	3.543	8	100.0	3	2	1	38.93	2.313	8	5.4	4	2	0	47.03	1.932	4	1.3
2	0	2	28.85	3.095	8	1.2	2	3	1	38.93	2.313	8	11.4	3	2	3	48.92	1.862	8	7.1
2	2	0	29.24	3.055	4	3.1	0	0	4	40.67	2.218	2	1.0	2	3	3	48.92	1.862	8	1.5
1	0	3	31.98	2.798	8	8.2	4	0	0	41.82	2.160	4	1.7	3	3	2	49.23	1.851	8	1.2
3	0	1	32.69	2.739	8	8.9	1	1	4	43.40	2.085	8	16.7							
3	1	0	32.78	2.732	4	5.9	3	0	3	43.88	2.063	8	22.6							

Tugtupite

SOD



STF SSZ-35, Calcined

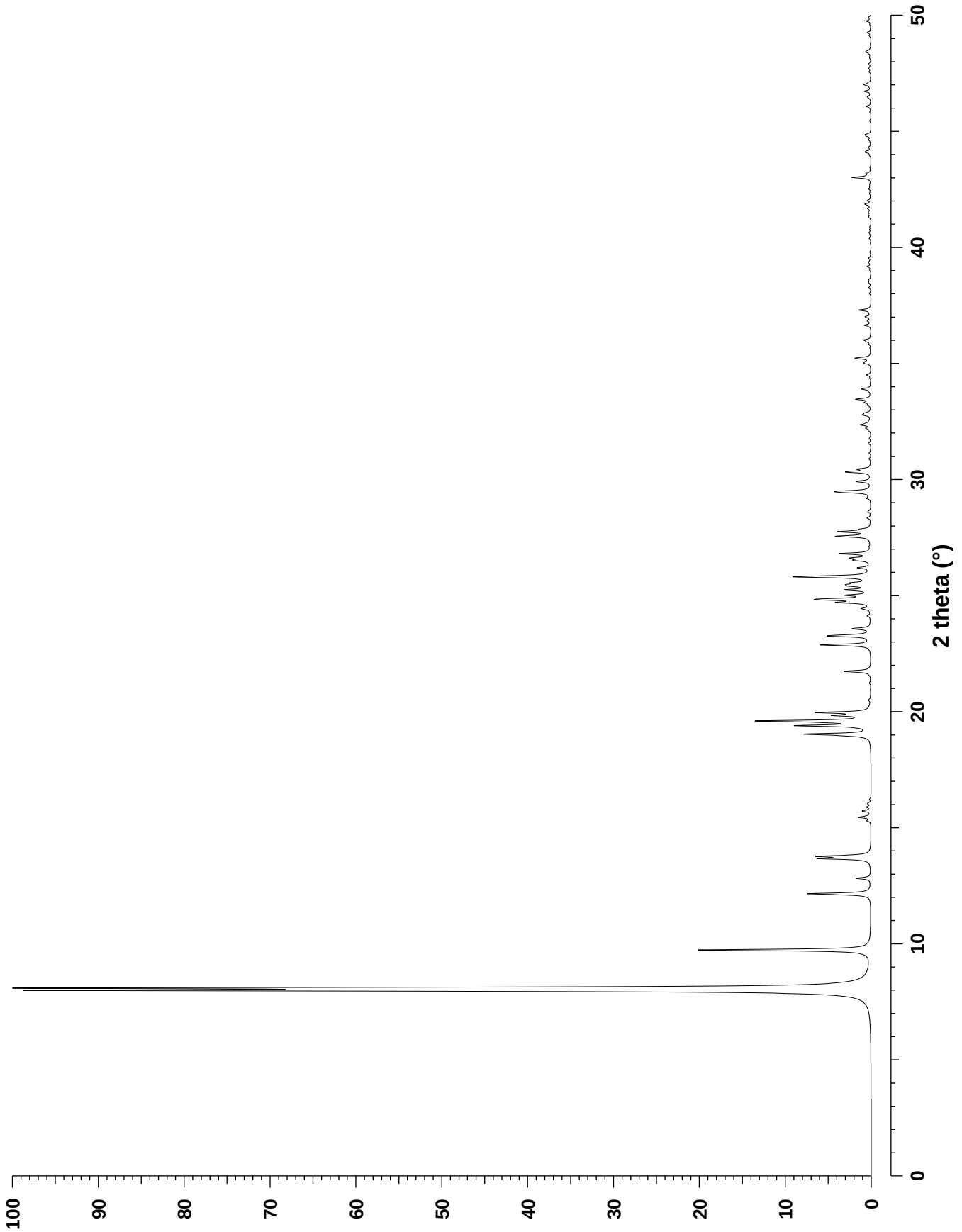
CHEMICAL COMPOSITION: $[Si_{16}O_{32}]$

REFINED COMPOSITION: $[Si_{16}O_{32}]$

CRYSTAL DATA: $P\bar{1}$ (No. 2)
$a = 11.4114$ Å $b = 11.5268$ Å $c = 7.3770$ Å
$\alpha = 94.661°$ $\beta = 96.206°$ $\gamma = 104.892°$
X-ray Rietveld refinement, $R_p = 0.0995$, $R_{wp} = 0.1188$

REFERENCE: P. Wagner, S. I. Zones, M. E. Davis and R. C. Medrud, *Angew. Chem., Int. ed.* **38** 1269–1272 (1999).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	7.99	11.068	2	98.4	-1	1	2	26.19	3.403	2	1.6	3	2	1	36.97	2.431	2	0.2
1	0	0	8.09	10.929	2	100.0	1	-1	2	26.52	3.361	2	1.9	0	0	3	37.01	2.429	2	0.6
1	-1	0	9.73	9.091	2	22.8	0	1	2	26.61	3.349	2	2.4	-1	-1	3	37.29	2.412	2	1.6
0	0	1	12.15	7.286	2	8.4	-2	-2	1	26.80	3.327	2	2.8	1	-4	2	38.27	2.352	2	0.2
1	1	0	12.82	6.905	2	2.0	1	0	2	26.81	3.325	2	1.3	-2	0	3	38.49	2.339	2	0.2
-1	0	1	13.67	6.476	2	6.3	1	3	0	27.51	3.242	2	0.3	2	2	2	38.61	2.332	2	0.2
0	-1	1	13.77	6.430	2	6.5	-2	0	2	27.55	3.238	2	4.4	-3	-3	1	39.17	2.300	2	0.5
0	1	1	15.30	5.791	2	0.5	-3	2	1	27.60	3.231	2	0.2	-4	2	2	39.36	2.289	2	0.2
-1	1	1	15.45	5.737	2	1.6	0	-2	2	27.75	3.215	2	4.1	-1	-2	3	39.53	2.280	2	0.3
1	0	1	15.49	5.719	2	0.2	2	-3	1	27.85	3.203	2	0.9	-2	-4	1	40.38	2.234	2	0.2
1	-1	1	15.72	5.636	2	1.1	0	3	1	28.33	3.150	2	0.4	-1	-4	2	40.63	2.220	2	0.2
1	-2	0	15.89	5.577	2	0.5	-3	-1	1	28.61	3.120	2	0.4	0	5	0	40.76	2.214	2	0.2
0	2	0	16.02	5.534	2	0.2	-2	-1	2	29.18	3.060	2	0.4	-5	2	1	40.88	2.207	2	0.2
2	-1	0	16.05	5.523	2	0.3	1	1	2	29.44	3.034	2	1.8	5	0	0	41.30	2.186	2	0.3
2	0	0	16.22	5.464	2	0.2	3	-3	0	29.48	3.030	2	3.9	-4	4	1	41.40	2.181	2	0.3
-2	0	1	18.95	4.683	2	1.6	-1	2	2	29.91	2.988	2	1.9	-5	0	1	41.51	2.175	2	0.3
0	-2	1	19.00	4.670	2	1.3	2	2	1	30.32	2.948	2	3.2	3	-5	0	41.67	2.167	2	0.4
1	1	1	19.03	4.663	2	7.6	2	-1	2	30.44	2.937	2	1.6	-2	2	3	41.85	2.159	2	0.3
-2	1	1	19.39	4.578	2	9.3	0	2	2	30.88	2.896	2	0.3	4	-4	1	41.85	2.158	2	0.5
2	-2	0	19.53	4.545	2	2.5	1	-4	0	31.14	2.872	2	0.3	5	-3	0	42.02	2.150	2	0.4
1	-2	1	19.60	4.530	2	14.2	4	-1	0	31.55	2.835	2	0.4	2	-2	3	42.52	2.126	2	0.2
1	2	0	19.83	4.477	2	4.2	3	-3	1	32.20	2.780	2	0.6	3	3	1	43.01	2.103	2	2.5
2	1	0	19.96	4.449	2	6.8	0	4	0	32.35	2.767	2	1.2	3	-5	1	43.17	2.095	2	0.4
-1	2	1	20.50	4.333	2	0.3	4	-2	0	32.42	2.761	2	0.4	0	5	1	44.09	2.054	2	0.6
0	2	1	21.23	4.184	2	0.2	4	0	0	32.78	2.732	2	0.9	-3	2	3	44.14	2.052	2	0.4
-1	-2	1	21.72	4.091	2	0.9	-2	-2	2	32.85	2.727	2	0.5	-5	1	2	44.63	2.030	2	0.3
-2	-1	1	21.74	4.089	2	2.8	3	2	0	32.86	2.726	2	0.2	1	-5	2	44.79	2.024	2	0.4
-2	2	1	22.87	3.888	2	6.7	-2	-3	1	33.19	2.699	2	0.3	2	-3	3	44.84	2.021	2	0.4
2	-2	1	23.25	3.825	2	4.5	0	-4	1	33.31	2.690	2	0.7	5	0	1	44.86	2.020	2	0.3
1	-3	0	23.29	3.820	2	2.3	-4	0	1	33.45	2.679	2	2.0	-2	3	3	45.82	1.980	2	0.2
3	-1	0	23.57	3.774	2	2.4	-4	2	1	33.79	2.652	2	0.2	-4	-3	1	46.07	1.970	2	0.5
0	3	0	24.12	3.689	2	0.4	2	-4	1	33.89	2.645	2	1.2	-4	1	3	46.48	1.954	2	0.4
0	0	2	24.43	3.643	2	0.2	-1	4	1	34.50	2.600	2	0.6	3	-2	3	46.70	1.945	2	0.2
3	0	0	24.43	3.643	2	0.9	-2	4	1	34.98	2.565	2	0.2	-5	4	1	46.72	1.944	2	0.7
-1	0	2	24.70	3.604	2	4.0	2	-3	2	35.01	2.563	2	0.7	4	-5	1	47.00	1.933	2	0.7
1	2	1	24.82	3.587	2	4.5	3	-4	0	35.07	2.559	2	0.4	0	3	3	47.07	1.930	2	0.2
0	-1	2	24.85	3.583	2	3.4	4	-1	1	35.20	2.549	2	0.4	-3	3	3	47.55	1.912	2	0.2
2	1	1	25.01	3.560	2	2.9	-1	3	2	35.22	2.548	2	1.5	-4	2	3	47.89	1.899	2	0.3
2	-3	0	25.24	3.528	2	3.2	4	-3	0	35.24	2.546	2	0.3	-5	-2	1	48.40	1.881	2	0.3
3	-2	0	25.41	3.505	2	2.1	-2	3	2	35.82	2.507	2	0.2	2	-6	1	48.41	1.880	2	0.3
-3	1	1	25.47	3.497	2	2.1	3	-1	2	35.93	2.499	2	0.4	3	-3	3	48.46	1.879	2	0.3
1	-3	1	25.55	3.486	2	1.9	0	4	1	36.00	2.494	2	0.9	2	2	3	49.10	1.855	2	0.2
0	-3	1	25.80	3.453	2	2.2	4	0	1	36.64	2.453	2	0.8	-4	-3	2	49.25	1.850	2	0.4
2	2	0	25.80	3.453	2	6.8	-1	0	3	36.82	2.441	2	0.3	-1	-1	4	49.74	1.833	2	0.6
-3	0	1	25.84	3.448	2	2.4	-4	3	1	36.84	2.439	2	0.2	3	4	1	49.90	1.828	2	0.3


100
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40
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0
0
10
20
30
40
50
2 theta (°)

STI Stilbite

CHEMICAL COMPOSITION: $|Na_{1.28}Ca_{4.18}Mg_{0.18}(H_2O)_{34.1}|\ [Si_{25.7}Al_{10.3}O_{72}]$
Iceland

REFINED COMPOSITION: $|Na_{1.76}Ca_4(H_2O)_{29.4}|\ [Si_{25.68}Al_{10.32}O_{72}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 13.64$ Å $b = 18.24$ Å $c = 11.27$ Å
$\alpha = 90°$ $\beta = 128.0°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.123$

REFERENCE: E. Galli,
Acta Cryst. **B27** 833–841 (1971).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
-1	1	1	9.46	9.349	4	0.6	1	3	2	29.93	2.985	4	14.6	-6	2	3	40.91	2.206	4	1.6
0	2	0	9.70	9.120	2	100.0	0	0	3	30.19	2.960	2	5.5	3	1	2	41.27	2.187	4	1.1
0	0	1	9.96	8.881	2	24.7	0	6	1	31.09	2.876	4	2.3	-5	5	3	41.60	2.171	4	0.5
-2	0	1	12.98	6.819	2	4.2	0	2	3	31.78	2.816	4	4.4	-5	5	2	41.71	2.165	4	1.4
0	2	1	13.92	6.363	4	4.0	-3	5	1	31.89	2.806	4	6.0	0	2	4	41.88	2.157	4	2.7
-2	2	1	16.23	5.461	4	2.5	-3	1	4	32.15	2.784	4	1.2	0	6	3	42.63	2.121	4	5.7
-2	0	2	16.28	5.444	2	5.3	-2	6	1	32.24	2.777	4	26.1	-2	0	5	42.66	2.119	2	1.7
2	0	0	16.49	5.374	2	4.8	3	1	1	32.57	2.749	4	2.3	-2	8	2	43.01	2.103	4	4.1
-1	3	1	16.70	5.308	4	7.7	-2	0	4	32.82	2.729	2	1.6	2	8	0	43.10	2.099	4	0.6
1	3	0	16.75	5.292	4	3.1	-4	0	4	32.90	2.722	2	19.0	-3	3	5	43.24	2.092	4	0.6
-1	1	2	16.96	5.229	4	2.6	4	0	0	33.34	2.687	2	2.2	-1	7	3	43.53	2.079	4	1.4
-2	2	2	18.98	4.674	4	39.7	-4	4	1	34.46	2.602	4	1.8	1	7	2	43.64	2.074	4	0.5
2	2	0	19.17	4.630	4	41.4	2	2	2	34.62	2.591	4	9.6	-2	2	5	43.85	2.064	4	4.3
0	4	0	19.47	4.560	2	2.4	4	2	0	34.80	2.578	4	3.3	-1	5	4	43.90	2.063	4	2.0
0	0	2	20.00	4.440	2	5.8	-3	5	3	34.87	2.573	4	9.9	-5	5	4	44.03	2.057	4	1.0
-3	1	2	20.68	4.294	4	28.0	-3	3	4	35.10	2.556	4	5.1	1	5	3	44.05	2.056	4	2.9
-3	1	1	20.81	4.268	4	12.2	3	5	0	35.11	2.556	4	8.2	-5	3	5	44.18	2.050	4	6.3
-1	3	2	21.88	4.061	4	61.9	1	7	0	35.45	2.532	4	2.4	2	2	3	44.20	2.049	4	1.1
0	4	1	21.91	4.057	4	35.8	3	3	1	35.49	2.529	4	2.1	-5	5	1	44.35	2.042	4	2.0
1	3	1	22.00	4.039	4	60.4	0	6	2	35.80	2.508	4	4.9	-6	4	3	44.54	2.034	4	2.2
0	2	2	22.27	3.992	4	14.5	-1	5	3	35.83	2.506	4	0.5	-2	6	4	44.62	2.031	4	1.5
-2	4	1	23.47	3.791	4	2.4	0	4	3	36.18	2.483	4	4.6	0	8	2	44.68	2.028	4	1.9
-2	0	3	23.76	3.744	2	12.3	-1	1	4	36.26	2.477	4	0.5	5	3	0	44.71	2.027	4	7.7
2	0	1	24.06	3.699	2	13.2	-5	3	3	36.39	2.469	4	3.1	4	6	0	45.03	2.013	4	0.4
-3	1	3	25.02	3.560	4	0.5	-5	1	4	36.41	2.467	4	3.3	-6	0	1	45.04	2.013	2	1.2
-3	3	1	25.02	3.559	4	1.8	1	1	3	36.44	2.466	4	2.6	4	4	1	45.43	1.997	4	2.4
-2	4	2	25.48	3.496	4	2.2	-5	3	2	36.52	2.461	4	4.2	0	4	4	45.43	1.996	4	0.7
2	4	0	25.62	3.477	4	6.2	-5	1	1	36.79	2.443	4	9.2	-6	2	5	45.69	1.986	4	0.9
1	5	0	25.79	3.454	4	2.4	-2	6	3	38.13	2.360	4	3.9	-6	4	2	45.88	1.978	4	2.1
2	2	1	26.00	3.427	4	4.0	-1	7	2	38.28	2.351	4	2.1	-2	8	3	46.64	1.947	4	0.5
-4	0	2	26.13	3.410	2	22.4	2	6	1	38.33	2.349	4	1.8	-7	1	4	47.12	1.929	4	0.9
-1	1	3	26.30	3.389	4	11.3	1	7	1	38.35	2.347	4	2.1	-2	4	5	47.29	1.922	4	1.1
1	1	2	26.47	3.368	4	8.7	-2	4	4	38.44	2.342	4	0.7	-1	9	2	47.88	1.900	4	0.9
-4	0	3	27.90	3.197	2	16.4	2	4	2	38.73	2.325	4	0.5	1	9	1	47.94	1.898	4	1.8
-4	2	2	27.94	3.194	4	25.1	4	4	0	38.90	2.315	4	3.6	-4	8	2	48.00	1.895	4	2.6
0	4	2	28.05	3.181	4	4.7	-5	3	4	39.09	2.304	4	0.8	3	5	2	48.25	1.886	4	1.9
-4	0	1	28.16	3.169	2	14.6	1	3	3	39.11	2.303	4	2.3	-5	7	3	48.54	1.875	4	4.6
-3	3	3	28.64	3.116	4	9.3	-6	0	3	39.65	2.273	2	3.8	-4	0	6	48.64	1.872	2	0.6
3	3	0	28.92	3.087	4	3.7	-4	0	5	40.07	2.250	2	1.4	-5	5	5	48.70	1.870	4	3.6
0	6	0	29.38	3.040	2	4.8	-3	7	1	40.25	2.241	4	1.4	-5	1	6	48.95	1.861	4	0.6
-1	5	2	29.45	3.033	4	24.4	-3	5	4	40.45	2.230	4	2.4	5	5	0	49.20	1.852	4	1.3
1	5	1	29.54	3.024	4	28.1	4	0	1	40.62	2.221	2	1.0	-4	8	1	49.23	1.851	4	0.8
-4	2	3	29.60	3.017	4	10.2	0	0	4	40.63	2.220	2	2.0	-7	3	4	49.31	1.848	4	1.4
-1	3	3	29.78	3.000	4	10.4	-3	1	5	40.79	2.212	4	1.7	-3	9	2	49.48	1.842	4	0.8
-4	2	1	29.85	2.993	4	5.1	3	5	1	40.80	2.212	4	1.3	5	1	1	49.65	1.836	4	1.8

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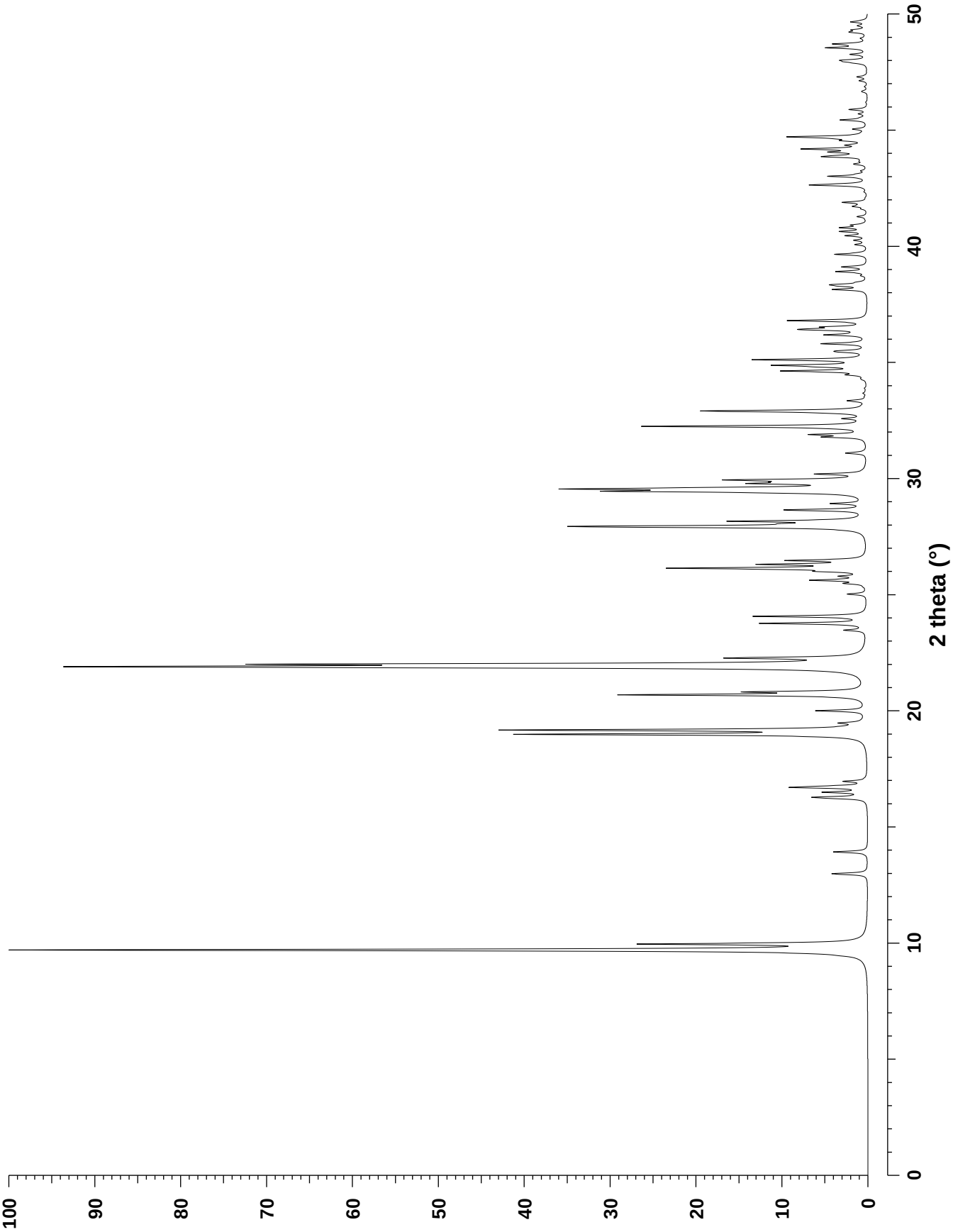
STI



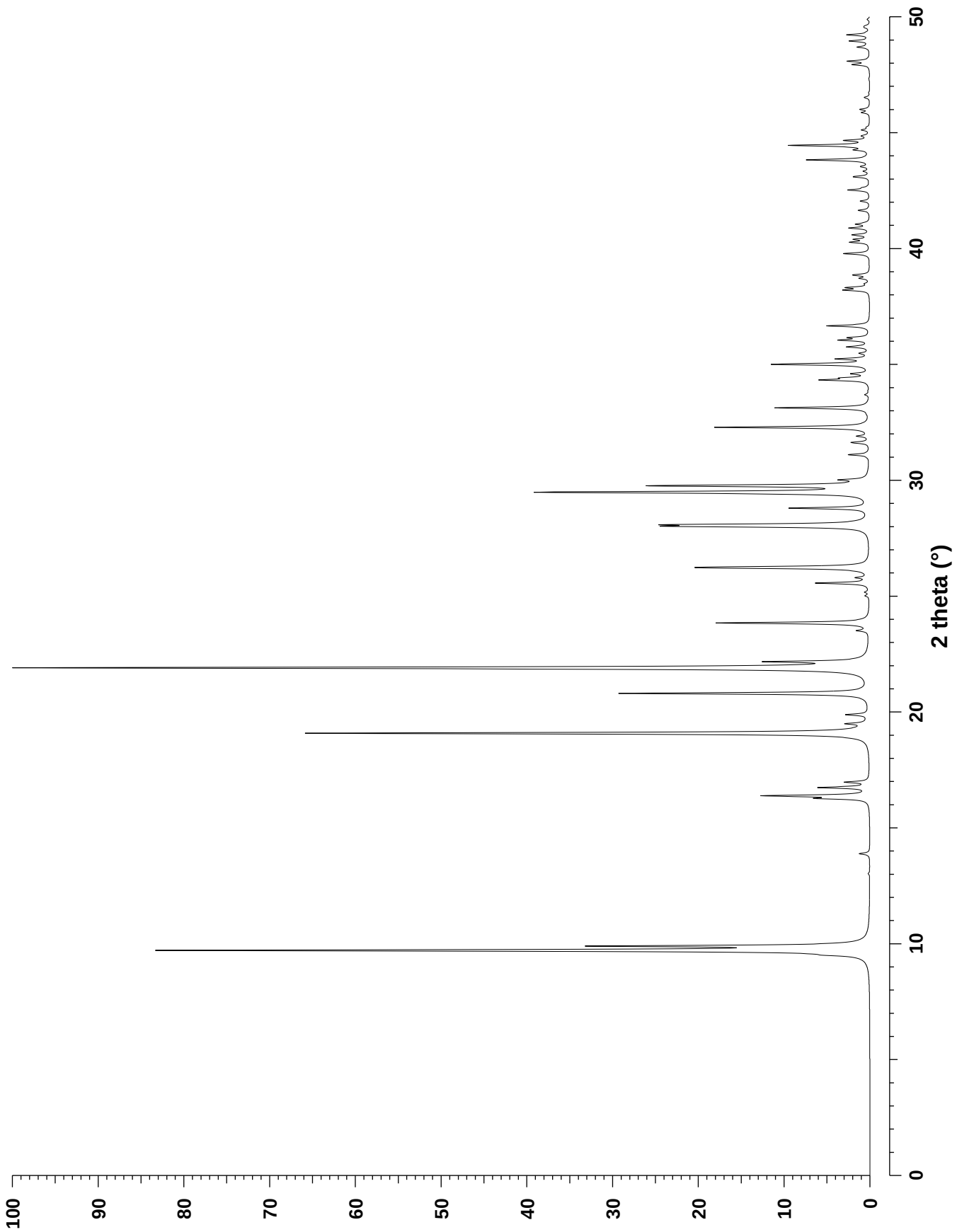
CHEMICAL COMPOSITION: $|Ca_{7.56}Mg_{0.06}Sr_{0.02}Na_{0.34}K_{0.28}(H_2O)_{56.2}|\ [Si_{56.04}Al_{15.86}Fe_{0.12}O_{144}]$
Villanova-Monteleone, Sardinia, Italy

REFINED COMPOSITION: $|Ca_8(H_2O)_{55.52}|\ [Si_{56}Al_{16}O_{144}]$

CRYSTAL DATA: *Fmmm* (No. 69)
$a = 13.599$ Å $b = 18.222$ Å $c = 17.863$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.082$

REFERENCE: E. Galli and A. Alberti,
Bull. Soc. Fr. Minéral. Crystallogr. **98** 11–18 (1975).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	9.51	9.304	8	2.7	0	6	2	31.10	2.875	4	3.0	5	1	5	42.04	2.149	8	1.3
0	2	0	9.71	9.111	2	100.0	0	2	6	31.62	2.830	4	2.5	0	6	6	42.52	2.126	4	3.0
0	0	2	9.90	8.932	2	36.2	3	5	1	31.90	2.805	8	1.6	2	0	8	42.62	2.121	4	0.8
2	0	0	13.02	6.799	2	0.2	3	1	5	32.28	2.773	8	3.8	2	8	2	43.09	2.099	8	2.3
0	2	2	13.88	6.378	4	1.5	2	6	0	32.28	2.773	4	18.2	3	3	7	43.33	2.088	8	0.8
2	2	0	16.27	5.449	4	6.3	4	0	4	33.12	2.705	4	13.5	1	7	5	43.53	2.079	8	1.1
2	0	2	16.38	5.410	4	14.7	5	1	1	33.69	2.660	8	0.6	2	2	8	43.82	2.066	8	3.3
1	3	1	16.74	5.297	8	7.1	2	6	2	33.85	2.648	8	0.1	1	5	7	43.82	2.066	8	5.6
1	1	3	16.97	5.225	8	3.4	2	2	6	34.32	2.613	8	6.6	5	5	3	44.25	2.047	8	1.8
2	2	2	19.08	4.652	8	80.2	4	4	2	34.41	2.606	8	3.2	5	3	5	44.44	2.039	8	11.4
0	4	0	19.49	4.556	2	2.8	4	2	4	34.59	2.593	8	2.3	6	4	0	44.65	2.029	4	0.7
0	0	4	19.88	4.466	2	3.2	3	5	3	35.00	2.564	8	13.8	2	6	6	44.66	2.029	8	0.7
3	1	1	20.80	4.271	8	35.5	3	3	5	35.23	2.547	8	4.5	0	8	4	44.66	2.029	4	2.0
1	3	3	21.90	4.058	8	90.3	1	7	1	35.47	2.531	8	1.3	6	0	4	44.84	2.021	4	0.7
0	4	2	21.90	4.058	4	31.4	0	6	4	35.75	2.511	4	3.0	4	6	4	44.87	2.020	8	0.3
0	2	4	22.17	4.010	4	12.7	1	5	5	35.81	2.507	8	0.4	4	4	6	45.11	2.010	8	1.1
2	4	0	23.51	3.785	4	1.5	0	4	6	36.04	2.492	4	4.2	0	4	8	45.22	2.005	4	0.4
2	0	4	23.84	3.733	4	21.8	1	1	7	36.15	2.485	8	2.7	6	4	2	45.86	1.979	8	1.1
3	3	1	25.01	3.560	8	0.6	5	3	1	36.55	2.459	8	0.1	6	2	4	46.00	1.973	8	1.4
3	1	3	25.17	3.538	8	0.6	5	1	3	36.66	2.451	8	6.1	1	1	9	46.51	1.953	8	0.8
2	4	2	25.56	3.485	8	7.6	2	6	4	38.20	2.356	8	3.5	2	8	4	46.72	1.944	8	0.1
2	2	4	25.79	3.454	8	1.5	1	7	3	38.31	2.349	8	3.1	3	5	7	47.92	1.898	8	0.7
1	5	1	25.79	3.454	8	0.2	2	4	6	38.47	2.340	8	0.5	1	9	3	47.93	1.898	8	1.7
4	0	0	26.21	3.400	2	16.0	4	4	4	38.71	2.326	8	1.3	4	8	0	48.08	1.892	4	3.1
1	1	5	26.25	3.395	8	15.0	1	3	7	38.85	2.318	8	2.3	5	7	1	48.68	1.870	8	1.7
0	4	4	27.98	3.189	4	3.0	6	0	0	39.77	2.266	2	3.7	1	3	9	48.73	1.869	8	0.1
4	2	0	28.01	3.185	4	21.9	4	6	0	39.80	2.265	4	0.1	4	0	8	48.79	1.866	4	0.2
4	0	2	28.08	3.177	4	24.1	4	0	6	40.26	2.240	4	2.1	5	5	5	48.95	1.861	8	2.8
3	3	3	28.79	3.101	8	11.1	3	7	1	40.27	2.240	8	0.6	5	1	7	49.21	1.851	8	2.5
0	6	0	29.41	3.037	2	5.2	0	0	8	40.39	2.233	2	2.0	4	8	2	49.22	1.851	8	0.8
1	5	3	29.48	3.030	8	45.7	3	5	5	40.58	2.223	8	2.4	6	4	4	49.33	1.847	8	0.2
1	3	5	29.75	3.003	8	22.7	3	1	7	40.88	2.207	8	2.8	7	3	1	49.52	1.841	8	0.5
4	2	2	29.78	3.000	8	11.7	6	2	0	41.04	2.199	4	1.8	3	9	1	49.57	1.839	8	0.4
0	0	6	30.01	2.977	2	3.4	4	6	2	41.11	2.195	8	0.3	7	1	3	49.61	1.837	8	0.3
2	4	4	30.97	2.887	8	0.1	0	2	8	41.64	2.169	4	1.6	4	2	8	49.88	1.828	8	0.4


100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
2 theta (°)

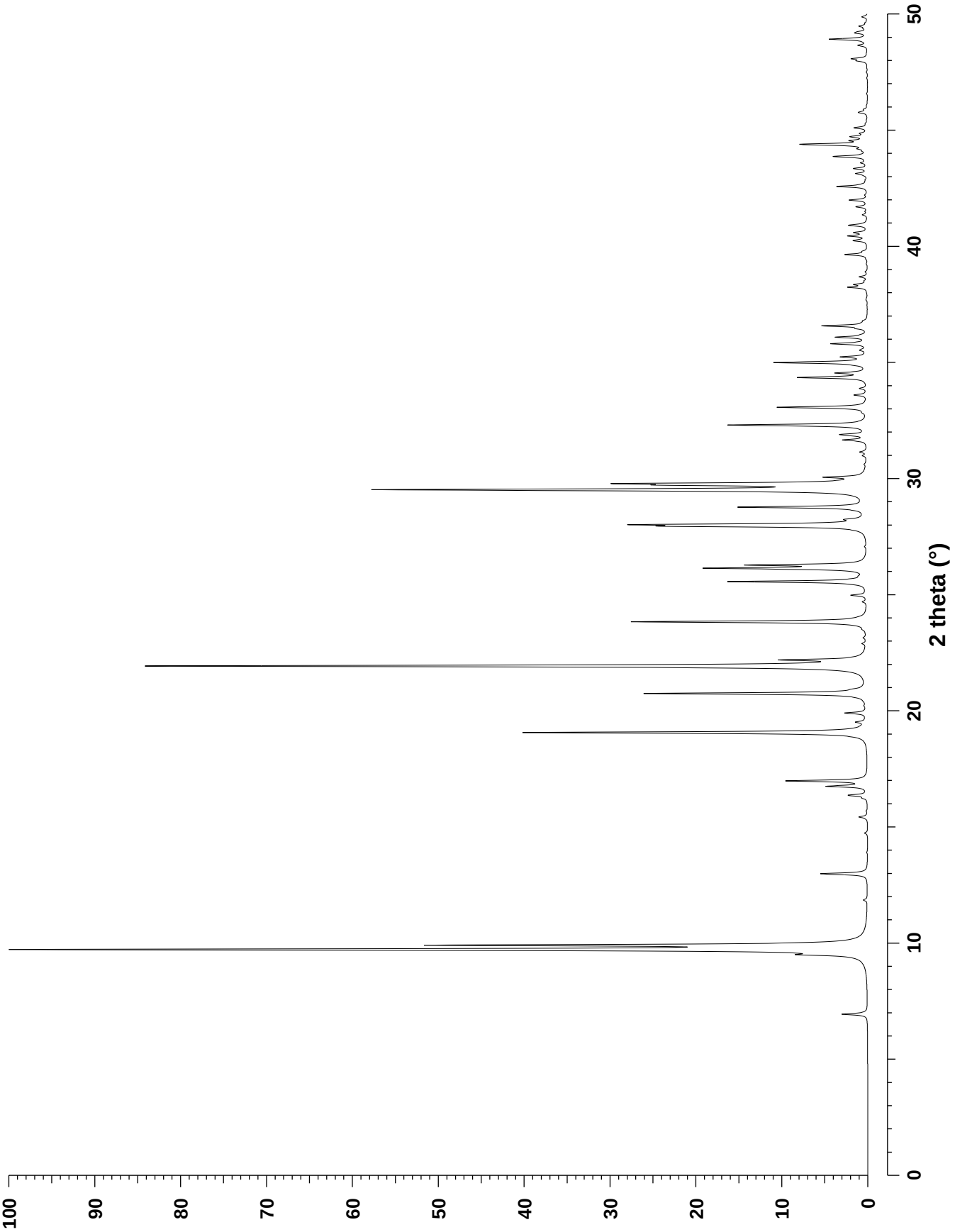
CHEMICAL COMPOSITION: $|Na_{10.9}K_{2.1}Mg_{0.3}Ca_{1.7}(H_2O)_{51.6}|\ [Si_{55.6}Al_{16.4}O_{144}]$
Capo Pula, Sardinia, Italy

REFINED COMPOSITION: $|Na_{9.812}K_{1.912}Mg_{0.032}Ca_{1.52}(H_2O)_{58.56}|\ [Si_{55.58}Al_{16.42}O_{144}]$

CRYSTAL DATA: *Amma* (No. 63) **cab** setting
$a = 13.643$ Å $b = 18.200$ Å $c = 17.842$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.067$

REFERENCE: E. Galli and A. Alberti,
Bull. Soc. Fr. Minéral. Crystallogr. **98** 331–340 (1975).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	1	6.94	12.741	4	3.1	4	2	2	29.71	3.007	8	16.5	3	1	7	40.89	2.207	8	1.4
1	1	1	9.50	9.312	8	5.0	3	2	4	29.72	3.006	8	0.4	6	2	0	40.91	2.206	4	0.9
0	2	0	9.72	9.100	2	100.0	1	3	5	29.78	3.000	8	25.0	0	8	2	40.94	2.204	4	0.3
0	0	2	9.91	8.921	2	48.5	0	0	6	30.05	2.974	2	4.2	3	4	6	41.35	2.184	8	0.6
1	0	2	11.85	7.466	4	0.5	4	1	3	30.61	2.920	8	0.2	4	2	6	41.49	2.176	8	0.2
2	0	0	12.98	6.821	2	5.6	2	4	4	30.98	2.886	8	0.5	5	5	1	41.68	2.167	8	0.3
2	1	1	14.73	6.014	8	0.4	0	6	2	31.14	2.872	4	0.8	0	2	8	41.70	2.166	4	1.1
0	3	1	15.43	5.744	4	1.0	0	2	6	31.65	2.827	4	2.8	5	1	5	41.98	2.152	8	2.1
2	2	0	16.24	5.458	4	0.4	1	6	2	31.84	2.810	8	0.8	6	2	2	42.20	2.142	8	0.2
2	0	2	16.36	5.419	4	2.2	3	5	1	31.89	2.806	8	2.7	0	6	6	42.57	2.123	4	3.6
1	3	1	16.75	5.294	8	4.7	3	1	5	32.26	2.775	8	1.7	2	0	8	42.65	2.120	4	0.4
1	1	3	16.98	5.223	8	9.6	2	6	0	32.30	2.772	4	15.7	0	7	5	43.04	2.101	4	0.2
2	2	2	19.06	4.656	8	41.0	4	4	0	32.82	2.729	4	0.2	2	8	2	43.12	2.098	8	1.3
0	4	0	19.51	4.550	2	1.1	4	0	4	33.06	2.709	4	10.7	3	3	7	43.34	2.088	8	1.6
0	0	4	19.90	4.460	2	2.6	5	1	1	33.59	2.668	8	1.5	1	7	5	43.58	2.077	8	0.7
2	3	1	20.21	4.394	8	0.2	2	6	2	33.87	2.647	8	0.8	5	4	4	43.68	2.072	8	0.2
3	1	1	20.74	4.283	8	26.5	2	2	6	34.34	2.611	8	7.3	2	2	8	43.85	2.065	8	2.0
0	3	3	20.92	4.247	4	0.6	4	4	2	34.36	2.610	8	1.0	1	5	7	43.87	2.064	8	2.3
1	0	4	20.95	4.240	4	0.2	4	2	4	34.54	2.597	8	3.5	4	7	1	44.09	2.054	8	0.3
1	3	3	21.92	4.055	8	69.6	0	7	1	34.87	2.573	4	0.6	5	5	3	44.19	2.050	8	0.8
0	4	2	21.93	4.053	4	17.0	3	5	3	34.99	2.564	8	11.0	5	3	5	44.38	2.041	8	7.8
3	0	2	21.94	4.052	4	0.2	3	3	5	35.23	2.548	8	2.8	6	4	0	44.54	2.034	4	1.6
0	2	4	22.19	4.005	4	8.7	1	7	1	35.51	2.528	8	0.6	2	6	6	44.69	2.028	8	0.7
1	4	2	22.89	3.885	8	0.4	0	1	7	35.56	2.524	4	0.2	0	8	4	44.72	2.027	4	1.2
1	2	4	23.14	3.843	8	0.3	0	6	4	35.80	2.508	4	4.1	6	0	4	44.73	2.026	4	0.2
2	4	0	23.50	3.785	4	0.2	0	4	6	36.08	2.489	4	3.7	4	6	4	44.85	2.021	8	0.7
2	0	4	23.83	3.733	4	28.1	1	1	7	36.19	2.482	8	0.4	4	4	6	45.09	2.011	8	1.4
2	3	3	24.69	3.605	8	0.5	4	5	1	36.45	2.465	8	0.3	0	9	1	45.12	2.009	4	0.3
3	3	1	24.97	3.565	8	1.8	5	3	1	36.45	2.465	8	0.6	0	4	8	45.28	2.003	4	0.2
0	1	5	25.44	3.502	4	0.4	5	1	3	36.57	2.457	8	5.3	3	8	2	45.74	1.984	8	0.3
2	4	2	25.56	3.485	8	16.5	1	4	6	36.70	2.449	8	0.3	6	4	2	45.75	1.983	8	0.7
2	2	4	25.79	3.454	8	0.3	4	1	5	36.78	2.443	8	0.4	1	4	8	45.79	1.981	8	0.3
4	0	0	26.13	3.411	2	18.5	2	5	5	37.68	2.387	8	0.2	6	2	4	45.89	1.977	8	0.3
1	1	5	26.27	3.392	8	13.2	2	6	4	38.23	2.354	8	2.2	1	9	3	47.98	1.896	8	1.0
4	1	1	27.06	3.295	8	0.2	1	7	3	38.35	2.347	8	1.5	2	1	9	48.05	1.893	8	0.2
4	2	0	27.94	3.194	4	18.9	2	4	6	38.50	2.338	8	0.3	4	8	0	48.07	1.893	4	1.6
4	0	2	28.01	3.186	4	19.7	4	4	4	38.68	2.328	8	0.6	5	7	1	48.64	1.872	8	1.1
0	4	4	28.01	3.185	4	3.9	5	0	4	38.68	2.328	4	0.4	5	5	5	48.90	1.862	8	4.5
3	0	4	28.02	3.184	4	0.2	1	3	7	38.89	2.316	8	0.2	5	1	7	49.17	1.853	8	1.1
2	5	1	28.23	3.161	8	1.6	6	0	0	39.64	2.274	2	2.7	4	8	2	49.21	1.851	8	0.2
2	1	5	28.65	3.115	8	0.2	4	6	0	39.77	2.267	4	0.5	6	4	4	49.23	1.851	8	0.6
3	3	3	28.76	3.104	8	15.1	4	0	6	40.23	2.241	4	1.5	7	3	1	49.38	1.846	8	0.3
0	6	0	29.45	3.033	2	3.1	3	7	1	40.27	2.239	8	0.3	7	1	3	49.47	1.843	8	0.9
1	5	3	29.51	3.027	8	56.1	0	0	8	40.44	2.230	2	2.2	3	9	1	49.60	1.838	8	0.2
3	4	2	29.52	3.026	8	0.8	3	5	5	40.58	2.223	8	1.5	4	2	8	49.87	1.829	8	0.7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2 theta (°)

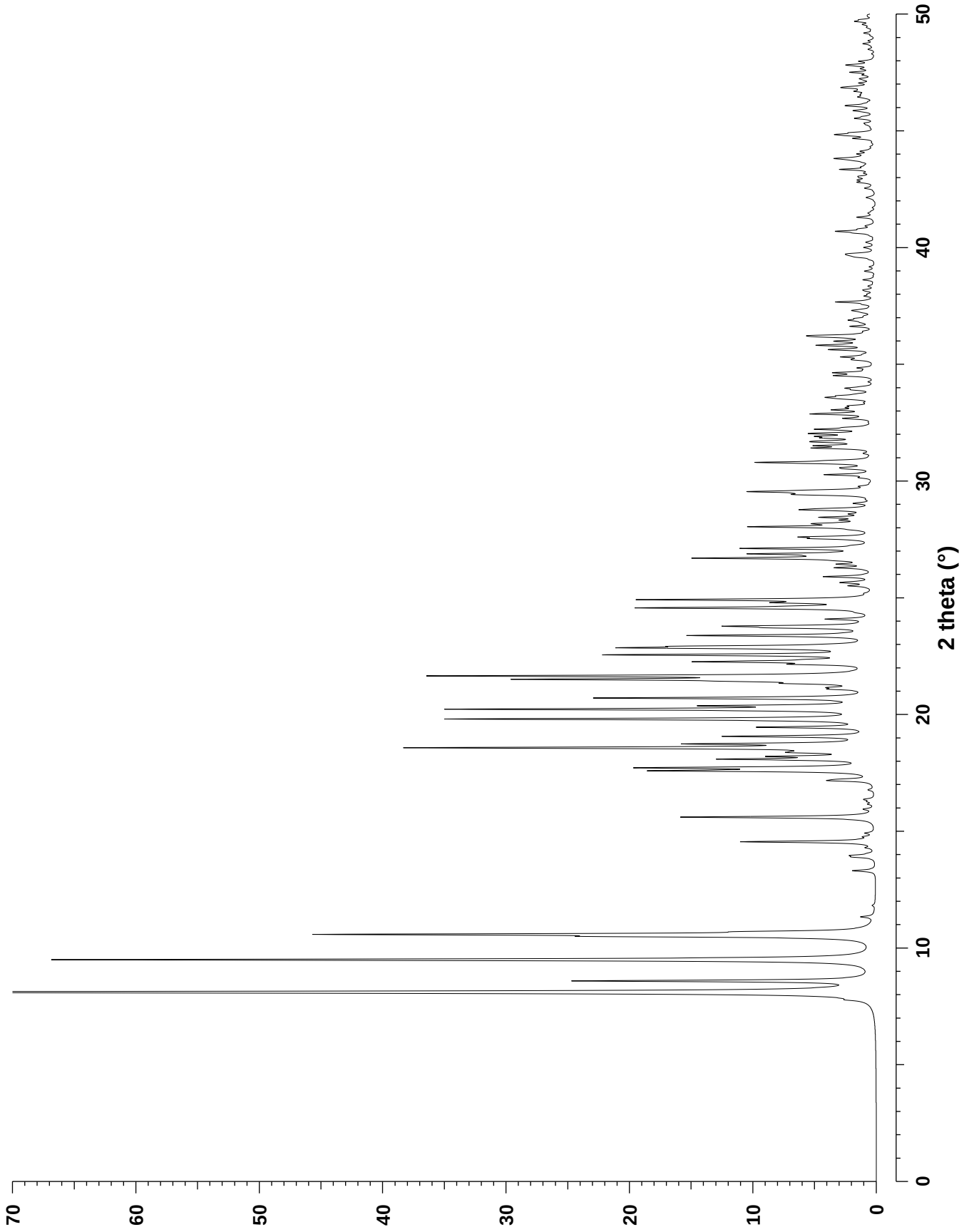
CHEMICAL COMPOSITION: $|(C_{13}H_{24}N)_{4.1}F_{3.3}(OH)_{0.8}(H_2O)_{1.6}|\ [Si_{64}O_{128}]$
$C_{13}H_{24}NF$ = *N,N,N*-trimethyl-1-adamantammonium fluoride

REFINED COMPOSITION: $|C_{52}N_4F_{2.84}|\ [Si_{64}O_{128}]$

CRYSTAL DATA: $P1\,2_1/n\,1$ (No. 14) unique axis **b**, cell choice 2
$a = 12.9594$ Å $b = 21.7919$ Å $c = 13.5980$ Å
$\alpha = 90.0°$ $\beta = 101.855°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_{F_{obs}} = 0.0811$, $wR_{F^2} = 0.1657$

REFERENCE: M. A. Camblor, M.-J. Diaz-Cabanas, J. Perez-Pariente, S. J. Teat, W. Clegg, I. J. Shannon, P. Lightfoot, P. A. Wright and R. E. Morris, *Angew. Chem., Int. Ed.* **37** 2122–2126 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.07	10.962	4	11.0	1	1	3	22.92	3.879	4	12.3	1	3	4	31.66	2.826	4	3.2
0	2	0	8.11	10.896	2	100.0	2	4	1	23.38	3.805	4	15.4	-3	2	4	31.70	2.823	4	2.6
-1	0	1	8.59	10.298	2	25.2	3	1	1	23.71	3.753	4	6.4	0	6	3	31.84	2.810	4	3.1
-1	1	1	9.50	9.311	4	70.5	-2	4	2	23.78	3.742	4	11.2	-1	7	2	31.91	2.805	4	3.6
0	2	1	10.49	8.431	4	17.5	-3	3	1	24.08	3.695	4	3.7	2	7	0	32.03	2.795	4	4.9
1	0	1	10.58	8.363	2	44.6	2	3	2	24.56	3.624	4	19.4	-4	2	3	32.21	2.779	4	4.1
1	2	0	10.70	8.265	4	7.1	-1	5	2	24.64	3.614	4	2.8	-3	6	1	32.29	2.772	4	1.7
0	0	2	13.31	6.654	2	2.0	2	5	0	24.79	3.592	4	6.1	4	4	0	32.68	2.740	4	2.0
0	3	1	13.89	6.376	4	1.4	-2	5	1	24.91	3.574	4	19.5	2	0	4	32.87	2.725	2	4.9
2	0	0	13.96	6.341	2	1.6	1	6	0	25.51	3.492	4	1.9	-3	3	4	33.04	2.711	4	3.0
2	1	0	14.55	6.089	4	11.6	-3	3	2	25.65	3.474	4	2.6	-3	5	3	33.22	2.697	4	1.6
0	2	2	15.60	5.679	4	16.7	0	4	3	25.90	3.440	4	4.2	0	8	1	33.58	2.669	4	2.8
2	1	1	17.17	5.165	4	3.2	-3	1	3	26.28	3.391	4	3.0	1	8	0	33.65	2.663	4	2.1
-2	0	2	17.22	5.149	2	1.7	2	5	1	26.44	3.371	4	2.2	-1	2	5	33.97	2.639	4	1.5
0	4	1	17.59	5.042	4	17.4	-1	1	4	26.58	3.353	4	1.4	-4	5	1	34.51	2.599	4	3.0
-2	1	2	17.70	5.011	4	7.5	3	4	0	26.69	3.340	4	14.7	1	8	1	34.63	2.590	4	3.2
1	4	0	17.72	5.006	4	12.3	2	4	2	26.88	3.317	4	9.5	-3	4	4	34.84	2.575	4	1.3
0	3	2	18.08	4.907	4	12.1	2	1	3	27.10	3.290	4	3.2	2	3	4	35.18	2.551	4	1.2
1	2	2	18.20	4.874	4	7.2	0	1	4	27.11	3.289	4	8.0	-4	4	3	35.31	2.542	4	2.4
-1	3	2	18.37	4.829	4	4.3	3	1	2	27.53	3.240	4	3.5	-5	2	1	35.61	2.521	4	1.7
-1	4	1	18.42	4.816	4	2.2	-2	0	4	27.60	3.232	2	5.3	5	1	0	35.63	2.520	4	1.9
2	3	0	18.57	4.777	4	38.5	2	2	3	28.03	3.183	4	2.9	1	5	4	35.80	2.508	4	2.4
-2	3	1	18.74	4.735	4	14.1	0	2	4	28.04	3.182	4	7.3	3	7	0	35.82	2.507	4	2.4
-2	2	2	19.06	4.656	4	12.4	4	0	0	28.14	3.171	2	1.5	-2	8	1	35.97	2.497	4	1.3
1	4	1	19.45	4.565	4	9.3	-1	6	2	28.18	3.166	4	3.5	-5	2	2	36.16	2.484	4	1.8
-1	0	3	19.80	4.484	2	36.3	2	6	0	28.32	3.152	4	2.0	3	4	3	36.19	2.482	4	2.3
-1	1	3	20.22	4.392	4	35.5	3	2	2	28.44	3.138	4	3.4	-3	1	5	36.23	2.479	4	3.8
1	3	2	20.37	4.359	4	12.3	-3	3	3	28.76	3.104	4	4.3	2	6	3	36.62	2.454	4	1.6
2	3	1	20.70	4.290	4	23.3	-2	2	4	28.81	3.099	4	2.8	2	4	4	36.88	2.437	4	1.2
0	4	2	21.08	4.215	4	2.4	-1	3	4	29.04	3.075	4	1.5	3	7	1	37.30	2.411	4	1.3
-2	3	2	21.15	4.201	4	2.3	1	1	4	29.41	3.037	4	3.6	4	6	0	37.66	2.389	4	3.1
-1	4	2	21.33	4.166	4	4.8	3	5	0	29.43	3.035	4	2.0	4	7	0	40.61	2.221	4	1.2
3	1	0	21.41	4.150	4	2.4	0	7	1	29.47	3.031	4	1.9	-5	4	3	40.69	2.217	4	1.7
-1	2	3	21.43	4.147	4	2.7	2	3	3	29.52	3.026	4	2.1	3	4	4	41.29	2.186	4	1.2
2	4	0	21.50	4.132	4	27.0	1	7	0	29.54	3.023	4	7.3	-5	6	2	43.34	2.088	4	2.9
0	2	3	21.63	4.109	4	1.2	2	5	2	29.60	3.017	4	3.1	4	8	0	43.81	2.066	4	2.6
2	1	2	21.64	4.107	4	2.3	1	2	4	30.27	2.952	4	4.0	1	3	6	44.67	2.028	4	1.4
-2	4	1	21.65	4.105	4	33.0	-3	5	2	30.52	2.929	4	1.7	4	7	2	44.83	2.022	4	2.1
-1	5	1	22.15	4.014	4	5.2	4	1	1	30.57	2.924	4	1.9	-5	6	3	44.91	2.018	4	1.6
-3	2	1	22.26	3.993	4	13.9	4	3	0	30.77	2.906	4	2.4	1	4	6	46.08	1.970	4	1.3
-2	1	3	22.35	3.978	4	2.6	-3	4	3	30.79	2.904	4	7.8	-1	0	7	46.84	1.939	2	1.5
1	0	3	22.55	3.942	2	14.7	-3	1	4	30.87	2.897	4	2.4	-5	7	3	47.50	1.914	4	1.6
3	2	0	22.56	3.941	4	8.1	-4	1	3	31.40	2.849	4	2.0	4	8	2	47.81	1.902	4	1.4
2	2	2	22.78	3.904	4	1.5	4	2	1	31.41	2.848	4	2.8	-4	4	6	47.97	1.897	4	1.2
-3	1	2	22.85	3.891	4	18.1	0	4	4	31.51	2.839	4	4.1	-4	5	6	49.68	1.835	4	1.3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2 theta (°)
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TER Terranovaite

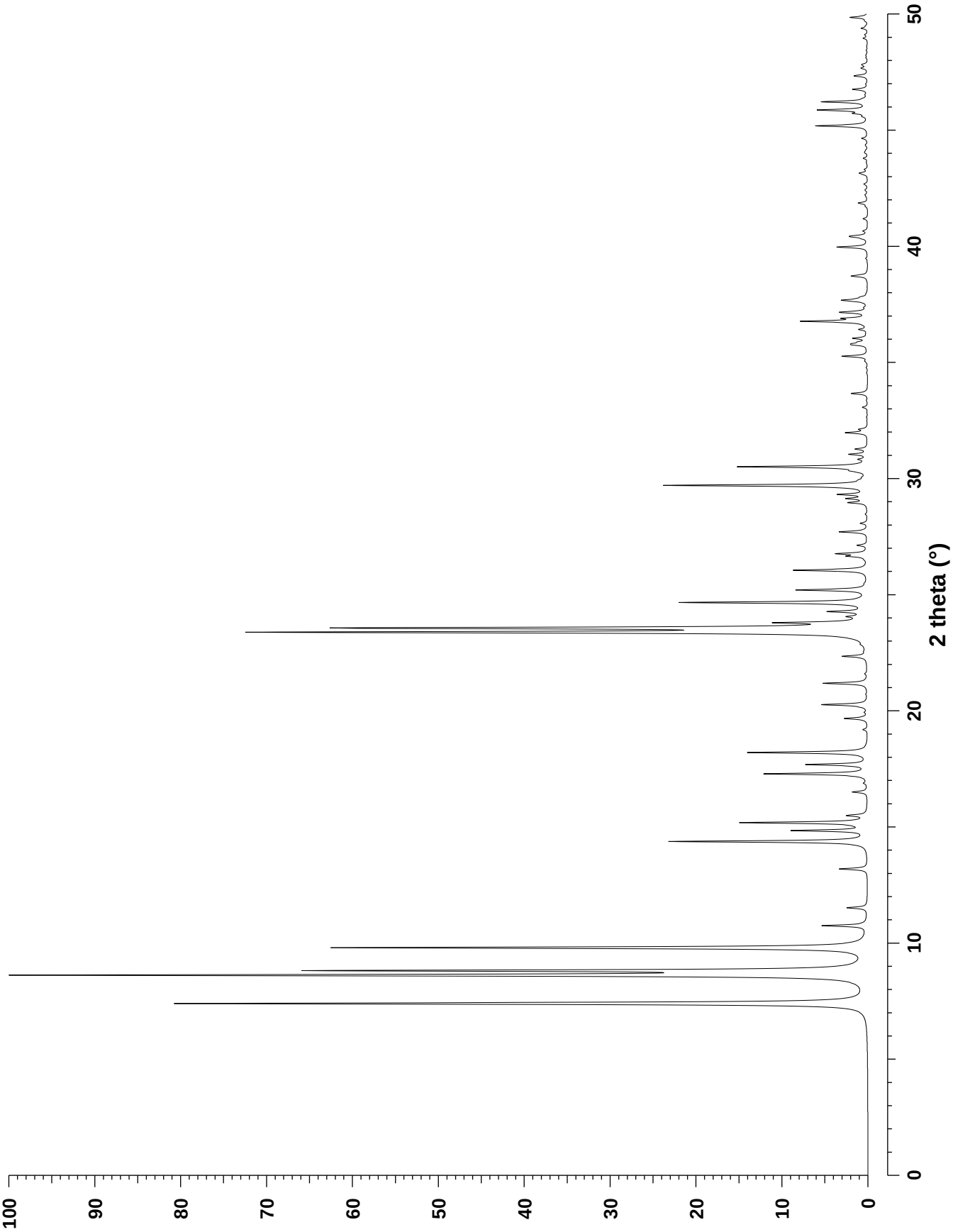
CHEMICAL COMPOSITION: $|Na_{4.2}K_{0.2}Mg_{0.2}Ca_{3.7}(H_2O)_{>29}|\ [Al_{12.3}Si_{67.7}O_{160}]$
Mt. Adamson, N. Victoria Land, Antarctica

REFINED COMPOSITION: $|Na_{4.23}K_{0.167}Mg_{0.167}Ca_{3.74}|\ [Al_{12.32}Si_{67.68}O_{160}]$

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 9.747$ Å $b = 23.880$ Å $c = 20.068$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.071$, $R_w = 0.068$

REFERENCE: E. Galli, S. Quartieri, G. Vezzalini, A. Alberti and M. Franzini, *American Mineralogist* **82** 423–429 (1997).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	2	0	7.40	11.940	2	82.9	3	1	1	28.07	3.179	8	0.7	3	5	5	40.40	2.232	8	1.3
0	2	1	8.62	10.261	4	100.0	1	1	6	28.46	3.136	8	0.2	2	0	8	40.44	2.230	4	1.3
0	0	2	8.81	10.034	2	63.4	2	6	0	28.96	3.083	4	2.2	3	7	3	40.65	2.219	8	0.5
1	1	0	9.80	9.024	4	64.1	1	7	2	29.13	3.066	8	0.4	0	2	9	41.18	2.192	4	0.4
1	1	1	10.75	8.230	8	5.3	3	1	2	29.13	3.065	8	1.8	1	5	8	41.71	2.165	8	0.2
0	2	2	11.52	7.682	4	2.4	2	6	1	29.31	3.047	8	3.3	1	9	5	41.85	2.158	8	1.1
1	1	2	13.19	6.710	8	3.4	2	4	4	29.61	3.017	8	0.5	2	10	0	42.14	2.144	4	0.1
1	3	0	14.37	6.165	4	23.7	3	3	0	29.70	3.008	4	24.3	3	1	7	42.21	2.141	8	0.3
0	4	0	14.84	5.970	2	8.8	0	8	0	29.93	2.985	2	0.3	2	10	1	42.39	2.132	8	0.2
1	3	1	15.03	5.893	8	0.3	3	3	1	30.04	2.975	8	0.2	3	7	4	42.43	2.130	8	0.2
0	2	3	15.18	5.836	4	15.2	0	8	1	30.27	2.953	4	0.4	1	11	0	42.67	2.119	4	0.4
0	4	1	15.49	5.722	4	2.3	2	6	2	30.33	2.947	8	1.1	2	6	7	43.09	2.099	8	0.3
1	1	3	16.50	5.374	8	1.8	1	3	6	30.40	2.940	8	0.4	2	10	2	43.14	2.097	8	0.9
1	3	2	16.88	5.253	8	0.4	1	5	5	30.50	2.931	8	15.4	2	4	8	43.30	2.089	8	0.4
0	4	2	17.28	5.131	4	12.4	1	7	3	30.82	2.901	8	0.5	0	8	7	43.78	2.068	4	0.5
0	0	4	17.68	5.017	2	7.3	3	1	3	30.82	2.901	8	0.3	4	4	4	44.01	2.058	8	0.2
2	0	0	18.20	4.873	2	14.4	3	3	2	31.04	2.881	8	2.1	3	9	0	44.06	2.055	4	0.2
0	2	4	19.19	4.625	4	0.5	0	8	2	31.26	2.861	4	1.4	4	2	5	44.13	2.052	8	0.1
2	2	0	19.67	4.512	4	2.8	2	6	3	31.97	2.800	8	2.6	2	10	3	44.36	2.042	8	0.2
0	4	3	19.93	4.454	4	0.3	0	2	7	32.11	2.788	4	0.9	3	7	5	44.64	2.030	8	0.7
2	2	1	20.17	4.402	8	0.2	1	7	4	33.06	2.710	8	0.6	0	0	10	45.18	2.007	2	6.2
1	1	4	20.25	4.385	8	0.8	3	5	1	33.66	2.663	8	2.0	0	12	0	45.58	1.990	2	0.4
2	0	2	20.26	4.384	4	4.8	3	3	4	34.77	2.580	8	0.2	4	6	3	45.71	1.985	8	1.4
1	5	0	20.71	4.289	4	0.1	1	9	0	35.05	2.560	4	0.2	0	12	1	45.82	1.980	4	0.4
1	5	1	21.18	4.194	8	5.3	2	8	0	35.26	2.545	4	3.1	0	2	10	45.85	1.979	4	0.2
2	2	2	21.59	4.115	8	0.2	3	1	5	35.75	2.511	8	1.3	1	7	8	45.86	1.979	8	5.5
0	6	0	22.34	3.980	2	2.9	0	0	8	35.80	2.509	2	1.2	3	9	3	46.21	1.964	8	5.5
1	5	2	22.55	3.944	8	0.1	2	4	6	35.87	2.504	8	0.7	1	1	10	46.35	1.959	8	0.2
1	3	4	22.85	3.891	8	0.3	3	5	3	36.03	2.493	8	1.7	5	1	0	46.75	1.943	4	1.7
0	4	4	23.16	3.841	4	0.2	2	8	2	36.41	2.467	8	1.0	5	1	1	46.98	1.934	8	0.2
0	2	5	23.38	3.804	4	71.6	2	6	5	36.76	2.445	8	7.8	0	8	8	47.33	1.920	4	1.6
2	4	0	23.56	3.775	4	60.7	4	0	0	36.89	2.437	2	2.5	1	3	10	47.65	1.908	8	0.3
2	2	3	23.79	3.741	8	8.9	2	2	7	37.15	2.420	8	3.2	5	1	2	47.67	1.908	8	0.4
0	6	2	24.05	3.700	4	1.5	1	1	8	37.20	2.417	8	0.2	0	12	3	47.68	1.907	4	0.1
1	1	5	24.27	3.667	8	4.2	3	3	5	37.36	2.407	8	0.3	2	8	7	47.78	1.903	8	0.3
1	5	3	24.66	3.610	8	22.4	1	9	3	37.62	2.391	8	0.8	0	4	10	47.82	1.902	4	0.5
2	4	2	25.20	3.533	8	8.4	0	10	0	37.67	2.388	2	1.9	2	10	5	48.11	1.891	8	0.2
2	0	4	25.48	3.496	4	0.1	4	2	0	37.67	2.388	4	0.8	4	8	0	48.21	1.888	4	0.2
0	6	3	26.05	3.420	4	8.9	1	5	7	37.74	2.383	8	0.6	4	8	1	48.43	1.879	8	0.2
0	0	6	26.65	3.345	2	2.1	2	8	3	37.81	2.379	8	0.6	5	3	2	48.95	1.861	8	0.5
0	4	5	26.76	3.331	4	3.6	0	6	7	38.71	2.326	4	1.8	2	0	10	49.09	1.856	4	0.2
2	4	3	27.12	3.288	8	1.2	0	10	2	38.76	2.323	4	0.4	4	6	5	49.38	1.845	8	0.8
0	2	6	27.70	3.221	4	0.2	2	4	7	39.47	2.283	8	0.2	2	12	0	49.47	1.842	4	0.2
1	7	0	27.70	3.220	4	2.6	4	4	0	39.96	2.256	4	3.7	0	10	7	49.69	1.835	4	0.2
3	1	0	27.71	3.219	4	0.7	3	3	6	40.32	2.237	8	0.4	3	9	5	49.85	1.829	8	2.1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THO Thomsonite

CHEMICAL COMPOSITION: $|Na_4Ca_{7.5}Sr_{0.5}(H_2O)_{24}|\ [Si_{20}Al_{20}O_{80}]$
Death Valley, California, U.S.A.

REFINED COMPOSITION: $|Na_4Ca_{11.2}Sr_{0.8}(H_2O)_{24}|\ [Si_{20}Al_{20}O_{80}]$

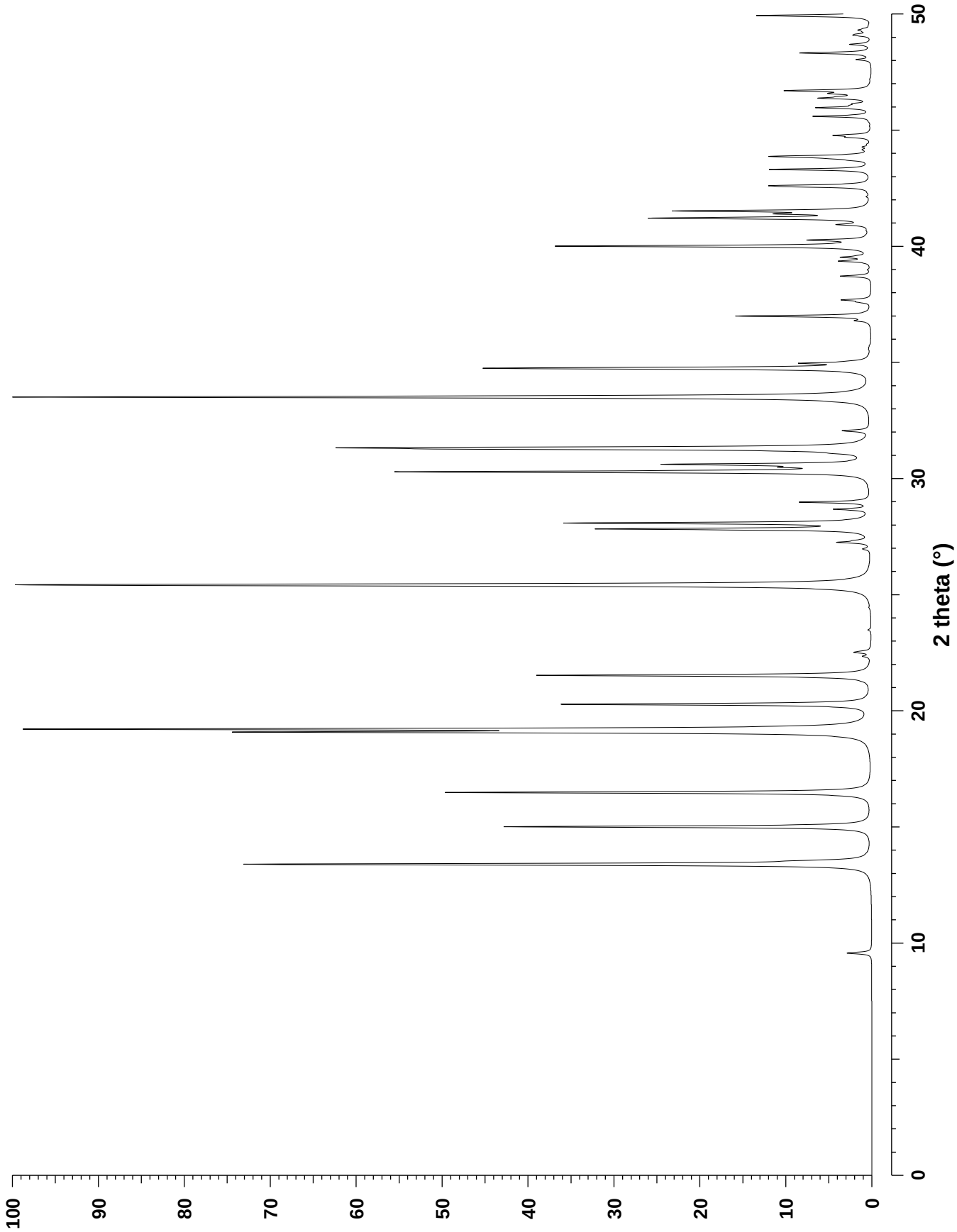
CRYSTAL DATA: *Pncn* (No. 52) **bca** setting
$a = 13.088$ Å $b = 13.052$ Å $c = 13.229$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{F^2} = 0.048$

REFERENCE: J. J. Pluth, J. V. Smith and Å. Kvick,
Zeolites **5** 74–80 (1985).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	9.57	9.242	4	3.0	2	2	4	33.31	2.689	8	0.6	2	0	6	43.30	2.089	4	11.0
0	0	2	13.39	6.615	2	76.6	4	2	2	33.50	2.675	8	100.0	0	2	6	43.31	2.089	4	1.4
2	0	0	13.53	6.544	2	4.3	2	4	2	33.55	2.671	8	13.2	6	0	2	43.69	2.072	4	1.4
0	2	0	13.57	6.526	2	1.1	3	1	4	34.72	2.583	8	20.2	6	2	0	43.76	2.069	4	2.2
1	0	2	15.01	5.903	4	45.0	1	3	4	34.75	2.581	8	33.0	0	6	2	43.81	2.066	4	2.6
1	1	2	16.48	5.379	8	52.2	4	1	3	34.83	2.576	8	0.1	2	6	0	43.86	2.064	4	8.8
2	0	2	19.08	4.652	4	69.8	5	1	0	34.96	2.566	4	6.9	1	2	6	43.89	2.063	8	3.6
2	2	0	19.21	4.621	4	97.9	4	3	1	34.98	2.565	8	0.1	5	0	4	44.12	2.053	4	0.2
2	1	2	20.26	4.382	8	11.1	1	5	0	35.05	2.560	4	0.8	4	3	4	44.15	2.051	8	0.3
1	2	2	20.28	4.378	8	28.8	3	3	3	35.55	2.525	8	0.1	3	4	4	44.17	2.050	8	0.3
2	2	1	20.36	4.362	8	0.8	5	1	1	35.63	2.520	8	0.1	6	1	2	44.27	2.046	8	0.8
0	1	3	21.27	4.178	4	0.2	1	5	1	35.72	2.513	8	0.1	1	6	2	44.38	2.041	8	0.3
3	1	0	21.48	4.138	4	2.1	3	2	4	36.78	2.444	8	1.0	5	1	4	44.69	2.028	8	2.3
0	3	1	21.50	4.133	4	0.6	2	3	4	36.79	2.443	8	0.5	1	5	4	44.77	2.024	8	4.2
1	3	0	21.52	4.129	4	39.5	4	3	2	36.96	2.432	8	0.2	5	3	3	45.36	1.999	8	0.1
1	1	3	22.34	3.980	8	0.9	3	4	2	36.99	2.430	8	16.4	2	2	6	45.59	1.990	8	7.1
3	1	1	22.51	3.949	8	1.8	5	1	2	37.59	2.393	8	1.2	6	2	2	45.96	1.974	8	6.4
1	3	1	22.56	3.941	8	0.8	1	5	2	37.68	2.387	8	3.4	2	6	2	46.06	1.971	8	1.3
2	2	2	23.48	3.788	8	0.4	4	0	4	38.71	2.326	4	3.7	3	0	6	46.13	1.968	4	1.5
3	0	2	24.44	3.642	4	0.1	0	4	4	38.77	2.323	4	0.2	5	2	4	46.37	1.958	8	5.6
3	1	2	25.39	3.508	8	54.4	4	4	0	38.98	2.310	4	0.3	2	5	4	46.44	1.955	8	2.2
1	3	2	25.43	3.502	8	74.3	4	1	4	39.35	2.290	8	3.6	5	4	2	46.55	1.951	8	2.2
3	2	1	25.46	3.498	8	0.1	1	4	4	39.40	2.287	8	0.4	4	5	2	46.58	1.950	8	2.3
2	3	1	25.49	3.494	8	0.7	5	2	2	39.52	2.280	8	3.2	3	1	6	46.68	1.946	8	4.6
0	0	4	26.96	3.307	2	0.8	2	5	2	39.59	2.276	8	0.7	1	3	6	46.70	1.945	8	6.2
4	0	0	27.25	3.272	2	3.7	3	3	4	40.00	2.254	8	38.5	3	6	1	47.19	1.926	8	0.1
0	4	0	27.33	3.263	2	1.3	3	4	3	40.11	2.248	8	0.2	4	4	4	48.03	1.894	8	1.7
1	0	4	27.82	3.206	4	32.9	5	3	0	40.21	2.243	4	0.7	3	2	6	48.31	1.884	8	6.4
3	2	2	28.06	3.180	8	2.5	3	5	0	40.26	2.240	4	6.7	2	3	6	48.32	1.883	8	2.6
2	3	2	28.08	3.178	8	34.9	5	1	3	40.67	2.218	8	0.1	6	3	2	48.68	1.870	8	2.5
1	1	4	28.67	3.114	8	4.3	0	0	6	40.93	2.205	2	3.5	3	6	2	48.76	1.868	8	0.2
3	3	0	28.98	3.081	4	8.5	4	2	4	41.20	2.191	8	23.8	5	3	4	49.07	1.856	8	1.7
2	0	4	30.28	2.952	4	39.9	2	4	4	41.24	2.189	8	5.4	3	5	4	49.12	1.855	8	1.2
0	2	4	30.30	2.950	4	21.2	6	0	0	41.39	2.181	2	7.6	7	1	0	49.23	1.851	4	0.5
4	0	2	30.48	2.933	4	6.0	4	4	2	41.39	2.181	8	0.8	5	5	0	49.30	1.848	4	1.2
4	2	0	30.56	2.925	4	4.5	0	6	0	41.51	2.175	2	21.9	0	7	1	49.36	1.846	4	0.2
2	4	0	30.61	2.920	4	22.3	1	0	6	41.53	2.174	4	1.5	1	7	0	49.37	1.846	4	0.4
1	2	4	31.08	2.878	8	1.5	1	1	6	42.13	2.145	8	0.3	5	1	5	49.48	1.842	8	0.1
4	1	2	31.26	2.861	8	36.8	2	5	3	42.55	2.125	8	0.2	1	5	5	49.55	1.840	8	0.1
1	4	2	31.32	2.856	8	54.1	5	3	2	42.56	2.124	8	6.8	0	4	6	49.92	1.827	4	14.1
3	3	2	32.05	2.793	8	3.2	3	5	2	42.61	2.122	8	9.6							

Thomsonite

THO



TON Diethylamine Theta-1 (Silica ZSM-22)

CHEMICAL COMPOSITION: $|(C_2H_5)_2NH|\ [Si_{24}O_{48}]$
$(C_2H_5)_2NH$ = diethylamine

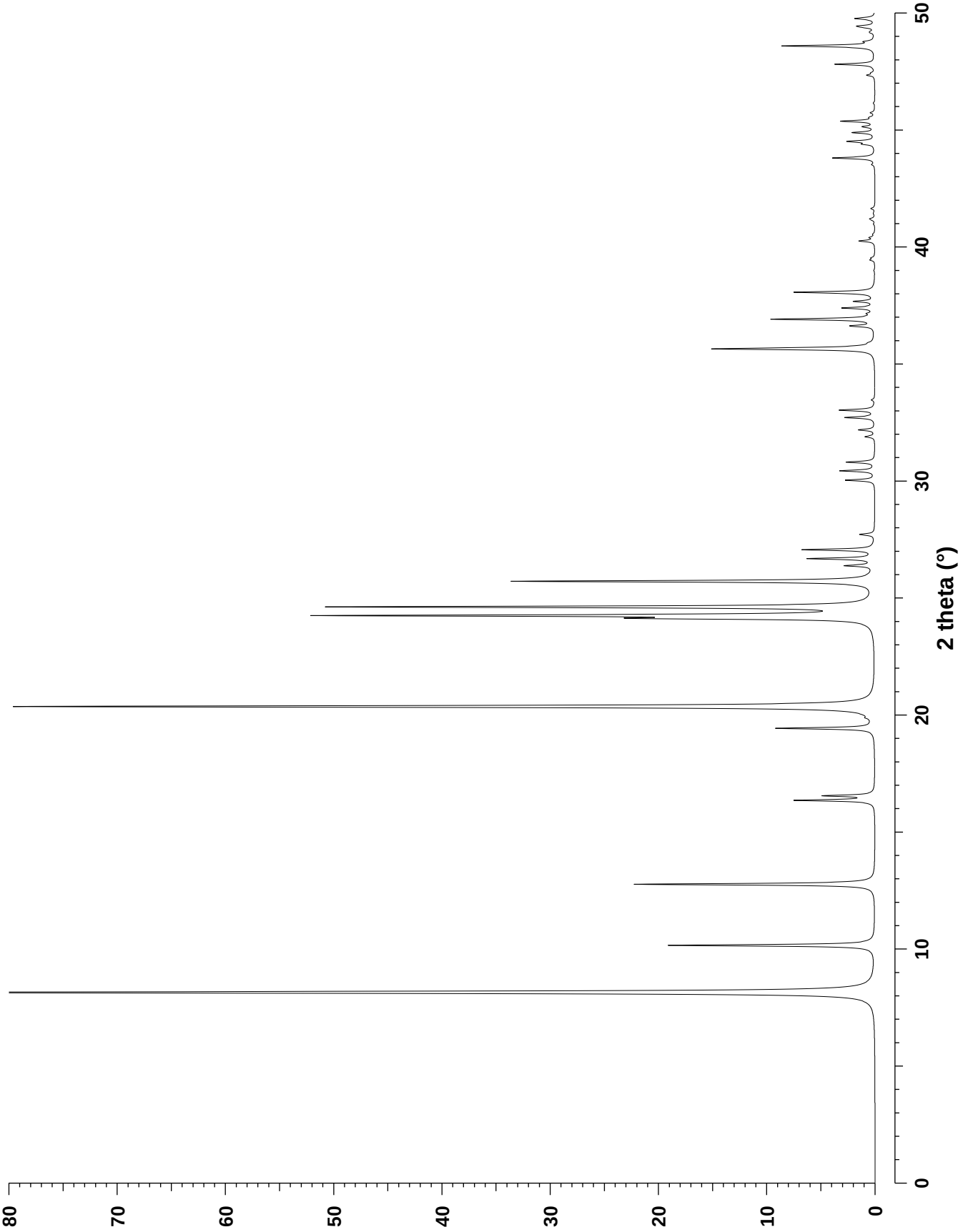
REFINED COMPOSITION: $|C_{5.1}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: $Cmc2_1$ (No. 36)
$a = 13.859$ Å $b = 17.420$ Å $c = 5.038$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.056$

REFERENCE: B. Marler,
Zeolites **7** 393–397 (1987).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	8.15	10.845	4	100.0	5	1	0	32.71	2.737	4	2.7	2	4	2	43.51	2.080	8	0.2
0	2	0	10.16	8.710	2	19.1	4	2	1	33.02	2.713	8	2.7	3	3	2	43.80	2.067	8	3.9
2	0	0	12.77	6.929	2	22.3	4	4	0	33.04	2.711	4	0.7	6	2	1	44.38	2.041	8	0.5
2	2	0	16.35	5.423	4	7.3	2	6	0	33.46	2.678	4	0.3	6	4	0	44.39	2.041	4	0.5
1	3	0	16.55	5.356	4	4.6	0	0	2	35.64	2.519	2	13.8	4	0	2	44.47	2.037	4	0.5
1	1	1	19.43	4.569	8	9.0	0	6	1	35.69	2.516	4	3.5	4	6	1	44.51	2.036	8	2.2
3	1	0	19.88	4.465	4	0.3	5	3	0	35.90	2.501	4	0.2	1	5	2	44.88	2.020	8	2.1
0	2	1	20.36	4.361	4	69.6	1	1	2	36.62	2.454	8	2.1	3	7	1	45.13	2.009	8	1.1
0	4	0	20.39	4.355	2	15.6	3	5	1	36.91	2.435	8	9.6	0	8	1	45.37	1.999	4	3.1
2	2	1	24.11	3.691	8	8.7	0	2	2	37.15	2.420	4	0.4	5	5	1	45.53	1.992	8	0.4
2	4	0	24.14	3.687	4	11.5	5	1	1	37.39	2.405	8	2.9	4	2	2	45.73	1.984	8	0.4
1	3	1	24.25	3.670	8	49.5	4	4	1	37.67	2.388	8	1.9	7	1	0	46.14	1.967	4	0.1
3	3	0	24.62	3.615	4	50.0	2	0	2	38.01	2.367	4	0.7	2	8	1	47.33	1.920	8	0.7
4	0	0	25.71	3.465	2	33.5	2	6	1	38.06	2.365	8	7.2	1	9	0	47.43	1.917	4	0.3
1	5	0	26.38	3.379	4	2.6	2	2	2	39.44	2.285	8	0.4	0	6	2	47.80	1.903	4	3.7
3	1	1	26.68	3.342	8	6.1	1	3	2	39.53	2.279	8	0.3	7	3	0	48.58	1.874	4	8.6
0	4	1	27.06	3.295	4	6.6	5	3	1	40.25	2.240	8	1.5	3	5	2	48.77	1.867	8	0.8
4	2	0	27.71	3.219	4	1.4	6	2	0	40.40	2.233	4	0.5	5	1	2	49.15	1.854	8	0.3
2	4	1	30.03	2.975	8	2.7	4	6	0	40.54	2.225	4	0.2	5	7	0	49.20	1.852	4	0.3
3	3	1	30.43	2.937	8	3.2	1	7	1	40.97	2.203	8	0.1	4	4	2	49.38	1.845	8	0.8
0	6	0	30.80	2.903	2	2.6	3	1	2	41.14	2.194	8	0.2	4	8	0	49.43	1.844	4	1.4
1	5	1	31.89	2.806	8	0.9	3	7	0	41.20	2.191	4	0.4	2	6	2	49.69	1.835	8	0.2
3	5	0	32.18	2.782	4	1.5	5	5	0	41.64	2.169	4	0.4	7	1	1	49.76	1.832	8	1.8

Diethylamine Theta-1 (Silica ZSM-22) TON



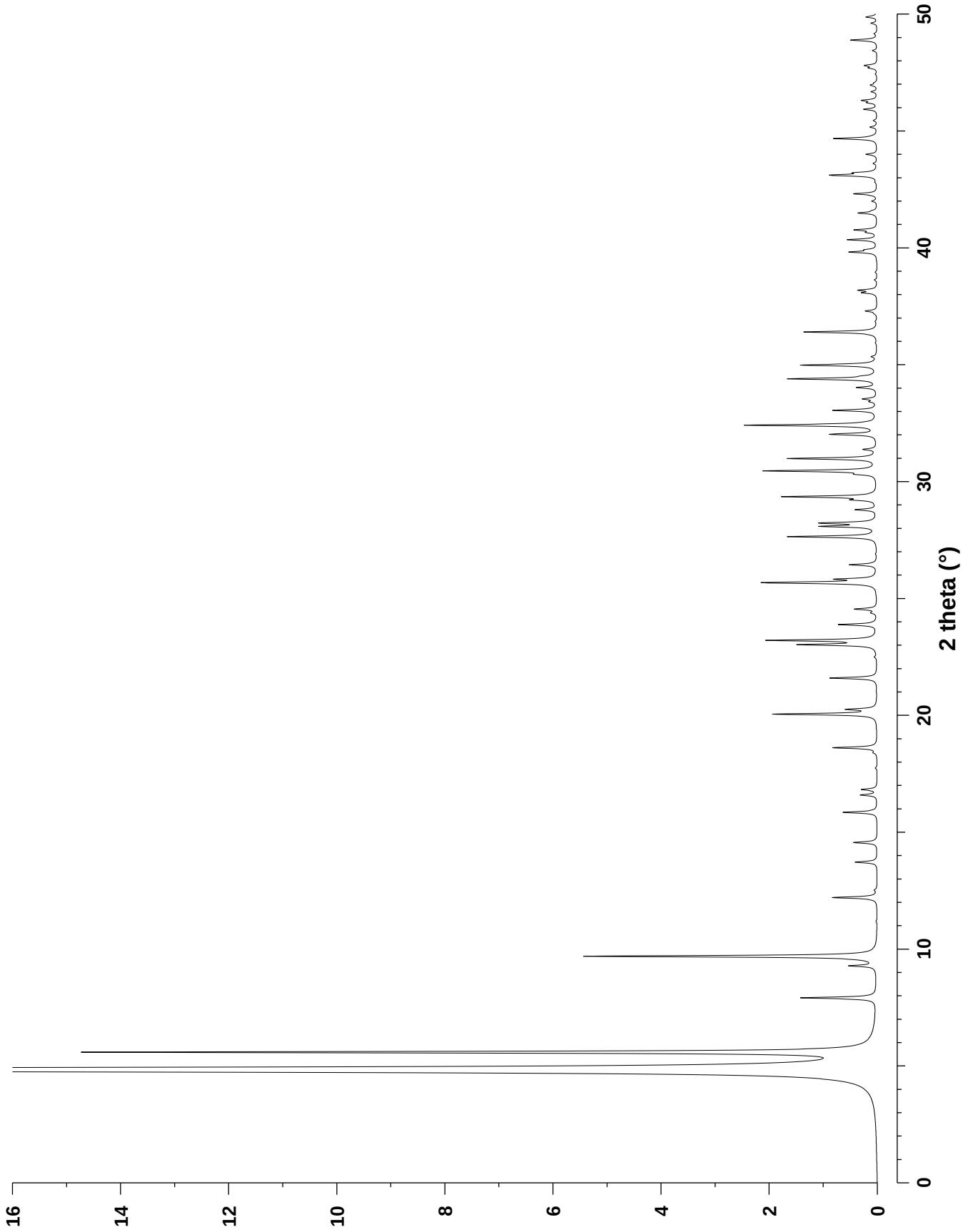
CHEMICAL COMPOSITION: $|K_{11.2}Ca_{89.6}Sr_{16.64}Ba_{4.8}Cu_{46.4}(H_2O)_{217}(OH)_{135.04}|\ [Fe_{1.44}Al_{189.6}Si_{192.96}O_{768}]$
Bellberg volcano, near Mayen, Eifel, Germany

REFINED COMPOSITION: $|K_{12}Ca_{76}Sr_{12}Ba_{12}Cu_{48}Cl_{0.896}O_{327.448}(OH)_{128}|\ [Si_{192}Al_{192}O_{768}]$

CRYSTAL DATA: $Fm\overline{3}m$ (No. 225)
$a = 31.62$ Å $b = 31.62$ Å $c = 31.62$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Single Crystal X-ray Refinement. $R_p = 0.065$, $R_{wp} = 0.156$

REFERENCE: H. Effenberger, G. Giester, W. Krause and H.-J. Bernhardt, *American Mineralogist* **83** 607–617 (1998).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	1	4.84	18.256	8	100.0	10	0	0	28.22	3.162	6	0.5	13	3	1	38.07	2.363	48	0.1
2	0	0	5.59	15.810	6	14.5	8	6	2	28.79	3.101	48	0.4	12	6	0	38.18	2.357	24	0.2
2	2	0	7.91	11.179	12	1.4	9	5	1	29.21	3.057	48	0.2	10	8	4	38.18	2.357	48	0.1
3	1	1	9.28	9.534	24	0.5	7	7	3	29.21	3.057	24	0.2	11	7	5	39.81	2.264	48	0.5
2	2	2	9.69	9.128	8	5.4	10	2	2	29.35	3.043	24	0.8	14	0	0	39.91	2.259	6	0.2
3	3	1	12.20	7.254	24	0.8	6	6	6	29.35	3.043	8	0.9	10	10	0	40.34	2.236	12	0.5
4	2	2	13.72	6.454	24	0.4	9	5	3	30.31	2.949	48	0.3	13	5	3	40.65	2.219	48	0.2
5	1	1	14.56	6.085	24	0.4	10	4	0	30.45	2.936	24	1.3	14	2	2	40.76	2.214	24	0.3
4	4	0	15.85	5.590	12	0.6	8	6	4	30.45	2.936	48	0.8	10	10	2	40.76	2.214	24	0.1
5	3	1	16.59	5.345	48	0.3	10	4	2	30.98	2.886	48	1.6	9	9	7	41.48	2.177	24	0.2
6	0	0	16.82	5.270	6	0.2	11	1	1	31.37	2.851	24	0.1	11	9	3	41.48	2.177	48	0.1
6	2	2	18.61	4.767	24	0.8	7	7	5	31.37	2.851	24	0.1	11	7	7	42.30	2.137	24	0.1
5	5	1	20.05	4.428	24	1.0	8	8	0	32.02	2.795	12	0.9	13	5	5	42.30	2.137	24	0.3
7	1	1	20.05	4.428	24	0.9	11	3	1	32.41	2.763	48	0.8	11	9	5	43.10	2.099	48	0.5
6	4	0	20.25	4.385	24	0.5	9	5	5	32.41	2.763	24	1.1	15	1	1	43.10	2.099	24	0.3
5	5	3	21.59	4.117	24	0.6	9	7	1	32.41	2.763	48	0.6	10	8	8	43.20	2.094	24	0.2
7	3	1	21.59	4.117	48	0.3	10	6	0	33.04	2.711	24	0.8	14	4	4	43.20	2.094	24	0.1
7	3	3	23.02	3.863	24	1.4	11	3	3	33.41	2.682	24	0.1	10	10	6	43.99	2.058	24	0.2
6	4	4	23.20	3.834	24	0.8	10	6	2	33.53	2.672	48	0.3	9	9	9	44.67	2.028	8	0.4
8	2	0	23.20	3.834	24	1.2	8	8	4	34.02	2.635	24	0.3	13	7	5	44.67	2.028	48	0.2
6	6	0	23.88	3.726	12	0.7	11	5	1	34.39	2.608	48	0.4	11	11	1	44.67	2.028	24	0.2
6	6	2	24.54	3.627	24	0.4	7	7	7	34.39	2.608	8	1.2	16	0	0	45.92	1.976	6	0.2
7	5	3	25.67	3.471	48	2.1	12	2	0	34.51	2.599	24	0.2	15	5	3	46.20	1.965	48	0.2
8	4	2	25.82	3.450	48	0.7	10	6	4	34.98	2.565	48	1.4	14	8	0	46.30	1.961	24	0.2
6	6	4	26.44	3.371	24	0.5	12	4	2	36.39	2.469	48	0.5	13	9	5	47.69	1.907	48	0.1
8	4	4	27.64	3.227	24	1.7	8	8	6	36.39	2.469	24	0.7	14	8	4	47.79	1.903	48	0.2
9	3	3	28.08	3.178	24	0.5	10	8	0	36.39	2.469	24	0.2	12	12	0	48.88	1.863	12	0.5
7	5	5	28.08	3.178	24	0.5	10	6	6	37.29	2.411	24	0.2	13	11	3	49.87	1.829	48	0.1
8	6	0	28.22	3.162	24	0.5	11	7	3	38.07	2.363	48	0.1							


0
10
20
30
40
50
2 theta (°)
0
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4
6
8
10
12
14
16

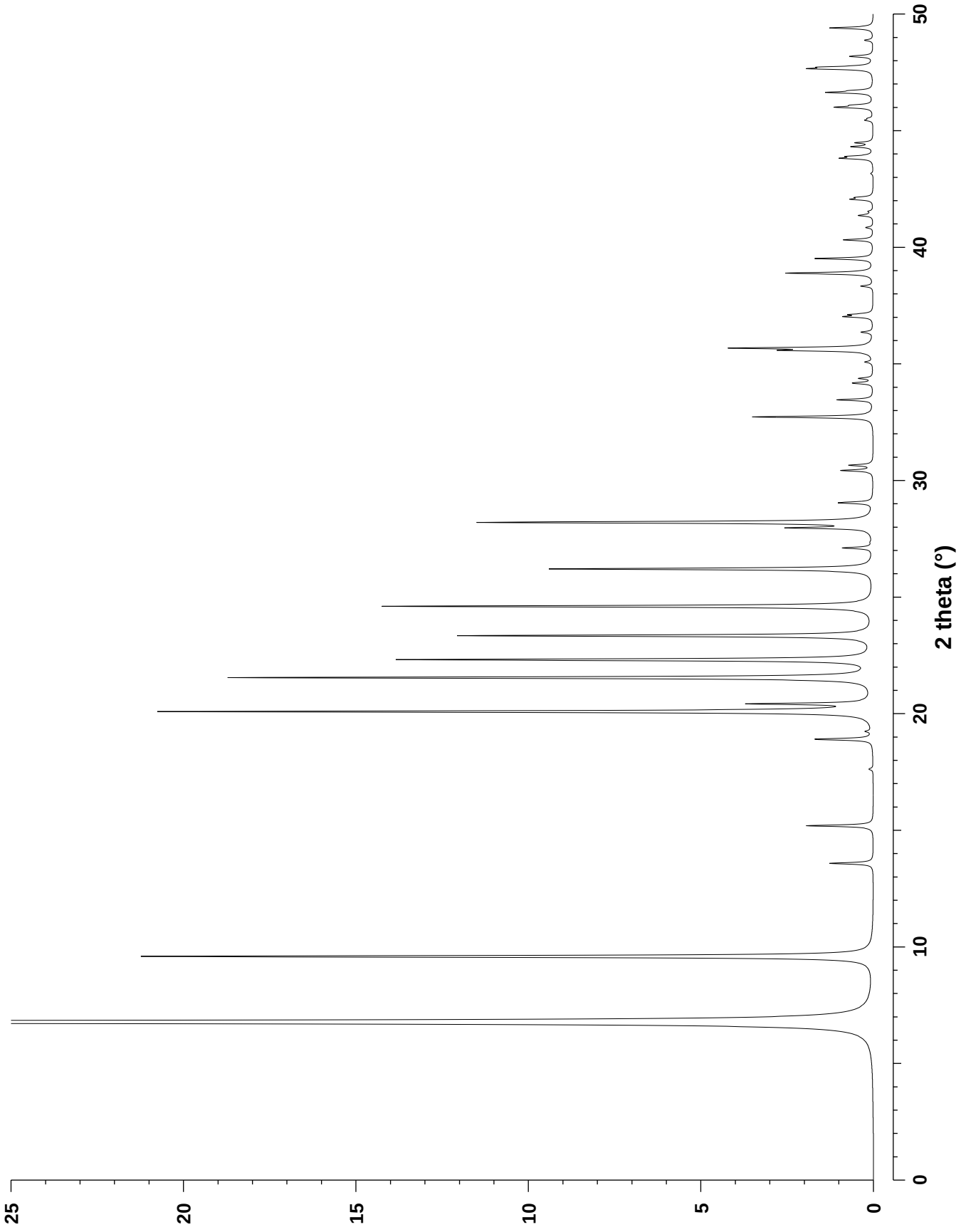
CHEMICAL COMPOSITION: $[Si_{17}O_{34}]$

REFINED COMPOSITION: $[Si_{17}O_{34}]$

CRYSTAL DATA: $P\overline{4}$ (No. 81)
$a = 13.045$ Å $b = 13.045$ Å $c = 5.034$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.125$, $R_p = 0.102$

REFERENCE: C. C. Freyhardt, R. F. Lobo, S. Khodabandeh, J. E. Lewis, Jr., M. Tsapatsis, M. Yoshikawa, M. A. Camblor, M. Pan, M. M. Helmkamp, S. I. Zones and M. E. Davis, *J. Am. Chem. Soc.* **118** 7299–7310 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	6.78	13.045	4	100.0	3	2	1	30.42	2.938	8	0.2	1	3	2	42.05	2.149	8	0.5
1	1	0	9.59	9.224	4	21.2	4	2	0	30.65	2.917	4	0.6	1	6	0	42.13	2.145	4	0.3
2	0	0	13.58	6.523	4	1.3	4	0	1	32.72	2.737	8	3.5	6	1	0	42.13	2.145	4	0.2
1	2	0	15.19	5.834	4	1.7	4	1	1	33.45	2.679	8	0.7	2	3	2	43.81	2.066	8	0.4
2	1	0	15.19	5.834	4	0.2	1	4	1	33.45	2.679	8	0.4	3	2	2	43.81	2.066	8	0.4
0	0	1	17.62	5.034	2	0.1	3	3	1	34.17	2.624	8	0.6	2	6	0	43.89	2.063	4	0.6
1	0	1	18.90	4.696	8	1.7	4	3	0	34.37	2.609	4	0.4	5	3	1	44.31	2.044	8	0.2
2	2	0	19.24	4.612	4	0.2	1	5	0	35.07	2.558	4	0.2	3	5	1	44.31	2.044	8	0.4
1	1	1	20.09	4.419	8	20.7	4	2	1	35.57	2.524	8	1.4	5	4	0	44.47	2.037	4	0.5
3	0	0	20.42	4.348	4	3.4	2	4	1	35.57	2.524	8	0.9	6	0	1	45.44	1.996	8	0.2
3	1	0	21.54	4.125	4	18.6	0	0	2	35.67	2.517	2	3.9	4	0	2	45.52	1.993	8	0.1
2	0	1	22.31	3.985	8	13.8	1	0	2	36.35	2.471	8	0.3	1	6	1	46.00	1.973	8	0.2
2	1	1	23.34	3.811	8	8.2	1	1	2	37.02	2.428	8	0.8	6	1	1	46.00	1.973	8	0.8
1	2	1	23.34	3.811	8	3.8	2	5	0	37.11	2.422	4	0.6	1	4	2	46.08	1.970	8	0.2
2	3	0	24.60	3.618	4	10.8	2	0	2	38.33	2.348	8	0.4	4	1	2	46.08	1.970	8	0.3
3	2	0	24.60	3.618	4	3.4	3	4	1	38.88	2.316	8	0.6	3	3	2	46.63	1.948	8	1.3
2	2	1	26.20	3.401	8	9.4	4	3	1	38.88	2.316	8	1.7	6	3	0	46.71	1.945	4	0.4
3	0	1	27.10	3.291	8	0.9	5	0	1	38.88	2.316	8	0.2	2	6	1	47.65	1.909	8	0.4
3	1	1	27.96	3.191	8	0.4	5	1	1	39.51	2.281	8	0.5	6	2	1	47.65	1.909	8	1.2
1	3	1	27.96	3.191	8	1.9	1	5	1	39.51	2.281	8	1.2	2	4	2	47.72	1.906	8	1.2
1	4	0	28.20	3.164	4	3.9	5	3	0	40.31	2.237	4	0.9	5	4	1	48.18	1.888	8	0.2
4	1	0	28.20	3.164	4	7.5	2	2	2	40.84	2.209	8	0.2	4	5	1	48.18	1.888	8	0.5
3	3	0	29.04	3.075	4	1.0	5	2	1	41.36	2.183	8	0.4	7	0	0	48.87	1.864	4	0.2
2	3	1	30.42	2.938	8	0.8	6	0	0	41.53	2.174	4	0.1	1	7	0	49.40	1.845	4	1.2


0
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2 theta (°)
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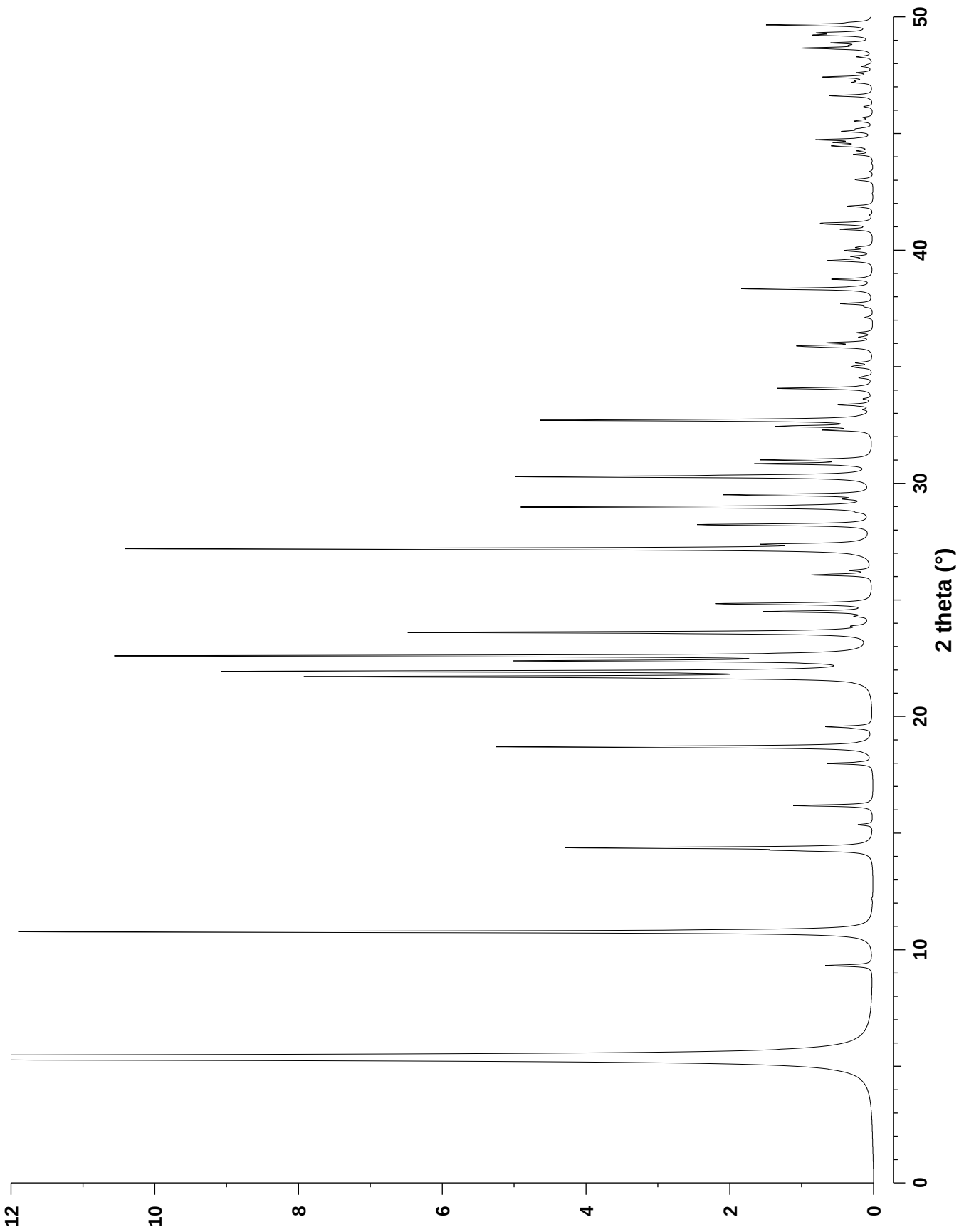
CHEMICAL COMPOSITION: $|(H_2O)_{42}|\ [Al_{18}P_{18}O_{72}]$

REFINED COMPOSITION: $|(H_2O)_{42}|\ [Al_{18}P_{18}O_{72}]$

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 18.9752$ Å $b = 18.9752$ Å $c = 8.1044$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.108$, $R_{wp} = 0.141$, $R_F = 0.086$

REFERENCE: L. B. McCusker, Ch. Baerlocher, E. Jahn and M. Bülow, *Zeolites* **11** 308–313 (1991).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	5.38	16.433	6	100.0	4	2	1	30.83	2.900	12	1.3	2	3	3	41.10	2.196	12	0.1
1	1	0	9.32	9.488	6	0.7	2	4	1	30.83	2.900	12	0.3	2	6	1	41.15	2.194	12	0.3
2	0	0	10.77	8.217	6	11.9	4	0	2	31.00	2.885	12	1.5	6	2	1	41.15	2.194	12	0.2
1	2	0	14.26	6.211	6	0.4	5	1	1	32.28	2.773	12	0.3	1	4	3	41.87	2.158	12	0.2
2	1	0	14.26	6.211	6	0.5	1	5	1	32.28	2.773	12	0.3	4	1	3	41.87	2.158	12	0.2
1	1	1	14.37	6.162	12	4.2	3	2	2	32.44	2.760	12	0.7	7	1	1	43.03	2.102	12	0.1
2	0	1	15.36	5.770	12	0.2	2	3	2	32.44	2.760	12	0.5	3	3	3	44.09	2.054	12	0.2
3	0	0	16.18	5.478	6	1.1	6	0	0	32.70	2.739	6	4.6	4	4	2	44.25	2.047	12	0.2
1	2	1	17.99	4.930	12	0.4	1	4	2	33.36	2.685	12	0.3	4	2	3	44.45	2.038	12	0.2
2	1	1	17.99	4.930	12	0.3	4	1	2	33.36	2.685	12	0.2	2	4	3	44.45	2.038	12	0.2
2	2	0	18.70	4.744	6	5.2	1	0	3	33.62	2.666	12	0.1	5	4	1	44.49	2.037	12	0.1
3	0	1	19.56	4.538	12	0.6	5	2	0	34.07	2.631	6	1.3	4	5	1	44.49	2.037	12	0.1
4	0	0	21.63	4.108	6	1.2	1	1	3	34.52	2.598	12	0.2	7	0	2	44.61	2.031	12	0.4
2	2	1	21.71	4.094	12	7.4	2	0	3	34.96	2.566	12	0.1	0	0	4	44.73	2.026	2	0.7
0	0	2	21.93	4.052	2	8.7	3	4	1	35.01	2.563	12	0.1	1	0	4	45.08	2.011	12	0.4
1	3	1	22.38	3.973	12	1.5	5	0	2	35.16	2.553	12	0.2	3	6	1	45.20	2.006	12	0.1
3	1	1	22.38	3.973	12	3.1	1	6	0	35.83	2.506	6	0.2	5	1	3	45.52	1.993	12	0.1
1	0	2	22.60	3.934	12	10.4	6	1	0	35.83	2.506	6	0.1	2	6	2	45.67	1.986	12	0.1
2	3	0	23.60	3.770	6	2.0	2	5	1	35.88	2.503	12	0.7	2	0	4	46.14	1.967	12	0.1
3	2	0	23.60	3.770	6	4.5	5	2	1	35.88	2.503	12	0.2	7	2	1	46.61	1.949	12	0.3
1	1	2	23.88	3.727	12	0.2	3	3	2	36.02	2.493	12	0.6	2	7	1	46.61	1.949	12	0.3
4	0	1	24.29	3.664	12	0.2	1	2	3	36.26	2.477	12	0.1	2	1	4	47.18	1.926	12	0.2
2	0	2	24.49	3.634	12	1.5	4	2	2	36.45	2.465	12	0.2	7	1	2	47.41	1.917	12	0.3
1	4	0	24.83	3.586	6	2.2	3	0	3	37.11	2.423	12	0.1	1	7	2	47.41	1.917	12	0.4
3	2	1	26.07	3.418	12	0.5	1	5	2	37.70	2.386	12	0.2	4	3	3	47.60	1.910	12	0.1
2	3	1	26.07	3.418	12	0.4	5	1	2	37.70	2.386	12	0.3	3	0	4	47.87	1.900	12	0.1
2	1	2	26.26	3.394	12	0.2	2	2	3	38.34	2.348	12	1.8	2	5	3	48.28	1.885	12	0.1
5	0	0	27.13	3.287	6	0.2	1	3	3	38.75	2.324	12	0.4	8	1	1	48.65	1.871	12	0.6
1	4	1	27.19	3.279	12	6.6	3	1	3	38.75	2.324	12	0.2	1	8	1	48.65	1.871	12	0.4
4	1	1	27.19	3.279	12	3.7	6	2	0	39.54	2.279	6	0.5	2	2	4	48.88	1.863	12	0.5
3	0	2	27.38	3.258	12	1.1	4	4	1	39.59	2.276	12	0.1	1	3	4	49.21	1.851	12	0.4
3	3	0	28.22	3.163	6	2.4	6	0	2	39.72	2.269	12	0.3	3	1	4	49.21	1.851	12	0.3
2	2	2	28.98	3.081	12	4.9	4	0	3	39.94	2.257	12	0.1	3	7	0	49.29	1.849	6	0.2
5	0	1	29.32	3.046	12	0.3	3	5	1	39.98	2.255	12	0.1	5	5	1	49.32	1.848	12	0.4
3	1	2	29.50	3.028	12	1.0	7	0	1	39.98	2.255	12	0.1	4	6	1	49.65	1.836	12	0.8
1	3	2	29.50	3.028	12	1.0	4	3	2	40.11	2.248	12	0.2	6	4	1	49.65	1.836	12	0.6
5	1	0	30.28	2.951	6	1.9	5	2	2	40.89	2.207	12	0.2	8	0	2	49.76	1.832	12	0.2
1	5	0	30.28	2.951	6	2.8	2	5	2	40.89	2.207	12	0.2							
3	3	1	30.34	2.946	12	0.7	3	2	3	41.10	2.196	12	0.3							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2 theta (°)
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4
6
8
10
12

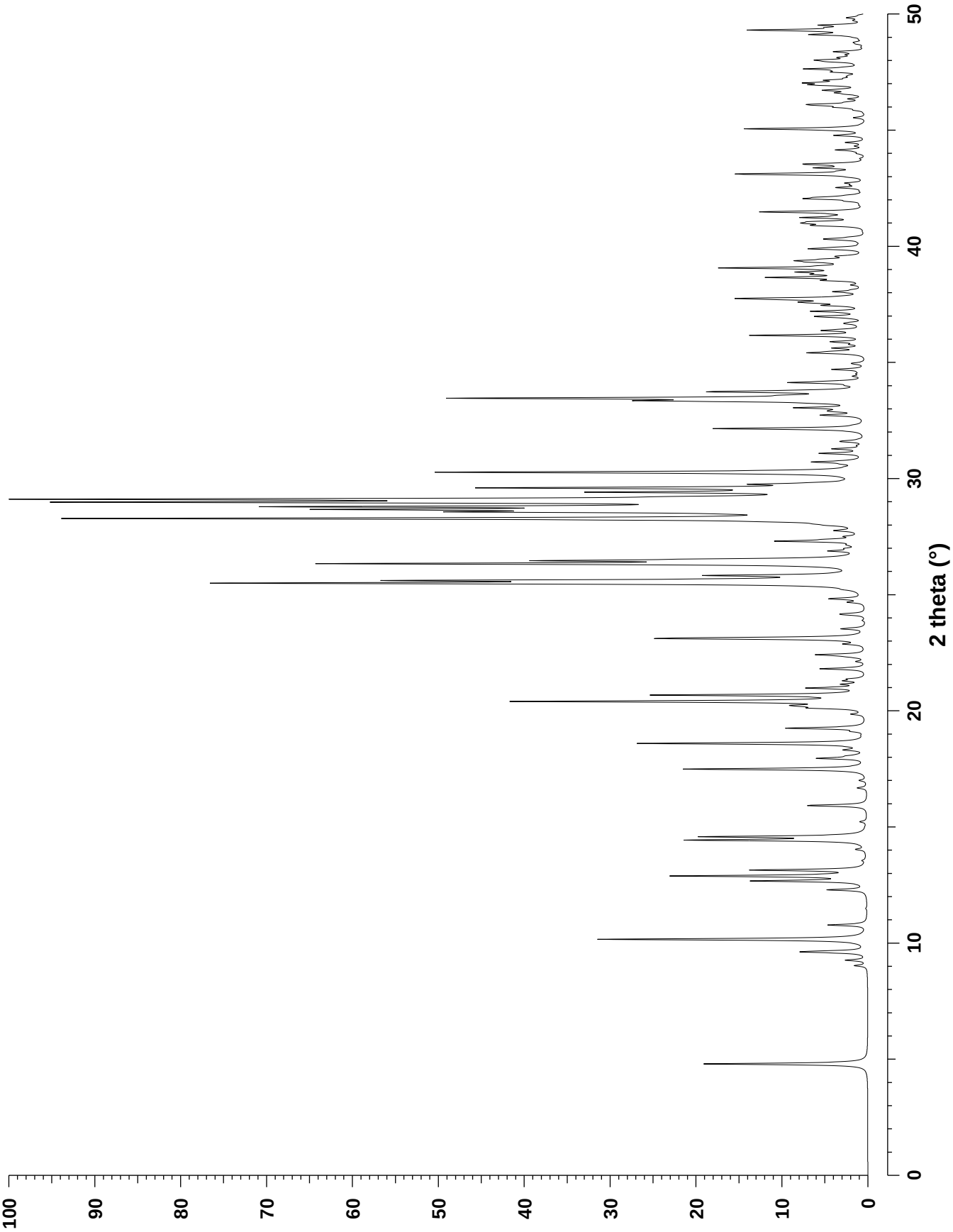
CHEMICAL COMPOSITION: $|Rb_{44}K_4(H_2O)_{48}|\ [Si_{96}Zn_{24}O_{240}]$

REFINED COMPOSITION: $|Rb_{44}K_4(H_2O)_{14}|\ [Si_{96}Zn_{24}O_{240}]$

CRYSTAL DATA: $P4_12_12$ (No. 92)
$a = 9.8837$ Å $b = 9.8837$ Å $c = 73.6505$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.099$, $R_{wp} = 0.147$, $R_F = 0.069$

REFERENCE: L. B. McCusker, R. W. Grosse-Kunstleve, Ch. Baerlocher, M. Yoshikawa, and M. E. Davis, *Microporous Materials* **6** 295–309 (1996).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	4	4.80	18.413	2	21.0	1	1	21	28.47	3.135	8	3.7	3	3	0	38.65	2.330	4	11.5
1	0	2	9.26	9.546	8	2.7	3	1	0	28.56	3.126	8	37.8	2	1	27	38.79	2.321	16	3.0
0	0	8	9.61	9.206	2	6.8	3	1	1	28.58	3.123	16	3.1	3	2	17	38.88	2.316	16	3.8
1	0	3	9.65	9.169	8	3.3	3	1	2	28.66	3.114	16	55.2	1	1	30	38.88	2.316	8	2.8
1	0	4	10.16	8.708	8	34.5	3	0	8	28.78	3.102	8	64.5	2	2	24	39.06	2.306	8	17.5
1	0	5	10.78	8.207	8	5.0	3	1	4	28.98	3.081	16	89.8	4	0	12	39.31	2.292	8	4.6
1	0	7	12.29	7.204	8	4.9	0	0	24	29.10	3.069	2	96.8	3	3	6	39.37	2.289	8	6.4
1	1	0	12.67	6.989	4	14.0	3	1	5	29.21	3.057	16	6.4	3	1	22	39.44	2.285	16	3.3
1	1	2	12.89	6.866	8	24.5	3	0	9	29.22	3.056	8	3.9	3	2	18	39.57	2.277	16	2.4
1	0	8	13.14	6.737	8	14.3	2	2	12	29.41	3.037	8	29.8	2	1	28	39.88	2.260	16	6.2
0	0	12	14.43	6.138	2	22.1	1	1	22	29.59	3.019	8	46.0	3	2	19	40.29	2.238	16	2.9
1	1	6	14.58	6.073	8	20.2	2	1	18	29.75	3.003	16	10.1	3	1	23	40.32	2.237	16	2.7
1	1	8	15.92	5.567	8	7.6	3	1	8	30.20	2.960	16	3.6	4	1	13	40.88	2.208	16	3.0
1	1	10	17.49	5.070	8	23.5	2	0	20	30.27	2.953	8	53.3	4	2	2	40.91	2.206	16	3.2
2	0	0	17.95	4.942	4	5.6	1	1	23	30.71	2.911	8	3.7	2	1	29	40.98	2.202	16	4.2
2	0	4	18.59	4.773	8	29.3	3	1	10	31.08	2.877	16	5.6	3	2	20	41.05	2.199	16	4.7
1	1	12	19.25	4.612	8	9.4	2	0	21	31.27	2.860	8	3.9	3	1	24	41.23	2.190	16	7.3
2	1	1	20.12	4.412	16	4.7	3	1	11	31.59	2.832	16	2.7	3	3	12	41.46	2.178	8	6.3
1	0	15	20.19	4.397	8	2.4	3	1	12	32.14	2.785	16	18.2	4	0	16	41.48	2.177	8	7.4
2	1	2	20.23	4.389	16	5.1	3	1	13	32.72	2.737	16	2.3	4	2	8	42.04	2.149	16	5.9
2	0	8	20.40	4.354	8	42.0	3	0	15	32.73	2.736	8	2.6	2	1	30	42.10	2.146	16	4.1
2	1	3	20.41	4.350	16	2.8	1	0	26	32.89	2.723	8	2.5	3	1	26	43.10	2.099	16	14.5
2	1	4	20.67	4.298	16	26.6	3	2	4	33.04	2.711	16	7.8	2	0	32	43.37	2.086	8	5.7
2	1	5	20.98	4.234	16	6.9	3	1	14	33.34	2.687	16	21.4	4	2	12	43.52	2.079	16	4.2
1	1	14	21.14	4.203	8	2.5	3	0	16	33.45	2.679	8	49.4	3	3	16	43.54	2.079	8	3.7
1	0	16	21.29	4.173	8	2.3	2	1	22	33.58	2.669	16	5.0	4	0	20	44.14	2.052	8	3.2
2	1	7	21.81	4.075	16	5.9	2	2	18	33.73	2.657	8	17.7	4	2	14	44.46	2.038	16	2.5
1	0	17	22.41	3.968	8	5.8	3	2	7	33.79	2.653	16	3.6	3	3	18	44.77	2.024	8	3.9
2	1	9	22.87	3.889	16	2.3	3	2	8	34.13	2.627	16	8.8	3	1	28	45.05	2.013	16	15.1
2	0	12	23.11	3.849	8	23.2	3	1	16	34.69	2.586	16	4.2	4	3	2	45.98	1.974	16	2.7
1	1	16	23.14	3.844	8	6.1	2	2	20	35.41	2.535	8	5.9	3	3	20	46.10	1.969	8	4.2
1	0	18	23.53	3.781	8	3.1	2	1	24	35.61	2.521	16	3.8	4	1	22	46.60	1.949	16	2.8
2	1	12	24.82	3.587	16	4.3	3	2	12	35.88	2.503	16	4.1	4	2	18	46.71	1.945	16	2.7
2	2	0	25.49	3.494	4	74.9	3	1	18	36.16	2.484	16	14.7	5	1	2	46.94	1.936	16	5.6
2	2	1	25.52	3.490	8	3.9	4	0	0	36.36	2.471	4	4.5	5	0	8	47.02	1.933	8	3.4
2	0	15	25.57	3.483	8	3.7	3	1	19	36.94	2.433	16	2.4	4	3	8	47.02	1.933	16	2.4
2	2	2	25.61	3.479	8	50.8	3	2	14	36.98	2.431	16	5.0	5	1	4	47.14	1.928	16	3.9
1	0	20	25.82	3.451	8	17.3	2	2	22	37.19	2.417	8	6.6	5	1	6	47.49	1.915	16	3.1
2	1	14	26.33	3.384	16	66.3	3	0	21	37.45	2.401	8	4.4	4	3	10	47.63	1.909	16	6.7
2	0	16	26.46	3.368	8	33.7	3	2	15	37.58	2.393	16	4.3	4	2	20	48.01	1.895	16	4.8
2	2	6	26.52	3.361	8	10.6	4	0	8	37.69	2.386	8	3.1	5	0	12	48.37	1.882	8	3.2
2	2	7	26.88	3.316	8	3.6	2	1	26	37.72	2.385	16	3.3	3	3	24	49.10	1.856	8	5.5
2	2	8	27.30	3.267	8	8.9	3	1	20	37.75	2.383	16	12.6	5	1	12	49.30	1.848	16	13.6
1	0	22	28.14	3.171	8	3.5	4	1	5	38.03	2.366	16	2.3	4	2	22	49.41	1.844	16	2.9
2	2	10	28.27	3.157	8	100.0	4	1	7	38.52	2.337	16	4.3	2	2	34	49.51	1.841	8	4.6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2 theta (°)
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90
100

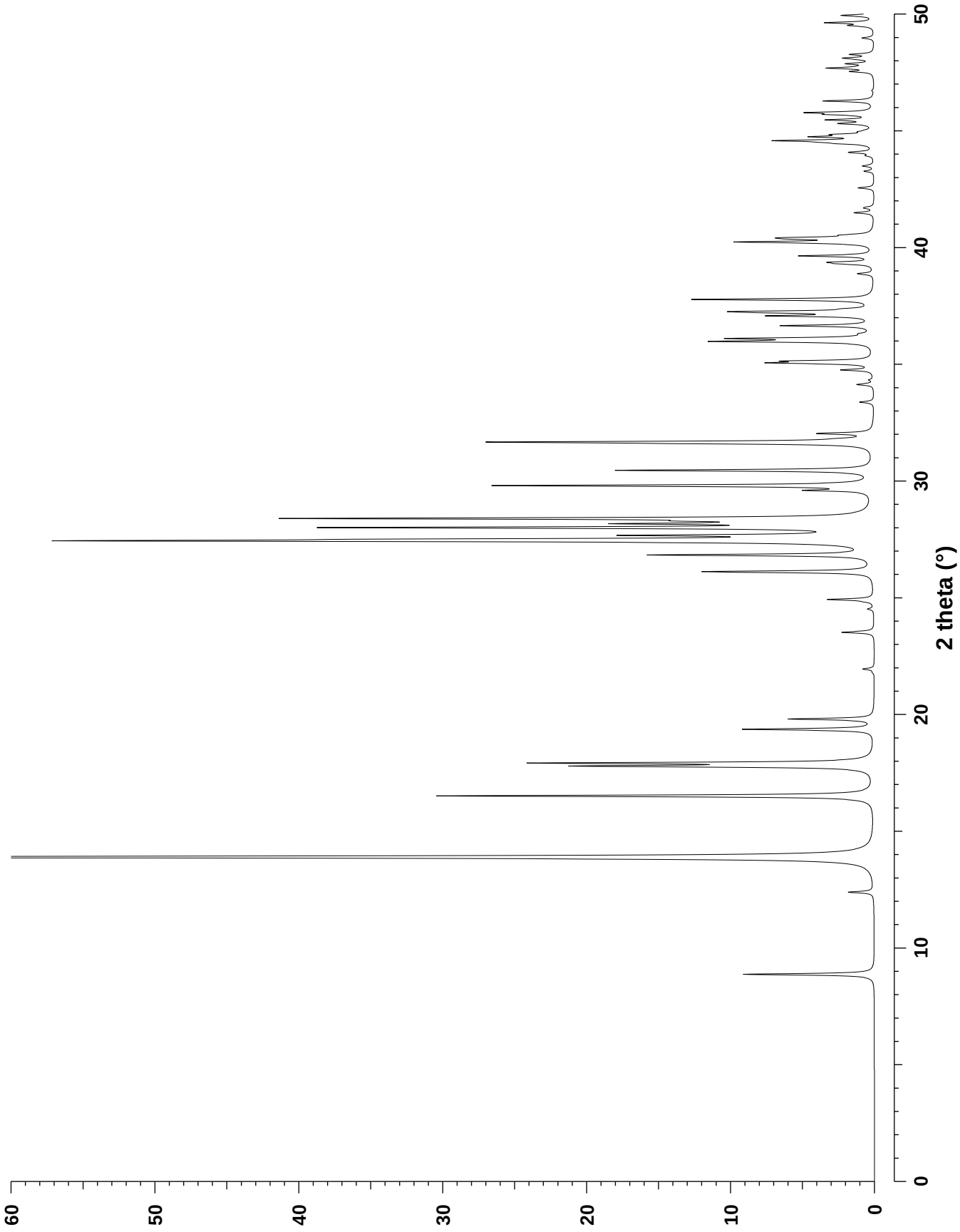
CHEMICAL COMPOSITION: $|Na_{32}(H_2O)_{40}|\ [Si_{56}Zn_{16}O_{144}]$

REFINED COMPOSITION: $|Na_{28.48}(H_2O)_{49.76}|\ [Si_{56}Zn_{16}O_{144}]$

CRYSTAL DATA: $Fdd2$ (No. 43)
$a = 39.88$ Å $b = 10.326$ Å $c = 10.219$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.248$, $R_{wp} = 0.162$, $R_I = 0.100$

REFERENCE: C. Röhrig, H. Gies and B. Marler,
Zeolites **14** 498–503 (1994).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
4	0	0	8.87	9.970	2	9.1	9	3	1	34.13	2.627	8	1.2	8	4	2	43.26	2.092	8	0.7
1	1	1	12.39	7.146	8	1.8	9	1	3	34.32	2.613	8	0.3	8	2	4	43.49	2.081	8	0.8
3	1	1	13.89	6.374	8	100.0	0	4	0	34.75	2.582	2	2.2	15	3	1	43.93	2.061	8	0.4
5	1	1	16.51	5.370	8	30.4	2	4	0	35.05	2.560	4	6.5	16	2	2	44.06	2.055	8	1.3
2	2	0	17.75	4.998	4	4.0	0	0	4	35.13	2.555	2	5.2	15	1	3	44.09	2.054	8	0.6
8	0	0	17.79	4.985	2	17.3	4	4	0	35.93	2.499	4	0.3	12	4	0	44.44	2.039	4	1.6
2	0	2	17.92	4.950	4	22.4	15	1	1	35.97	2.497	8	10.1	18	2	0	44.50	2.036	4	1.8
4	2	0	19.36	4.585	4	9.1	16	0	0	36.03	2.493	2	1.5	18	0	2	44.57	2.033	4	6.3
7	1	1	19.80	4.483	8	5.9	14	0	2	36.10	2.488	4	9.1	12	0	4	44.74	2.025	4	3.8
6	0	2	21.94	4.051	4	0.8	4	0	4	36.30	2.475	4	0.5	1	5	1	44.83	2.022	8	2.2
9	1	1	23.52	3.783	8	2.3	12	2	2	36.65	2.452	8	6.3	19	1	1	44.95	2.016	8	0.6
0	2	2	24.51	3.632	4	0.4	11	3	1	37.07	2.425	8	6.7	11	3	3	45.02	2.013	8	0.3
8	2	0	24.83	3.586	4	0.3	1	3	3	37.20	2.417	8	4.4	1	1	5	45.29	2.002	8	1.2
2	2	2	24.92	3.573	8	3.2	11	1	3	37.25	2.414	8	7.9	3	5	1	45.31	2.001	8	1.2
4	2	2	26.11	3.412	8	11.8	6	4	0	37.37	2.406	4	1.1	10	4	2	45.46	1.995	8	3.0
12	0	0	26.83	3.323	2	15.3	3	3	3	37.77	2.382	8	12.6	20	0	0	45.49	1.994	2	0.1
1	3	1	27.43	3.251	8	50.8	5	3	3	38.87	2.317	8	1.1	10	2	4	45.69	1.986	8	2.6
11	1	1	27.50	3.244	8	22.6	8	4	0	39.30	2.292	4	1.9	3	1	5	45.77	1.982	8	4.3
1	1	3	27.67	3.224	8	14.5	2	4	2	39.36	2.289	8	2.6	5	5	1	46.27	1.962	8	3.5
6	2	2	28.00	3.187	8	36.8	8	0	4	39.64	2.274	4	5.1	5	1	5	46.72	1.944	8	0.1
3	3	1	28.17	3.168	8	14.1	4	4	2	40.17	2.245	8	0.6	14	4	0	47.53	1.913	4	1.5
10	2	0	28.28	3.156	4	6.9	16	2	0	40.17	2.245	4	0.9	7	5	1	47.68	1.907	8	3.1
10	0	2	28.39	3.144	4	8.7	14	2	2	40.23	2.241	8	8.7	17	3	1	47.75	1.905	8	0.4
3	1	3	28.39	3.143	8	30.8	13	3	1	40.36	2.235	8	3.4	13	3	3	47.86	1.901	8	1.7
5	3	1	29.59	3.019	8	3.9	17	1	1	40.40	2.232	8	1.9	17	1	3	47.90	1.899	8	0.1
5	1	3	29.80	2.998	8	26.3	4	2	4	40.42	2.232	8	3.3	12	4	2	48.05	1.894	8	0.6
8	2	2	30.45	2.935	8	17.8	7	3	3	40.48	2.228	8	0.2	7	1	5	48.11	1.891	8	1.8
7	3	1	31.61	2.831	8	7.2	13	1	3	40.53	2.226	8	1.5	12	2	4	48.26	1.886	8	1.6
13	1	1	31.66	2.826	8	24.1	6	4	2	41.48	2.177	8	1.4	20	2	0	48.97	1.860	4	0.8
7	1	3	31.81	2.813	8	0.9	10	4	0	41.68	2.167	4	0.5	9	5	1	49.50	1.841	8	1.5
12	2	0	32.03	2.794	4	3.6	6	2	4	41.72	2.165	8	0.4	21	1	1	49.62	1.837	8	3.3
10	2	2	33.37	2.685	8	1.0	9	3	3	42.55	2.125	8	1.1	9	1	5	49.93	1.827	8	2.3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2 theta (°)
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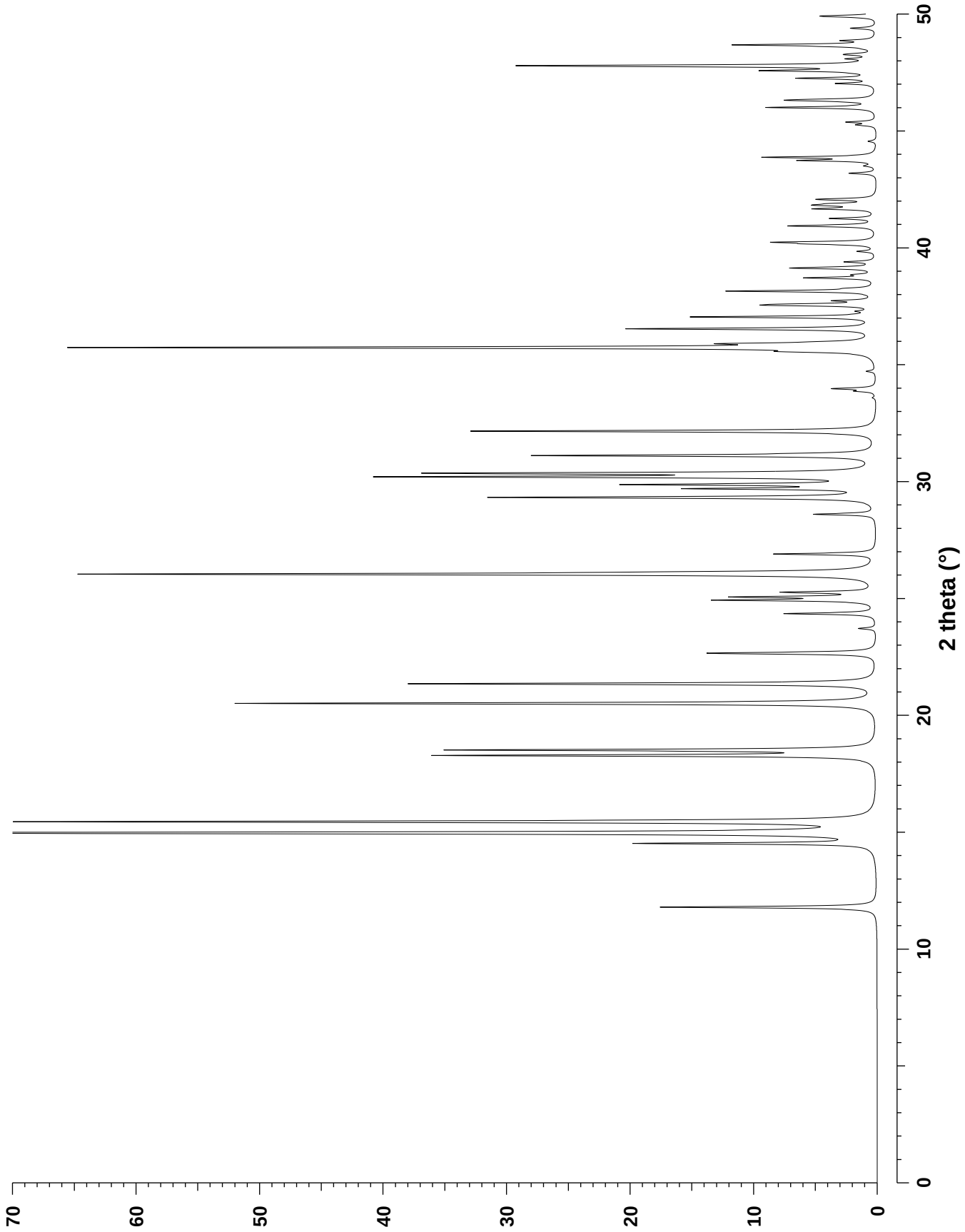
CHEMICAL COMPOSITION: $|Ca_4(H_2O)_{16}|\ [Be_{12}P_8O_{32}(OH)_8]$
Weinebene Pass, Koralpe, Austria

REFINED COMPOSITION: $|Ca_4(H_2O)_{16}|\ [Be_{12}P_8O_{32}(OH)_8]$

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 11.897$ Å $b = 9.707$ Å $c = 9.633$ Å
$\alpha = 90°$ $\beta = 95.76°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: F. Walter,
Eur. J. Mineral. **4** 1275–1283 (1992).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	1	0	11.79	7.506	4	17.7	1	3	2	34.71	2.584	4	0.7	0	2	4	42.05	2.149	4	2.4
-1	1	1	14.52	6.101	4	19.0	4	2	0	35.53	2.527	4	1.5	2	0	4	42.08	2.147	2	3.0
2	0	0	14.97	5.918	2	100.0	-3	1	3	35.56	2.525	4	3.8	-3	1	4	43.18	2.095	4	2.2
1	1	1	15.45	5.735	4	69.7	-2	2	3	35.73	2.513	4	65.1	-2	2	4	43.50	2.081	4	0.8
0	2	0	18.28	4.853	2	35.3	3	3	0	35.89	2.502	4	8.9	-4	2	3	43.73	2.070	4	5.8
0	0	2	18.51	4.792	2	34.2	-4	2	1	35.97	2.496	4	1.8	-2	4	2	43.87	2.064	4	8.9
0	2	1	20.51	4.330	4	52.2	-3	3	1	36.53	2.459	4	20.1	-3	3	3	44.55	2.034	4	0.7
-1	1	2	21.35	4.161	4	38.1	0	4	0	37.04	2.427	2	14.9	2	4	2	45.25	2.004	4	1.5
1	1	2	22.64	3.927	4	7.1	4	0	2	37.28	2.412	2	1.0	5	1	2	45.37	1.999	4	2.3
-2	0	2	22.67	3.922	2	8.6	0	0	4	37.54	2.396	2	6.9	6	0	0	46.00	1.973	2	8.9
2	2	0	23.71	3.753	4	1.4	4	2	1	37.58	2.393	4	4.2	2	2	4	46.23	1.964	4	0.8
3	1	0	24.35	3.655	4	7.4	3	3	1	37.73	2.384	4	2.9	-4	0	4	46.30	1.961	2	5.5
-2	2	1	24.92	3.573	4	12.5	2	2	3	38.14	2.360	4	12.0	-5	1	3	46.34	1.959	4	3.2
2	0	2	25.06	3.554	2	10.8	0	4	1	38.26	2.353	4	1.4	0	4	3	47.02	1.932	4	3.1
-3	1	1	25.26	3.526	4	7.1	-1	1	4	38.71	2.326	4	5.7	3	1	4	47.25	1.924	4	6.2
2	2	1	26.04	3.421	4	63.8	-4	2	2	38.84	2.318	4	1.4	1	5	0	47.46	1.916	4	0.6
0	2	2	26.13	3.410	4	7.4	-2	0	4	39.12	2.303	2	1.9	3	3	3	47.57	1.912	4	7.2
3	1	1	26.90	3.314	4	8.3	3	1	3	39.13	2.302	4	4.5	5	3	0	47.59	1.911	4	1.4
1	3	0	28.60	3.121	4	5.0	5	1	0	39.17	2.300	4	1.3	4	2	3	47.77	1.904	4	4.7
-2	2	2	29.28	3.050	4	2.2	-5	1	1	39.39	2.288	4	2.4	-5	3	1	47.78	1.904	4	24.6
-3	1	2	29.32	3.046	4	30.2	-1	3	3	39.84	2.263	4	1.4	-6	0	2	48.08	1.892	2	1.9
-1	1	3	29.69	3.009	4	14.3	2	4	0	40.16	2.245	4	4.3	-1	1	5	48.25	1.886	4	1.7
-1	3	1	29.87	2.991	4	19.3	1	1	4	40.23	2.242	4	7.6	-1	5	1	48.29	1.885	4	1.0
4	0	0	30.20	2.959	2	38.3	-2	4	1	40.93	2.205	4	5.6	1	3	4	48.50	1.877	4	0.3
1	3	1	30.35	2.945	4	34.3	1	3	3	40.95	2.204	4	2.0	1	5	1	48.61	1.873	4	1.1
1	1	3	31.11	2.874	4	27.5	5	1	1	41.25	2.189	4	3.7	-2	4	3	48.67	1.871	4	11.3
2	2	2	31.19	2.867	4	2.2	2	4	1	41.66	2.168	4	4.6	-4	4	1	48.86	1.864	4	2.5
3	1	2	32.15	2.784	4	33.0	0	4	2	41.72	2.165	4	0.8	5	3	1	49.39	1.845	4	2.1
0	2	3	33.58	2.669	4	0.3	3	3	2	41.78	2.162	4	0.3	1	1	5	49.84	1.830	4	0.4
-1	3	2	33.86	2.648	4	1.4	4	2	2	41.82	2.160	4	3.9	6	2	0	49.90	1.828	4	3.8
-4	0	2	33.97	2.639	2	3.5	-5	1	2	41.88	2.157	4	2.5	-6	2	1	49.92	1.827	4	0.9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2 theta (°)
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-WEN Wenkite

CHEMICAL COMPOSITION: $|Na_{0.5}K_{0.5}Ca_{5.5}Ba_{3.5}(SO_4)_3H_2O|\ [Si_{11}Al_9O_{41}(OH)_2]$
Candoglia, Italy

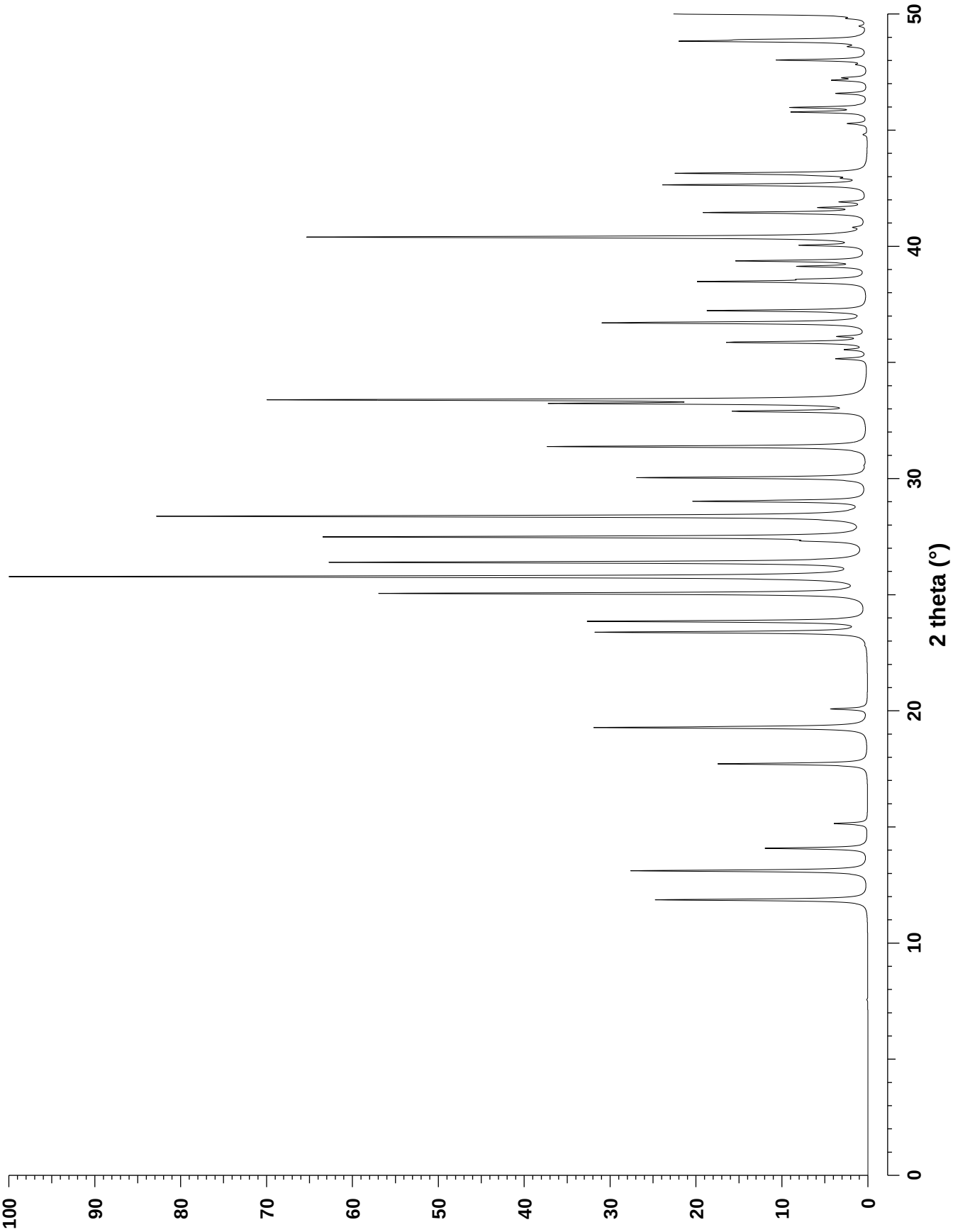
REFINED COMPOSITION: $|Na_{0.5}K_{0.5}Ca_{5.5}Ba_{3.5}S_3(OH)_{12}|\ [Si_{11}Al_9O_{41}(OH)_2]$

CRYSTAL DATA: $P\bar{6}2m$ (No. 189)
$a = 13.511$ Å $b = 13.511$ Å $c = 7.462$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.10$

REFERENCE: S. Merlino,
Acta Cryst. **B30** 1262–1266 (1974).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	0	7.56	11.701	6	0.1	2	1	2	31.37	2.852	24	37.4	4	2	1	42.64	2.120	24	23.8
0	0	1	11.86	7.462	2	24.9	4	0	1	32.89	2.723	12	15.0	4	1	2	42.92	2.107	24	1.7
1	1	0	13.11	6.755	6	27.7	3	0	2	33.23	2.696	12	32.7	5	1	0	43.04	2.102	12	2.5
1	0	1	14.08	6.292	12	12.0	3	2	0	33.38	2.684	12	68.0	3	0	3	43.13	2.097	12	21.9
2	0	0	15.14	5.850	6	3.9	4	1	0	35.15	2.553	12	3.6	5	1	1	44.80	2.023	24	0.5
1	1	1	17.71	5.008	12	17.5	3	2	1	35.54	2.526	24	2.4	2	2	3	45.27	2.003	12	2.3
2	0	1	19.28	4.604	12	32.1	2	2	2	35.86	2.504	12	16.3	5	0	2	45.77	1.982	12	8.6
2	1	0	20.08	4.423	12	4.3	0	0	3	36.11	2.487	2	3.1	3	1	3	45.97	1.974	24	8.8
3	0	0	22.80	3.900	6	0.1	3	1	2	36.70	2.449	24	30.9	6	0	0	46.57	1.950	6	3.7
2	1	1	23.38	3.805	24	31.6	4	1	1	37.22	2.416	24	18.6	3	3	2	47.14	1.928	12	3.9
0	0	2	23.85	3.731	2	32.5	5	0	0	38.47	2.340	6	19.1	4	3	0	47.25	1.924	12	2.5
1	0	2	25.05	3.555	12	56.8	1	1	3	38.57	2.334	12	5.5	4	2	2	47.81	1.902	24	0.9
3	0	1	25.77	3.457	12	100.0	4	0	2	39.13	2.302	12	7.7	4	0	3	48.01	1.895	12	10.6
2	2	0	26.39	3.378	6	62.5	2	0	3	39.36	2.289	12	15.1	5	2	0	48.59	1.874	12	1.6
1	1	2	27.31	3.266	12	4.2	3	3	0	40.04	2.252	6	7.1	0	0	4	48.82	1.865	2	19.5
3	1	0	27.48	3.245	12	63.2	5	0	1	40.39	2.233	12	65.5	4	3	1	48.89	1.863	24	10.2
2	0	2	28.37	3.146	12	83.0	4	2	0	40.81	2.211	12	1.1	1	0	4	49.47	1.842	12	0.7
2	2	1	29.02	3.077	12	20.1	3	2	2	41.44	2.179	24	19.0	5	1	2	49.80	1.831	24	1.6
3	1	1	30.03	2.976	24	26.9	2	1	3	41.66	2.168	24	5.1	3	2	3	49.99	1.824	24	22.6
4	0	0	30.56	2.925	6	0.1	3	3	1	41.90	2.156	12	3.0							

Wenkite -WEN



YUG Yugawaralite

CHEMICAL COMPOSITION: $|Ca_2(H_2O)_8|\ [Si_{12}Al_4O_{32}]$
Hvalfjördur, Iceland

REFINED COMPOSITION: $|Ca_2H_{15.82}O_{8.136}|\ [Si_{12}Al_4O_{32}]$

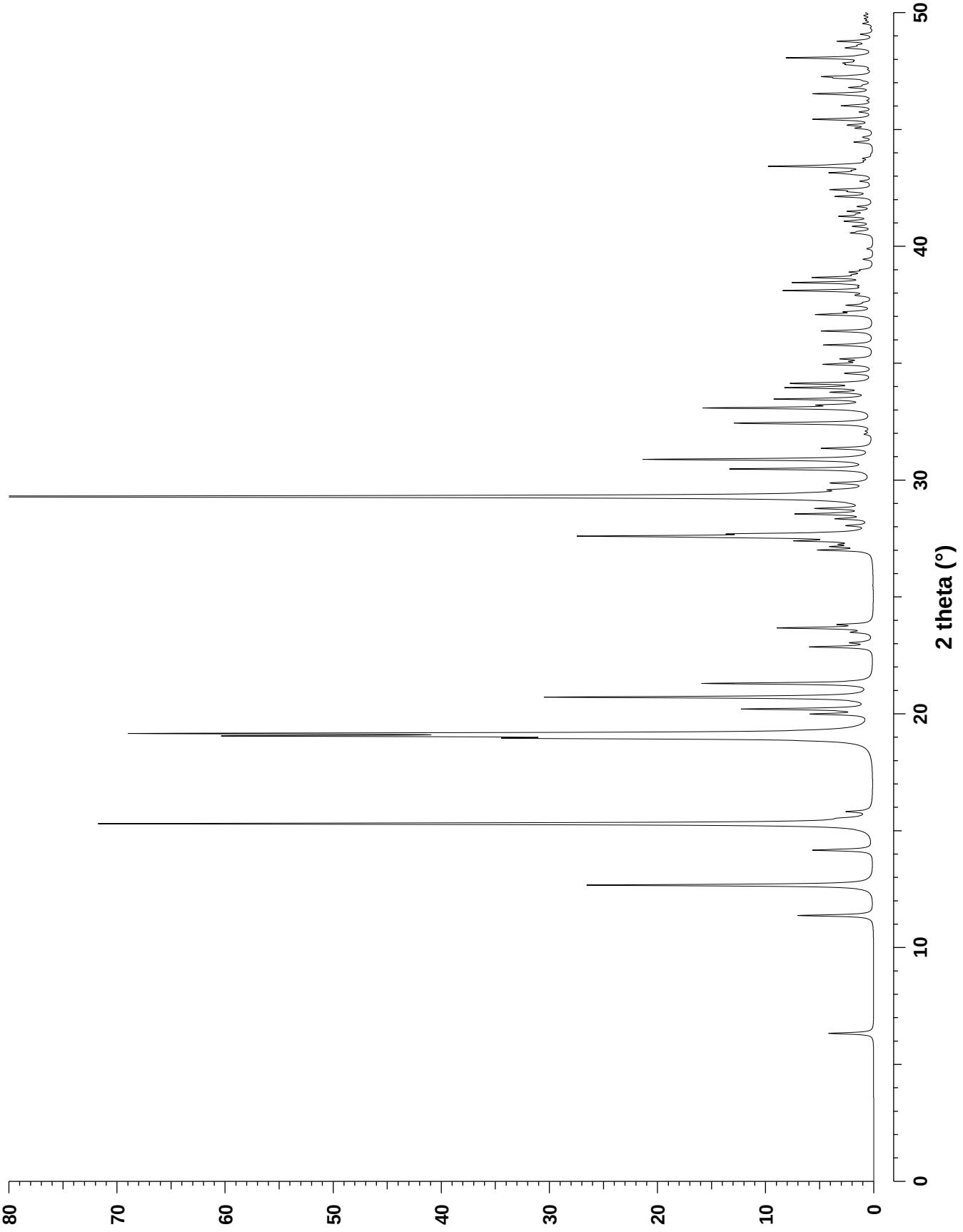
CRYSTAL DATA: $P1c1$ (No. 7) unique axis **b**, cell choice 1
$a = 6.700$ Å $b = 13.972$ Å $c = 10.039$ Å
$\alpha = 90°$ $\beta = 111.07°$ $\gamma = 90°$
Neutron single crystal refinement at $T = 13$K, $R_w = 0.045$

REFERENCE: Å. Kvick, G. Artioli and J. V. Smith,
Z. Kristallogr. **174** 265–281 (1986).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	1	0	6.33	13.972	2	4.8	0	5	1	33.46	2.678	4	10.1	-2	5	2	43.08	2.099	4	1.3
0	1	1	11.37	7.781	4	8.1	1	3	2	33.75	2.655	4	4.0	-3	1	3	43.14	2.097	4	3.9
0	2	0	12.67	6.986	2	30.6	2	1	1	33.95	2.641	4	8.8	0	3	4	43.24	2.092	4	1.2
1	0	0	14.17	6.252	2	6.4	-2	3	2	34.13	2.627	4	8.3	0	6	2	43.39	2.085	4	0.9
-1	1	1	15.30	5.790	4	82.6	2	3	0	34.56	2.596	4	2.6	3	0	0	43.42	2.084	2	8.9
1	1	0	15.53	5.707	4	1.5	-2	2	3	34.95	2.567	4	5.0	2	5	0	43.43	2.083	4	0.9
0	2	1	15.82	5.600	4	2.4	-1	5	1	35.07	2.559	4	1.7	0	5	3	43.46	2.082	4	1.2
0	0	2	18.95	4.684	2	29.3	1	5	0	35.18	2.551	4	3.2	-1	6	2	43.50	2.081	4	0.8
1	2	0	19.05	4.659	4	51.1	2	2	1	35.78	2.510	4	1.0	-2	3	4	43.65	2.074	4	0.6
0	3	0	19.06	4.657	2	6.4	-1	0	4	35.78	2.509	2	4.3	1	6	1	43.76	2.069	4	0.9
-1	0	2	19.16	4.632	2	71.5	-1	1	4	36.37	2.470	4	5.5	-1	4	4	44.45	2.038	4	2.0
0	1	2	19.99	4.441	4	5.9	1	1	3	37.08	2.425	4	5.9	-3	2	3	44.65	2.029	4	0.6
-1	1	2	20.20	4.397	4	13.5	-2	4	1	37.19	2.417	4	2.5	2	3	2	44.68	2.028	4	0.6
1	1	1	20.71	4.288	4	34.9	0	5	2	37.48	2.400	4	2.6	1	4	3	45.05	2.012	4	1.7
0	3	1	21.30	4.170	4	18.1	-1	5	2	37.59	2.393	4	0.7	-3	3	2	45.18	2.007	4	2.5
0	2	2	22.86	3.890	4	6.7	-2	3	3	37.89	2.375	4	0.9	3	2	0	45.41	1.997	4	0.9
-1	2	2	23.04	3.860	4	2.2	1	4	2	37.92	2.372	4	0.8	-3	3	1	45.43	1.996	4	4.7
1	2	1	23.49	3.787	4	1.9	-1	2	4	38.10	2.362	4	9.4	0	7	0	45.44	1.996	2	1.1
-1	3	1	23.67	3.758	4	10.0	-2	4	2	38.27	2.352	4	0.7	-1	1	5	45.74	1.983	4	1.3
1	3	0	23.82	3.735	4	3.2	0	0	4	38.44	2.342	2	8.3	1	0	4	46.01	1.973	2	3.3
0	3	2	27.00	3.303	4	5.4	2	4	0	38.65	2.329	4	1.4	-2	5	3	46.23	1.964	4	0.4
-1	3	2	27.15	3.284	4	3.5	2	3	1	38.66	2.329	4	3.2	1	1	4	46.49	1.953	4	1.3
0	4	1	27.25	3.273	4	2.1	0	6	0	38.66	2.329	2	0.5	0	7	1	46.52	1.952	4	5.5
-2	1	1	27.39	3.256	4	6.5	0	4	3	38.68	2.328	4	1.4	-3	0	4	46.79	1.942	2	2.3
1	3	1	27.54	3.238	4	8.2	1	2	3	38.78	2.322	4	1.3	2	5	1	46.89	1.938	4	0.6
1	0	2	27.60	3.232	2	27.2	-2	0	4	38.89	2.316	2	2.1	-2	1	5	47.19	1.926	4	2.2
-1	1	3	27.70	3.220	4	11.1	0	1	4	38.99	2.310	4	1.0	-1	2	5	47.19	1.926	4	0.7
-2	0	2	28.05	3.181	2	2.3	-2	1	4	39.44	2.285	4	1.1	-3	1	4	47.26	1.923	4	4.7
1	1	2	28.34	3.149	4	3.4	0	6	1	39.89	2.260	4	0.7	-1	6	3	47.76	1.904	4	2.1
2	0	0	28.55	3.126	2	7.7	2	1	2	40.56	2.224	4	1.0	3	3	0	47.81	1.902	4	0.7
-2	1	2	28.78	3.102	4	5.2	-3	0	2	40.56	2.224	2	1.2	1	7	0	47.84	1.901	4	1.8
2	1	0	29.28	3.051	4	1.6	0	2	4	40.63	2.221	4	1.1	1	2	4	47.92	1.898	4	0.8
1	4	0	29.29	3.049	4	100.0	-1	3	4	40.85	2.209	4	2.0	2	4	2	48.06	1.893	4	9.1
0	1	3	29.31	3.047	4	16.9	-2	2	4	41.06	2.198	4	2.5	3	1	1	48.48	1.878	4	0.5
-2	2	1	29.58	3.020	4	2.5	-3	1	2	41.10	2.196	4	0.8	2	1	3	48.48	1.878	4	1.9
-1	2	3	29.87	2.991	4	3.9	-1	6	1	41.28	2.187	4	3.3	-3	4	2	48.53	1.876	4	0.8
1	2	2	30.47	2.933	4	14.9	-3	1	1	41.37	2.183	4	0.5	-2	2	5	48.60	1.873	4	1.0
-2	2	2	30.88	2.895	4	24.3	1	6	0	41.37	2.182	4	0.5	2	6	0	48.76	1.867	4	1.6
2	2	0	31.35	2.853	4	4.6	1	3	3	41.49	2.177	4	2.5	-3	4	1	48.77	1.867	4	1.7
0	2	3	31.38	2.851	4	1.0	-2	4	3	41.70	2.166	4	1.6	0	1	5	49.06	1.857	4	1.3
0	4	2	31.96	2.800	4	0.7	-2	5	1	42.12	2.146	4	1.8	-1	3	5	49.52	1.841	4	1.0
-1	4	2	32.09	2.789	4	0.5	2	2	2	42.14	2.144	4	2.4	0	7	2	49.65	1.836	4	0.6
1	4	1	32.43	2.761	4	14.7	-1	5	3	42.33	2.135	4	1.9	-1	7	2	49.74	1.833	4	0.8
-2	1	3	33.08	2.708	4	17.6	2	4	1	42.42	2.131	4	4.2	3	2	1	49.86	1.829	4	0.5
-1	3	3	33.21	2.698	4	4.3	1	5	2	42.78	2.114	4	1.3	1	7	1	49.98	1.825	4	0.7

Yugawaralite

YUG



ZON Tetramethylammonium ZAPO-M1

CHEMICAL COMPOSITION: $|((CH_3)_4N)_8|\ [Al_{24}P_{32}Zn_8O_{128}]$
$((CH_3)_4N)^+$ = tetramethylammonium

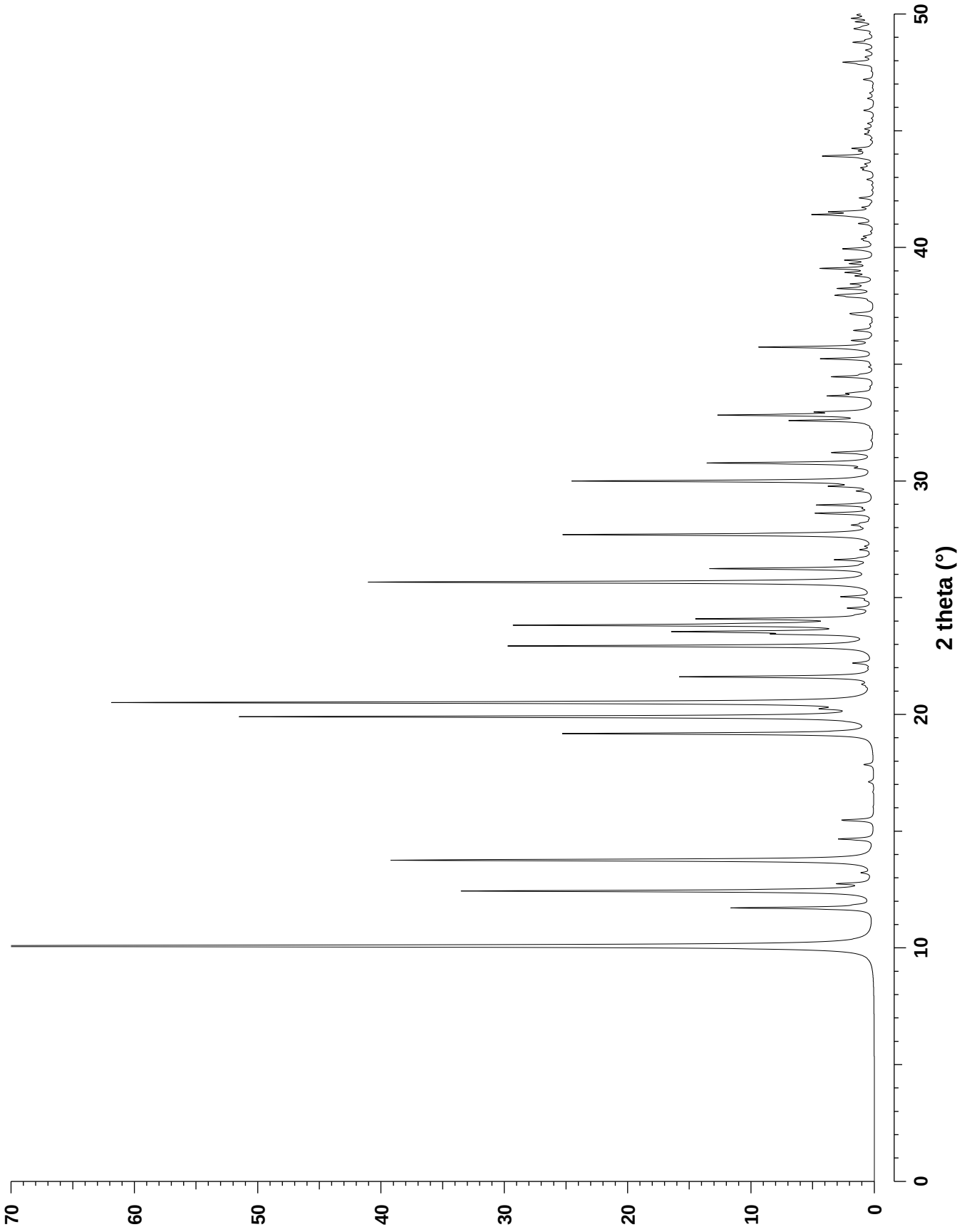
REFINED COMPOSITION: $|N_8C_{42.656}|\ [Al_{25}Zn_7P_{32}O_{128}]$

CRYSTAL DATA: *Pbca* (No. 61)
$a = 14.226$ Å $b = 15.117$ Å $c = 17.557$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.069$

REFERENCE: B. Marler, J. Patarin and L. Sierra,
Microporous Materials **5** 151–159 (1995).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	10.08	8.779	2	100.0	1	4	3	28.81	3.099	8	0.5	2	4	6	41.02	2.200	8	0.6
0	2	0	11.71	7.558	2	11.4	2	1	5	28.97	3.082	8	4.5	0	6	4	41.32	2.185	4	0.8
1	0	2	11.85	7.471	4	0.6	4	2	2	29.56	3.021	8	1.1	2	5	5	41.40	2.181	8	4.5
2	0	0	12.44	7.113	2	33.4	2	3	4	29.77	3.001	8	2.9	6	1	3	41.52	2.175	8	3.2
0	2	1	12.75	6.942	4	2.5	4	1	3	29.99	2.980	8	24.4	4	2	6	41.72	2.165	8	0.8
1	1	2	13.22	6.697	8	0.7	0	0	6	30.55	2.926	2	1.0	6	3	0	42.12	2.145	4	1.1
2	1	0	13.76	6.436	4	39.2	2	2	5	30.76	2.907	8	11.4	0	2	8	42.91	2.108	4	0.5
2	1	1	14.66	6.043	8	2.8	4	3	0	30.77	2.906	4	2.1	0	4	7	43.29	2.090	4	0.2
0	2	2	15.47	5.728	4	2.6	4	3	1	31.20	2.867	8	2.5	2	6	4	43.32	2.089	8	0.6
2	2	0	17.12	5.180	4	0.4	0	4	4	31.23	2.864	4	1.1	4	4	5	43.41	2.084	8	0.6
2	2	1	17.85	4.968	8	0.8	2	5	1	32.58	2.748	8	6.5	6	3	2	43.42	2.084	8	0.3
0	2	3	19.18	4.627	4	25.1	0	2	6	32.82	2.729	4	12.2	2	1	8	43.57	2.077	8	0.5
2	2	2	19.90	4.461	8	51.1	4	1	4	32.95	2.718	8	3.7	2	7	0	43.81	2.066	4	0.3
0	0	4	20.23	4.389	2	2.0	2	1	6	33.64	2.664	8	3.5	4	3	6	43.91	2.062	8	4.0
3	1	1	20.27	4.381	8	0.8	2	4	4	33.74	2.657	8	1.5	4	6	0	44.05	2.056	4	0.3
2	1	3	20.51	4.330	8	61.5	2	5	2	33.79	2.652	8	0.6	2	7	1	44.13	2.052	8	0.9
1	3	2	21.27	4.178	8	0.2	4	3	3	34.46	2.603	8	3.4	0	6	5	44.24	2.047	4	1.6
3	0	2	21.30	4.172	4	0.3	4	2	4	34.56	2.595	8	0.7	4	1	7	44.61	2.031	8	0.2
2	3	0	21.61	4.112	4	15.6	0	4	5	34.88	2.572	4	0.3	2	2	8	44.85	2.021	8	0.6
2	3	1	22.20	4.003	8	1.5	2	2	6	35.23	2.548	8	4.1	2	5	6	44.95	2.016	8	0.3
2	2	3	22.93	3.879	8	29.5	0	6	0	35.63	2.520	2	0.5	2	7	2	45.07	2.011	8	0.4
0	2	4	23.44	3.796	4	5.7	2	5	3	35.73	2.513	8	9.2	6	2	4	45.08	2.011	8	0.2
0	4	0	23.54	3.779	2	14.8	0	6	1	36.01	2.494	4	1.6	4	6	2	45.30	2.002	8	0.4
2	0	4	23.82	3.735	4	27.6	4	1	5	36.44	2.465	8	1.5	4	2	7	45.87	1.978	8	0.8
2	3	2	23.90	3.724	8	4.7	3	5	2	36.71	2.448	8	0.2	6	4	2	46.38	1.958	8	0.5
0	4	1	24.09	3.695	4	13.5	0	6	2	37.12	2.422	4	1.1	2	7	3	46.61	1.949	8	0.3
1	2	4	24.27	3.667	8	0.5	2	4	5	37.17	2.419	8	1.5	4	5	5	47.19	1.926	8	0.8
2	1	4	24.55	3.626	8	1.8	2	6	0	37.88	2.375	4	1.4	6	2	5	47.83	1.902	8	0.8
3	1	3	24.87	3.580	8	0.2	6	0	0	37.95	2.371	2	2.4	6	4	3	47.88	1.900	8	0.4
4	0	0	25.04	3.556	2	2.4	4	4	3	37.99	2.368	8	0.7	0	4	8	47.93	1.898	4	2.1
0	4	2	25.66	3.471	4	40.5	2	6	1	38.24	2.353	8	2.8	0	8	0	48.15	1.890	2	0.5
4	1	0	25.73	3.462	4	1.8	1	2	7	38.34	2.348	8	0.3	0	8	1	48.45	1.879	4	0.6
4	1	1	26.24	3.397	8	13.1	6	1	0	38.43	2.342	4	1.7	2	1	9	48.78	1.867	8	1.6
1	4	2	26.43	3.372	8	0.3	6	1	1	38.78	2.322	8	1.3	2	5	7	48.89	1.863	8	0.5
2	2	4	26.62	3.349	8	2.9	0	4	6	38.92	2.314	4	2.0	0	8	2	49.33	1.847	4	0.7
2	4	0	26.71	3.337	4	0.6	4	5	0	39.10	2.304	4	4.2	4	7	0	49.37	1.846	4	1.0
4	0	2	27.05	3.296	4	0.9	2	6	2	39.30	2.293	8	1.6	2	6	6	49.42	1.844	8	0.2
2	4	1	27.20	3.279	8	0.5	4	5	1	39.45	2.284	8	1.9	6	0	6	49.48	1.842	4	0.3
3	0	4	27.69	3.221	4	0.4	1	4	6	39.46	2.284	8	0.3	4	7	1	49.66	1.836	8	1.3
4	1	2	27.70	3.221	8	24.0	4	0	6	39.90	2.260	4	0.3	6	3	5	49.81	1.831	8	1.5
4	2	0	27.72	3.218	4	0.9	2	2	7	39.94	2.257	8	2.3	6	1	6	49.87	1.829	8	0.2
0	2	5	28.02	3.185	4	0.4	4	3	5	40.29	2.239	8	0.6	6	4	4	49.93	1.826	8	0.2
0	4	3	28.11	3.175	4	1.4	4	1	6	40.36	2.235	8	0.8	2	8	0	49.94	1.826	4	0.3
4	2	1	28.19	3.165	8	0.6	4	5	2	40.48	2.228	8	0.7	5	2	7	49.95	1.826	8	0.3
2	4	2	28.61	3.120	8	4.6	2	6	3	41.01	2.201	8	0.5	6	5	2	49.98	1.825	8	0.6

Tetramethylammonium ZAPO-M1 ZON



Alpha Cristobalite

CHEMICAL COMPOSITION: $[Si_4O_8]$
Ellora, Hyderabad, India

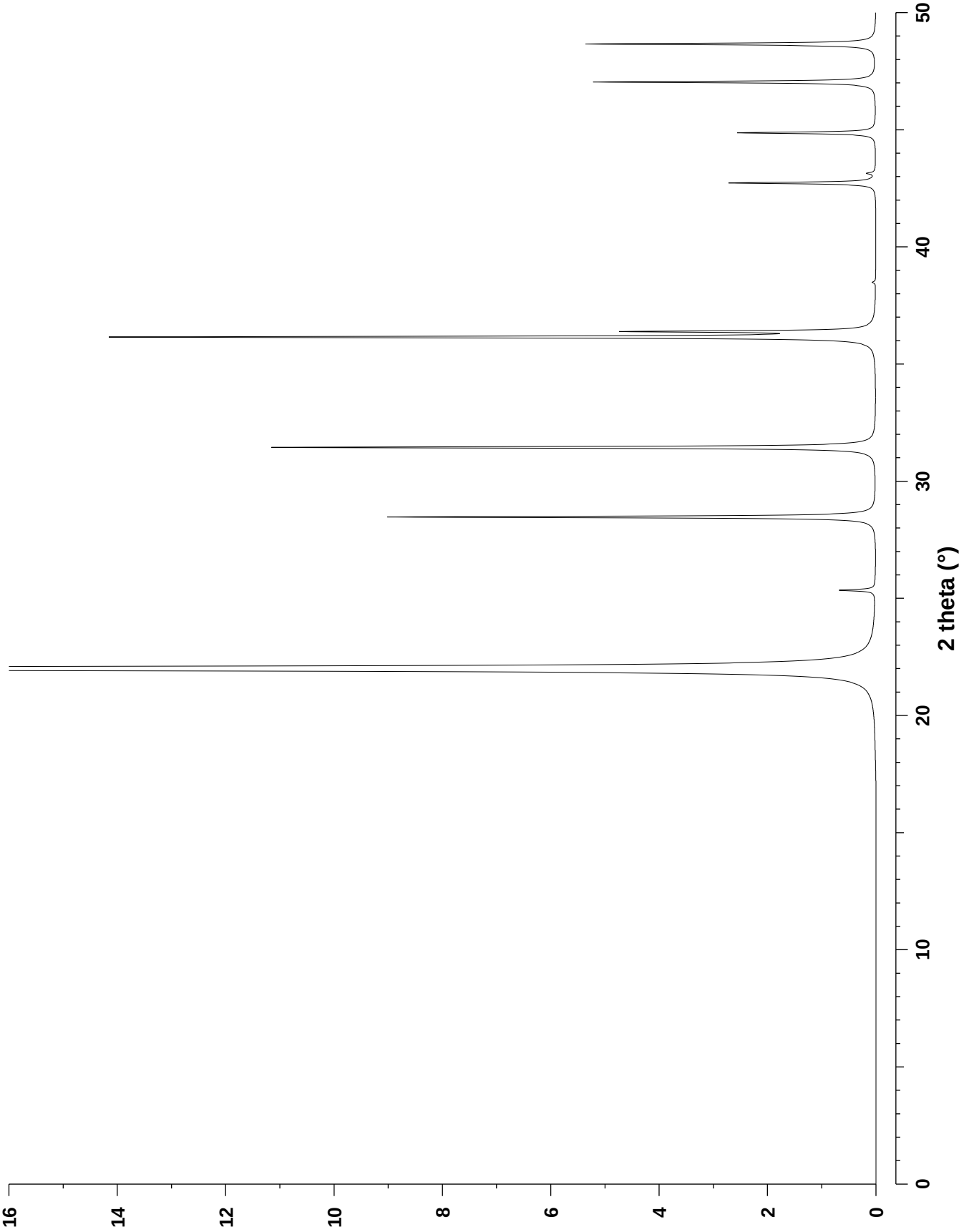
REFINED COMPOSITION: $[Si_4O_8]$

CRYSTAL DATA: $P4_12_12$ (No. 92)
$a = 4.97$ Å $b = 4.97$ Å $c = 6.94$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: W. A. Dollase,
Z. Kristallogr. **121** 369–377 (1965).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	22.00	4.041	8	100.0	2	0	0	36.15	2.485	4	14.0	2	0	2	44.86	2.020	8	2.6
1	1	0	25.34	3.514	4	0.7	1	1	2	36.38	2.469	8	4.3	1	1	3	47.03	1.932	8	5.2
1	1	1	28.47	3.135	8	9.0	2	1	1	42.72	2.117	16	2.7	2	1	2	48.65	1.872	16	5.4
1	0	2	31.44	2.845	8	11.2	1	0	3	43.13	2.097	8	0.2							

Alpha Cristobalite



Keatite

CHEMICAL COMPOSITION: $[Si_{12}O_{24}]$
Synthetic material

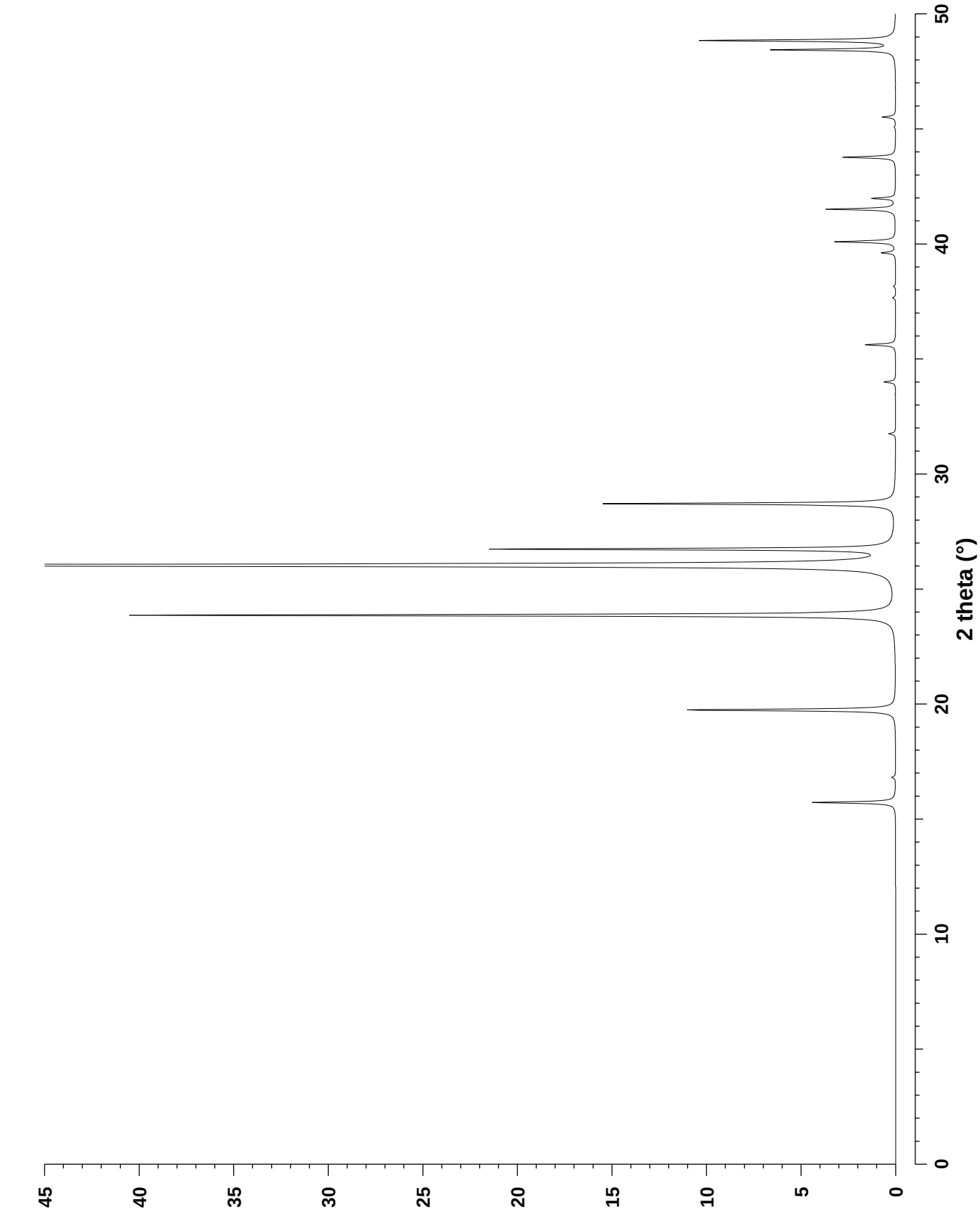
REFINED COMPOSITION: $[Si_{12}O_{24}]$

CRYSTAL DATA: $P4_32_12$ (No. 96)
$a = 7.46$ Å $b = 7.46$ Å $c = 8.61$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{hk0} = 0.129$, $R_{hhl} = 0.098$

REFERENCE: J. Shropshire, P. P. Keat and P. A. Vaughan,
Z. Kristallogr. **112** 409–413 (1959).

h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
1	0	1	15.72	5.638	8	4.4	2	0	2	31.74	2.819	8	0.4	0	0	4	41.97	2.152	2	1.2
1	1	0	16.81	5.275	4	0.2	2	2	0	33.99	2.638	4	0.3	3	2	0	43.75	2.069	8	0.2
1	1	1	19.74	4.498	8	11.0	2	1	2	34.00	2.637	16	0.3	3	1	2	43.76	2.069	16	1.9
2	0	0	23.86	3.730	4	0.7	1	1	3	35.61	2.521	8	1.6	1	0	4	43.77	2.068	8	0.8
1	0	2	23.86	3.729	8	39.8	3	0	1	37.65	2.389	8	0.2	1	1	4	45.51	1.993	8	0.7
2	0	1	26.03	3.423	8	100.0	3	1	0	38.15	2.359	8	0.1	3	0	3	48.43	1.879	8	6.5
2	1	0	26.72	3.336	8	0.5	3	1	1	39.61	2.275	16	0.7	4	0	0	48.83	1.865	4	7.8
1	1	2	26.73	3.335	8	20.7	2	2	2	40.09	2.249	8	3.2	3	2	2	48.84	1.865	16	2.6
2	1	1	28.70	3.111	16	15.5	2	1	3	41.50	2.176	16	3.7							

Keatite



Moganite

CHEMICAL COMPOSITION: $[Si_{12}O_{24}]$
Mogan formation, Gran Canaria, Canary Islands

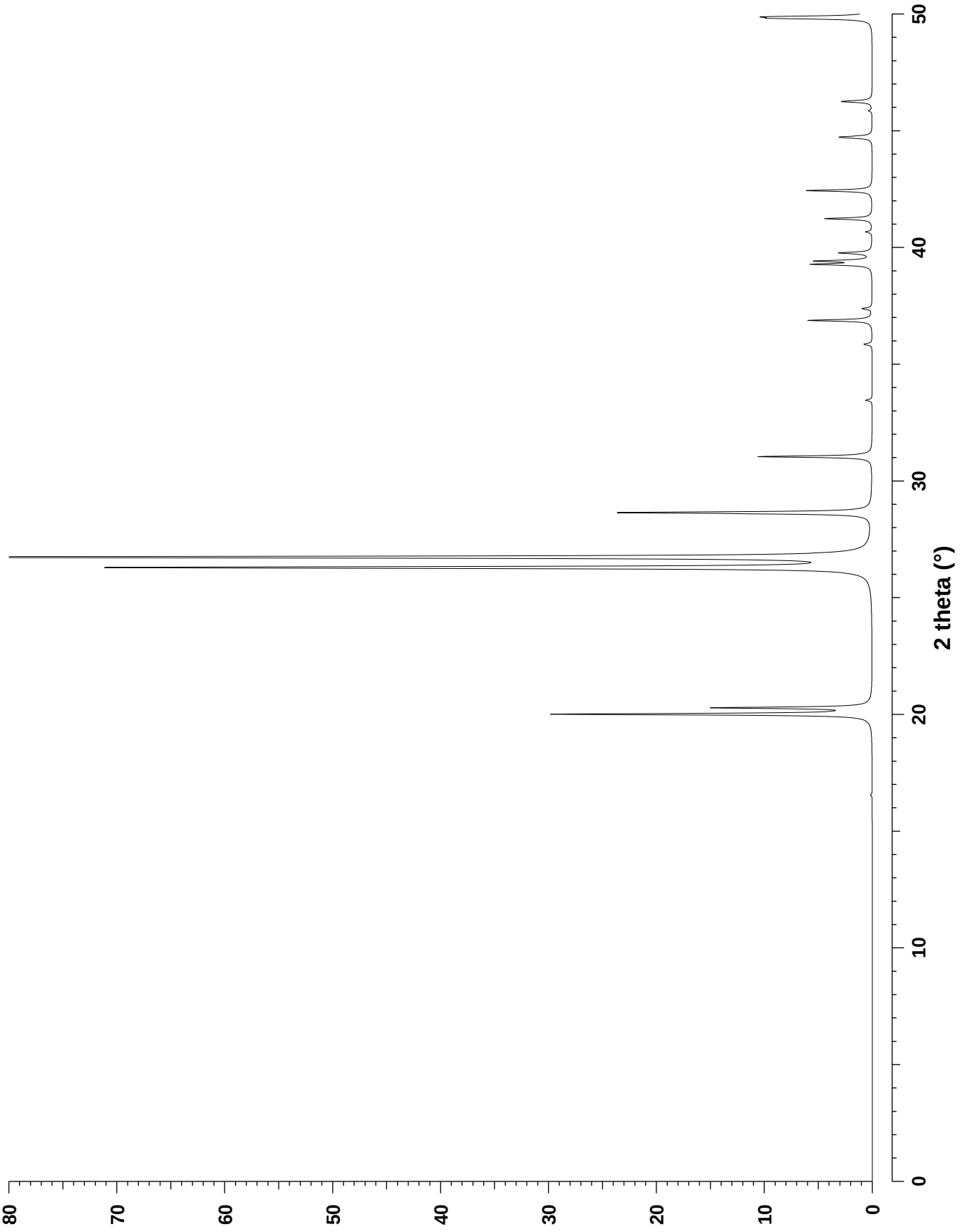
REFINED COMPOSITION: $[Si_{12}O_{24}]$

CRYSTAL DATA: $I1\,2/a\,1$ (No. 15) unique axis **b**, cell choice 3
$a = 8.758$ Å $b = 4.876$ Å $c = 10.715$ Å
$\alpha = 90°$ $\beta = 90.08°$ $\gamma = 90°$

REFERENCE: G. Miehe and H. Graetsch,
Eur. J. Mineral. **4** 693–706 (1992).

h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$	h	k	l	2θ	d	M	$I_{\rm rel}$
0	0	2	16.55	5.357	2	0.2	0	2	0	36.87	2.438	2	9.2	2	2	0	42.43	2.130	4	9.5
0	1	1	20.01	4.438	4	45.7	-2	1	3	37.34	2.408	4	0.1	-4	0	2	44.69	2.028	2	1.9
2	0	0	20.28	4.379	2	22.3	2	1	3	37.38	2.406	4	1.3	4	0	2	44.73	2.026	2	3.8
-2	0	2	26.27	3.393	2	47.4	-1	2	1	39.27	2.294	4	3.3	2	2	2	45.85	1.979	4	0.5
2	0	2	26.30	3.388	2	75.5	1	2	1	39.27	2.294	4	5.0	-4	1	1	46.22	1.964	4	0.4
-1	1	2	26.73	3.336	4	100.0	-2	0	4	39.41	2.287	2	7.6	4	1	1	46.24	1.963	4	3.0
1	1	2	26.74	3.333	4	57.3	2	0	4	39.46	2.284	2	0.6	-1	2	3	46.25	1.963	4	0.5
-2	1	1	28.63	3.118	4	26.7	-3	1	2	39.70	2.270	4	0.4	1	2	3	46.27	1.962	4	0.4
2	1	1	28.65	3.116	4	12.1	3	1	2	39.74	2.268	4	0.4	0	1	5	46.28	1.962	4	0.6
0	1	3	31.04	2.881	4	16.4	1	1	4	39.76	2.267	4	4.2	-3	1	4	49.81	1.831	4	11.2
0	0	4	33.45	2.679	2	1.0	0	2	2	40.66	2.219	4	0.9	3	1	4	49.87	1.828	4	12.5
3	1	0	35.85	2.505	4	1.2	4	0	0	41.23	2.189	2	6.8							

Moganite



Alpha Quartz

CHEMICAL COMPOSITION: $[Si_3O_6]$
Dextro-rotatory synthetic material

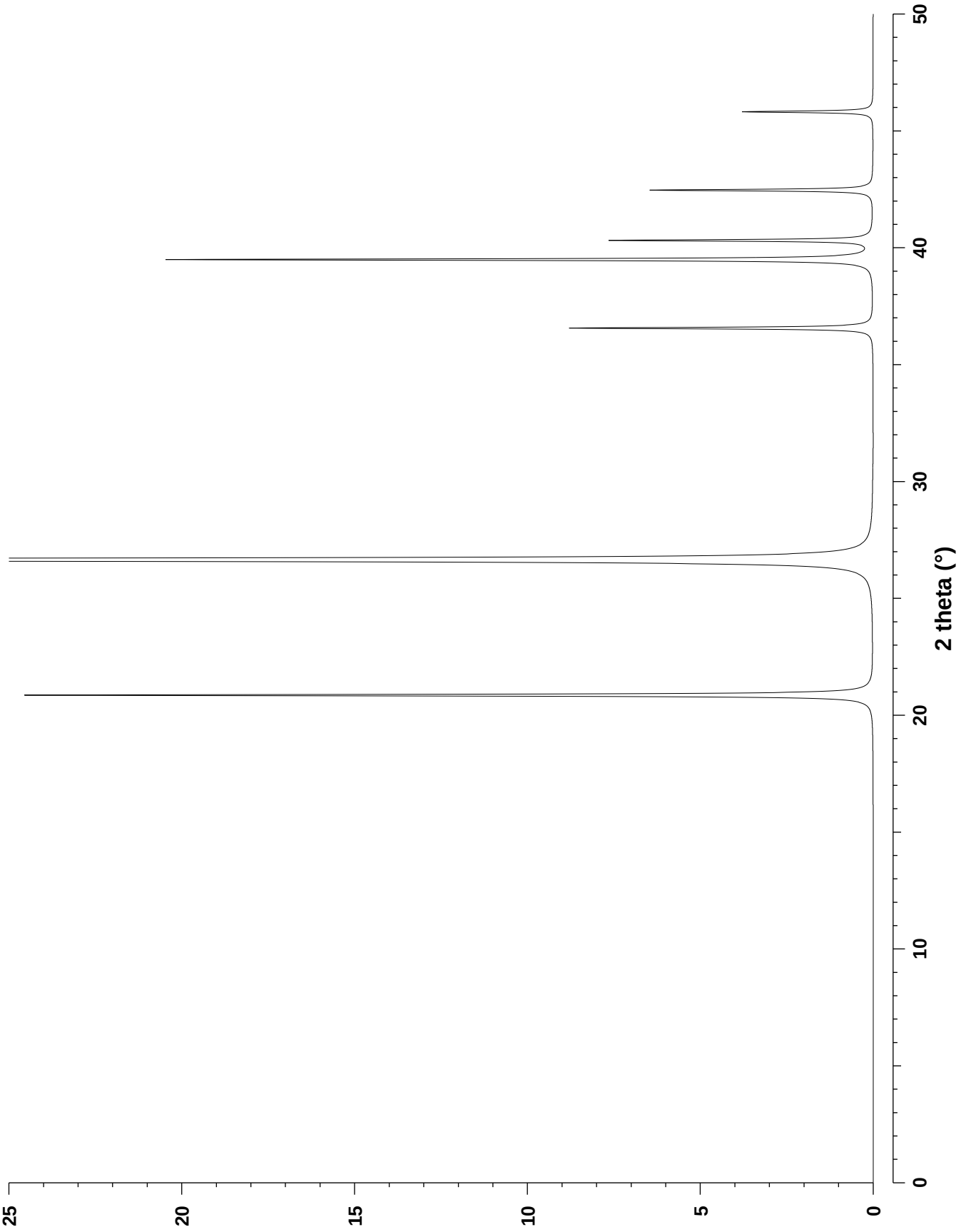
REFINED COMPOSITION: $[Si_3O_6]$

CRYSTAL DATA: $P3_221$ (No. 154)
$a = 4.916$ Å $b = 4.916$ Å $c = 5.4054$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.016$

REFERENCE: L. Levien, C. T. Prewitt and D. J. Weidner,
American Mineralogist **65** 920–930 (1980).

h	k	l	2θ	d	M	I_{rel}
1	0	0	20.86	4.257	6	26.7
0	1	1	26.65	3.345	6	8.9
1	0	1	26.65	3.345	6	100.0
1	1	0	36.56	2.458	6	9.6
1	0	2	39.49	2.282	6	1.1
0	1	2	39.49	2.282	6	21.2
1	1	1	40.31	2.238	12	8.3
2	0	0	42.46	2.129	6	7.0
2	0	1	45.81	1.981	6	2.8
0	2	1	45.81	1.981	6	1.3

Alpha Quartz



Tridymite

CHEMICAL COMPOSITION: $[Si_{48}O_{96}]$
From the Steinbach meteorite, Harvard Museum, U.S.A.

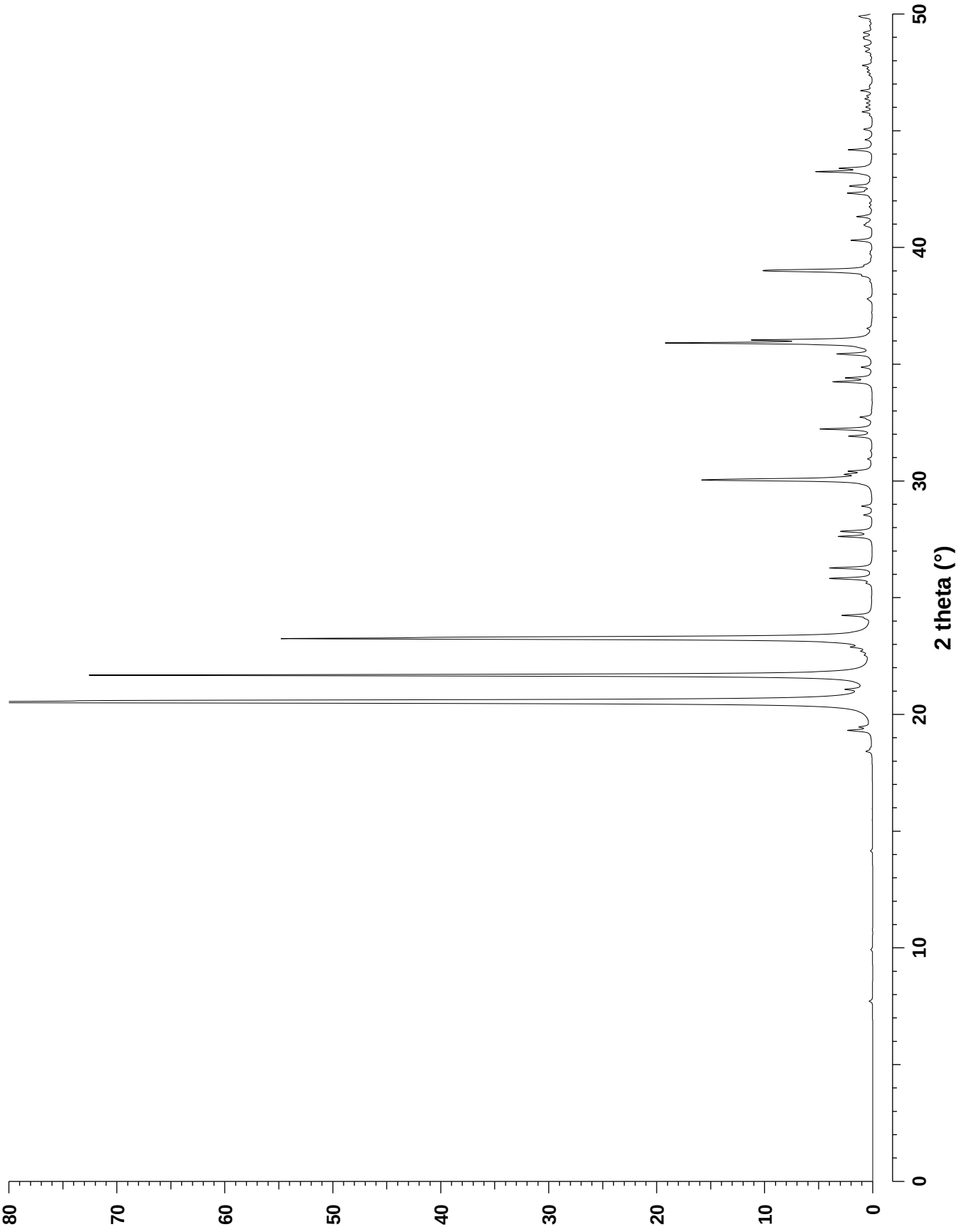
REFINED COMPOSITION: $[Si_{48}O_{96}]$

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 18.524$ Å $b = 5.0032$ Å $c = 23.810$ Å
$\alpha = 90°$ $\beta = 105.82°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.069$

REFERENCE: W. A. Dollase and W. H. Baur,
American Mineralogist **61** 971–978 (1976).

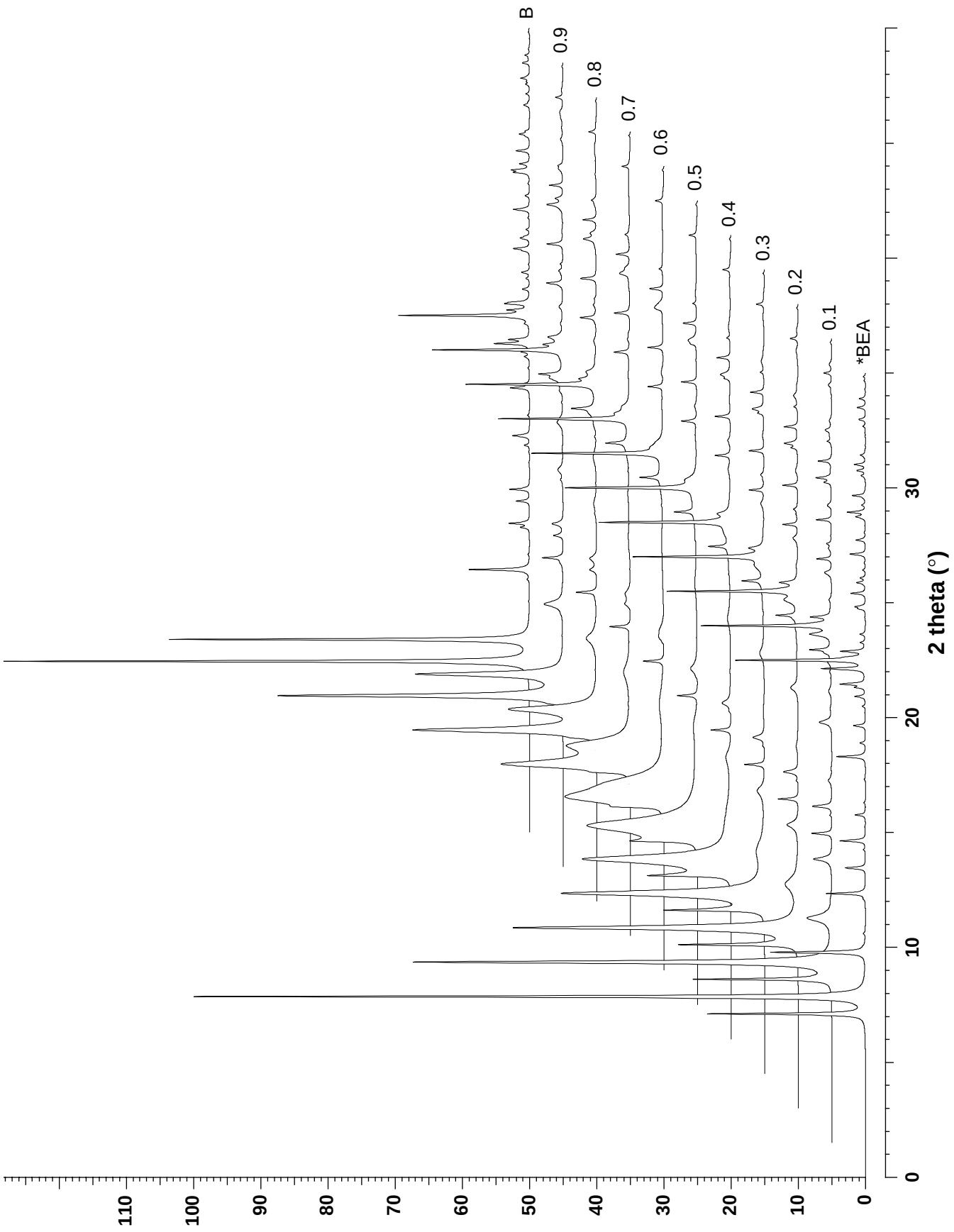
h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}	h	k	l	2θ	d	M	I_{rel}
0	0	2	7.72	11.454	2	0.4	1	1	7	34.24	2.619	4	4.1	-8	0	8	44.18	2.050	2	2.6
2	0	0	9.93	8.911	2	0.2	-5	1	6	34.41	2.607	4	2.6	-5	1	10	44.61	2.031	4	0.7
2	0	2	14.16	6.255	2	0.2	4	0	6	34.87	2.573	2	1.1	4	2	3	44.70	2.027	4	0.2
1	1	0	18.42	4.817	4	0.6	5	1	3	35.43	2.533	4	3.4	-4	2	6	45.03	2.013	4	0.2
-1	1	1	18.54	4.785	4	0.2	2	0	8	35.44	2.533	2	0.1	1	1	10	45.06	2.012	4	0.2
-4	0	2	19.31	4.597	2	2.4	-3	1	8	35.71	2.514	4	0.4	-2	2	7	45.06	2.012	4	0.6
-1	1	2	19.46	4.562	4	1.1	0	2	0	35.90	2.502	2	20.9	0	2	7	45.65	1.987	4	0.3
1	1	2	20.52	4.328	4	100.0	3	1	6	36.03	2.493	4	11.0	-3	1	11	45.80	1.981	4	0.7
2	0	4	20.59	4.313	2	56.5	0	2	1	36.12	2.487	4	0.1	-2	0	12	45.81	1.981	2	0.3
-1	1	3	21.07	4.217	4	1.7	-5	1	7	36.53	2.460	4	0.4	2	2	6	46.01	1.973	4	0.6
-4	0	4	21.68	4.100	2	82.5	-2	0	10	37.79	2.381	2	0.5	3	1	9	46.17	1.966	4	0.3
1	1	3	22.54	3.945	4	0.3	0	2	3	37.84	2.377	4	0.1	5	1	7	46.18	1.966	4	0.1
-2	0	6	22.70	3.917	2	0.6	-1	1	9	38.78	2.322	4	0.6	-1	1	11	46.20	1.965	4	0.1
-3	1	1	22.88	3.887	4	1.3	-3	1	9	38.90	2.315	4	0.2	-4	0	12	46.36	1.959	2	0.7
-1	1	4	23.24	3.828	4	27.0	-7	1	1	38.92	2.314	4	0.3	4	2	4	46.48	1.954	4	0.3
3	1	0	23.24	3.827	4	26.8	-5	1	8	38.97	2.311	4	1.8	7	1	4	46.49	1.953	4	0.2
0	0	6	23.30	3.818	2	15.7	-7	1	4	38.98	2.311	4	4.6	-7	1	9	46.71	1.945	4	1.2
4	0	2	23.31	3.816	2	15.0	-4	0	10	39.00	2.309	2	2.3	-6	2	3	46.88	1.938	4	0.1
-3	1	3	24.11	3.691	4	0.4	-8	0	2	39.03	2.308	2	6.7	-6	2	1	46.95	1.935	4	0.2
3	1	1	24.24	3.671	4	3.1	3	1	7	39.24	2.296	4	0.4	-6	2	4	47.37	1.919	4	0.3
-3	1	4	25.62	3.476	4	0.5	7	1	0	39.72	2.269	4	0.2	-2	2	8	47.50	1.914	4	0.2
3	1	2	25.81	3.452	4	2.5	-7	1	5	39.82	2.264	4	0.2	6	2	0	47.52	1.913	4	0.3
-1	1	5	25.83	3.449	4	2.3	5	1	5	40.30	2.238	4	2.3	0	0	12	47.63	1.909	2	0.2
-4	0	6	26.27	3.392	2	4.5	7	1	1	40.91	2.206	4	0.4	8	0	4	47.66	1.908	2	0.3
-3	1	5	27.62	3.229	4	3.5	-8	0	6	40.96	2.203	2	0.6	-5	1	11	47.76	1.904	4	0.1
2	0	6	27.82	3.207	2	1.5	-2	2	5	41.03	2.200	4	0.2	-9	1	3	47.79	1.903	4	0.9
1	1	5	27.84	3.204	4	1.3	-7	1	6	41.04	2.199	4	0.1	-9	1	2	48.02	1.895	4	0.1
3	1	3	27.85	3.203	4	0.8	0	2	5	41.11	2.196	4	0.1	-6	2	5	48.21	1.887	4	0.2
4	0	4	28.54	3.128	2	0.9	1	1	9	41.32	2.185	4	1.6	-9	1	5	48.38	1.881	4	0.6
-6	0	2	28.92	3.087	2	1.1	2	2	4	41.74	2.164	4	0.3	6	2	1	48.43	1.880	4	0.2
-6	0	4	29.87	2.991	2	0.1	4	0	8	41.89	2.156	2	0.3	2	2	7	48.55	1.875	4	0.1
-3	1	6	30.02	2.977	4	6.1	4	2	1	42.13	2.145	4	0.2	-9	1	1	48.59	1.874	4	0.3
-5	1	2	30.03	2.976	4	7.3	-3	1	10	42.27	2.138	4	0.4	-8	0	10	48.62	1.872	2	0.6
-2	0	8	30.06	2.972	2	4.5	-4	2	4	42.32	2.135	4	2.4	1	1	11	48.91	1.862	4	0.2
6	0	0	30.08	2.970	2	5.1	-1	1	10	42.43	2.131	4	0.2	7	1	5	48.93	1.861	4	0.6
-5	1	1	30.16	2.963	4	1.0	7	1	2	42.45	2.129	4	0.3	-4	2	8	49.00	1.859	4	0.8
3	1	4	30.28	2.951	4	2.1	-7	1	7	42.61	2.122	4	0.6	-7	1	10	49.17	1.853	4	0.2
-5	1	3	30.41	2.939	4	2.1	3	1	8	42.63	2.121	4	1.9	-9	1	6	49.19	1.852	4	0.3
1	1	6	30.94	2.890	4	0.5	-6	0	10	42.77	2.114	2	0.2	-6	0	12	49.20	1.852	2	0.3
-5	1	4	31.30	2.858	4	0.2	-2	2	6	42.89	2.108	4	0.1	-10	0	4	49.23	1.851	2	0.3
-1	1	7	31.91	2.805	4	0.5	5	1	6	43.13	2.097	4	0.4	9	1	0	49.50	1.841	4	0.2
5	1	1	31.92	2.803	4	1.9	0	2	6	43.24	2.092	4	3.0	6	2	2	49.67	1.836	4	0.2
-4	0	8	32.22	2.778	2	5.5	4	2	2	43.24	2.092	4	2.7	3	1	10	49.85	1.829	4	0.8
-5	1	5	32.64	2.743	4	0.4	2	0	10	43.38	2.086	2	2.0	6	0	8	49.90	1.828	2	1.1
-3	1	7	32.73	2.736	4	1.2	6	0	6	43.40	2.085	2	1.3							

Tridymite

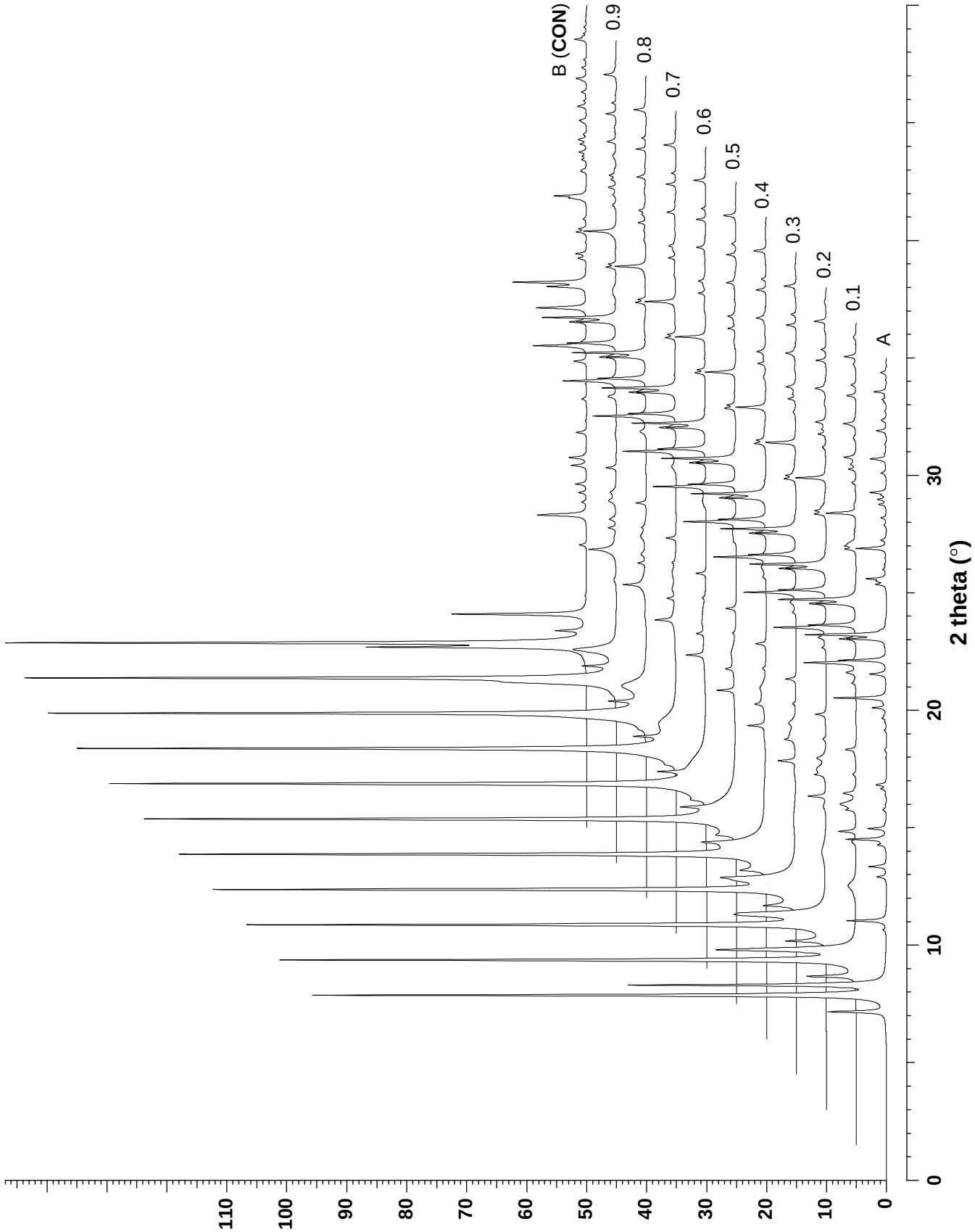


POWDER PATTERN SIMULATIONS OF DISORDERED INTERGROWTHS

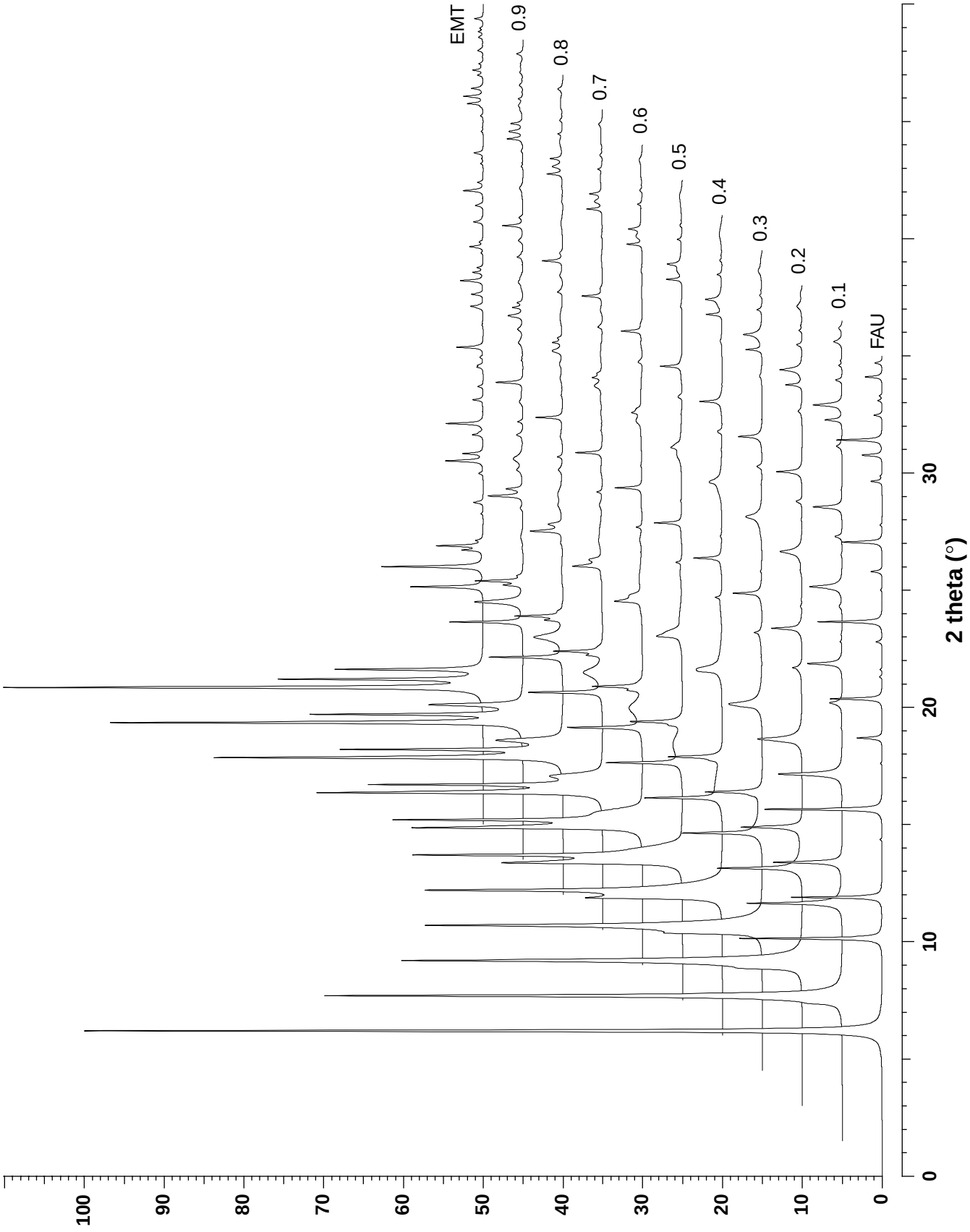
Beta family, polymorph A (*BEA) – polymorph B



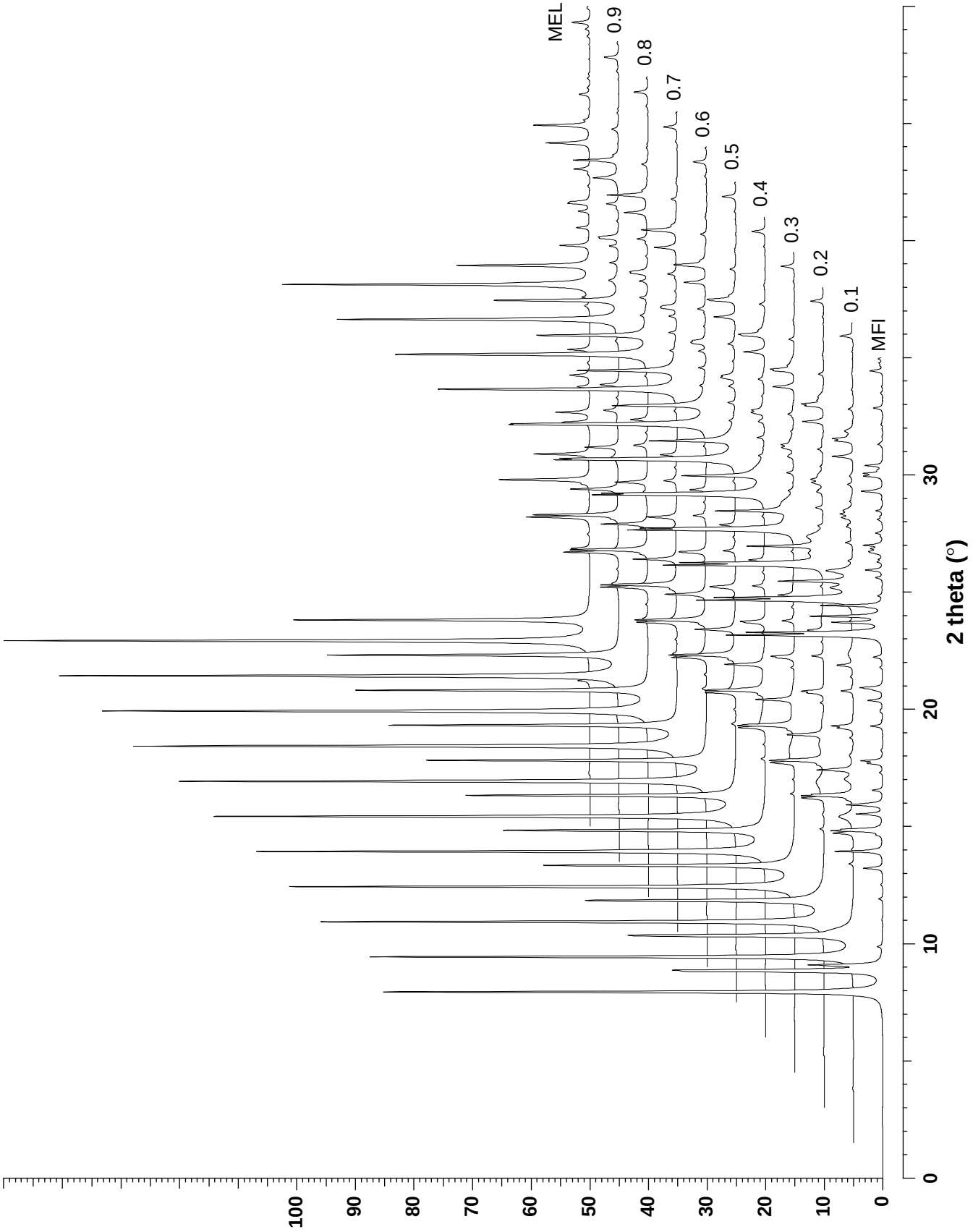
SSZ33/SSZ26 family, polymorph A – polymorph B

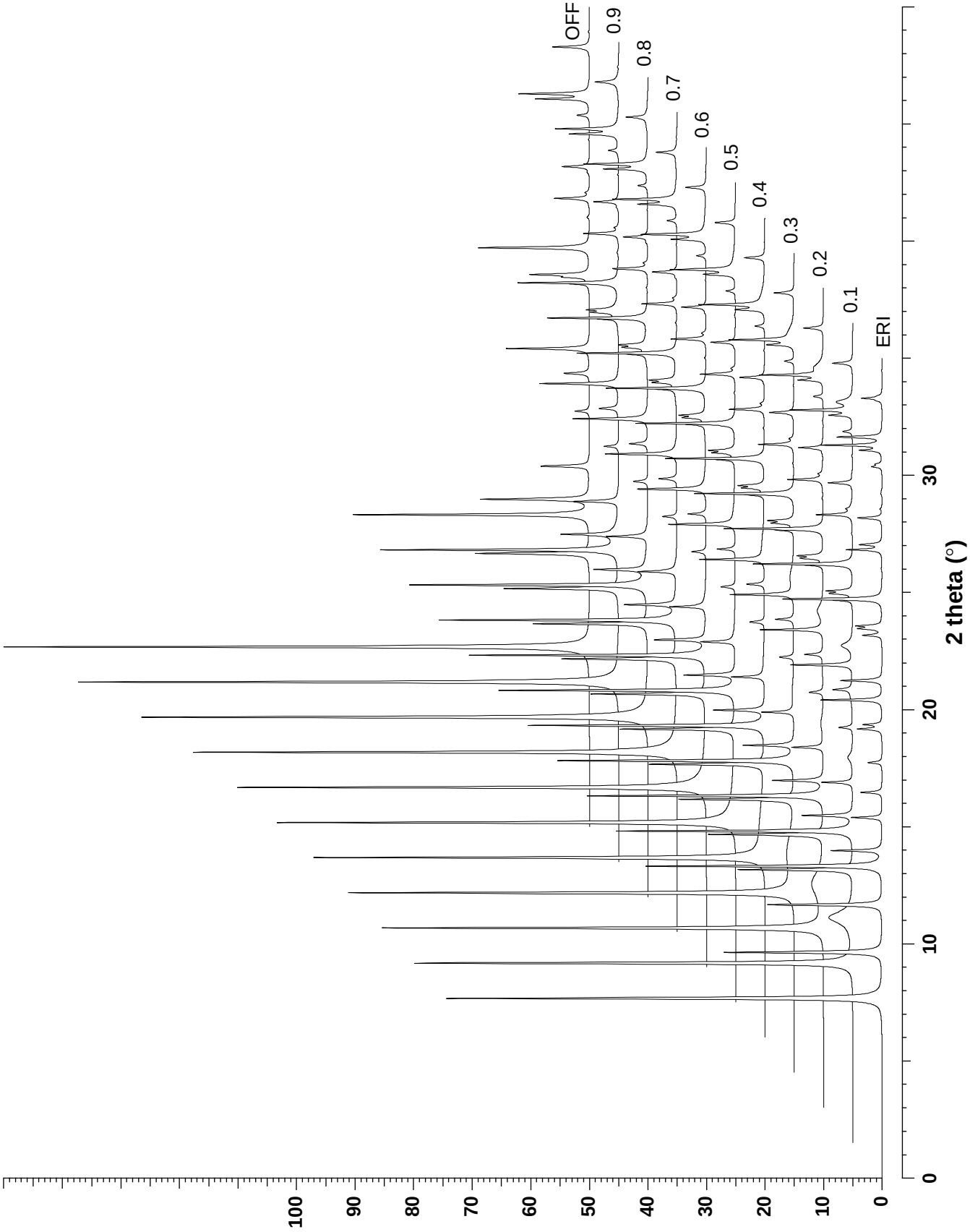


Faujasite family, FAU – EMT



ZSM5/ZSM11 family, MFI – MEL

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30
2 theta (°)
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80
90
100

ATOMIC COORDINATES

REFINED COMPOSITION: $|Li_4(H_2O)_4|$ $[Si_4Al_4O_{16}]$

CRYSTAL DATA: $Pna2_1$ (No. 33)
$a = 10.313$ Å $b = 8.194$ Å $c = 4.993$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.081$

REFERENCE: E. Krogh Andersen and G. Ploug-Sørensen, *Z. Kristallogr.* **176** 67–73 (1986).

Atom	x	y	z	B_{iso}	occ
Li	0.1862	0.6849	0.2520	1.57	1.0
Si	0.3544	0.3757	0.2492	0.44	1.0
Al	0.1593	0.0810	0.2500	0.4	1.0
O 1	0.0061	0.1584	0.1970	0.75	1.0
O 2	0.2736	0.2198	0.1391	0.97	1.0
O 3	0.1912	0.0399	0.5907	0.76	1.0
O 4	0.1804	-0.1008	0.0689	0.68	1.0
H 1	0.5497	0.1798	0.8651	4.0	1.0
H 2	0.4965	0.0587	0.5773	4.2	1.0
O 5	0.4891	0.0903	-0.2395	2.93	1.0

REFINED COMPOSITION: $|C_8N_8O_2|$ $[Co_8P_8O_{32}]$

CRYSTAL DATA: $I\bar{4}2m$ (No. 121)
$a = 10.240$ Å $b = 10.240$ Å $c = 9.652$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_p = 0.0775$

REFERENCE: P. Feng, X. Bu and G. D. Stucky,
Nature **388** 735–741 (1997).

Atom	x	y	z	B_{iso}	occ
Co	0.6332	0.3668	0.1316	3.79	0.89
Al	0.6332	0.3668	0.1316	3.79	0.11
P	0.6647	0.3353	0.8092	4.34	1.0
O 1	0.6999	0.3001	0.9553	5.37	1.0
O 2	0.4818	0.3036	0.2179	6.0	1.0
O 3	0.7417	0.2583	0.7049	11.2	1.0
N	0.5	0.1847	0.5	4.03	1.0
C	0.5017	0.0444	0.568	3.0	0.5
O 10	0.5	0.5	0.0	4.82	0.5
O 20	0.5	0.5	0.5	8.37	0.5

REFINED COMPOSITION: $[Al_{24}P_{24}O_{96}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 13.7114$ Å $b = 12.7315$ Å $c = 18.5706$ Å
$\alpha = 90°$ $\beta = 90.01°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.047$, $R_{wp} = 0.108$, $R_F = 0.032$

REFERENCE: A. Simmen, L. B. McCusker, Ch. Baerlocher and W. M. Meier, *Zeolites* **11** 654–661 (1991). Ch. Baerlocher, Private communication.

Atom	x	y	z	B_{iso}	occ
Al 1	0.88997	0.95872	0.16598	0.75	1.0
Al 2	0.88129	0.22661	0.93877	0.96	1.0
Al 3	0.22953	0.09687	0.04922	1.42	1.0
P 1	0.77251	0.09559	0.05384	1.42	1.0
P 2	0.10981	0.23135	0.93763	0.96	1.0
P 3	0.11634	0.96983	0.16394	0.75	1.0
O 1	0.17723	0.05318	0.12913	0.72	1.0
O 2	0.14278	0.16702	0.00209	0.72	1.0
O 3	0.00371	0.25884	0.94574	0.72	1.0
O 4	0.84714	0.16747	0.02039	0.72	1.0
O 5	0.81686	0.04552	0.12009	0.72	1.0
O 6	0.01022	0.99732	0.15632	0.72	1.0
O 7	0.13601	0.86260	0.13230	0.72	1.0
O 8	0.33199	0.16953	0.06981	0.72	1.0
O 9	0.85795	0.96546	0.25665	0.72	1.0
O 10	0.81531	0.33988	0.92509	0.72	1.0
O 11	0.12779	0.16274	0.87230	0.72	1.0
O 12	0.26213	-0.01281	0.99849	0.72	1.0

AEL AlPO–11, Calcined

REFINED COMPOSITION: $[Al_{20}P_{20}O_{80}]$

CRYSTAL DATA: *Ibm*2 (No. 46) **ba$\overline{\mathbf{c}}$** setting
$a = 13.5336$ Å $b = 18.4821$ Å $c = 8.3703$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.027$, $R_{F^2} = 0.058$

REFERENCE: J. W. Richardson, Jr., J. J. Pluth and J. V. Smith,
Acta Cryst. **B44** 367–373 (1988).

Atom	x	y	z	B_{iso}	occ
Al 1	0.134	0.035	-0.199	2.76	1.0
Al 2	0.949	0.102	0.317	3.54	1.0
Al 3	0.850	0.250	-0.185	1.89	1.0
P 1	0.143	0.025	0.182	2.76	1.0
P 2	0.953	0.104	-0.306	3.54	1.0
P 3	0.857	0.250	0.185	1.89	1.0
O 1	0.143	0.039	0.000	12.15	1.0
O 2	0.945	0.105	0.517	6.09	1.0
O 3	0.860	0.250	0.024	9.72	1.0
O 4	0.242	0.068	0.243	5.04	1.0
O 5	0.068	0.088	0.252	5.37	1.0
O 51	0.057	0.091	-0.257	5.37	1.0
O 6	0.118	0.955	0.232	8.52	1.0
O 61	0.125	0.954	-0.264	8.52	1.0
O 7	0.913	0.179	0.232	8.76	1.0
O 71	0.909	0.177	-0.263	8.76	1.0
O 8	0.762	0.250	0.234	7.02	1.0

REFINED COMPOSITION: $|C_{15.5}N_{2.58}|\ [Al_{20.54}P_{18.22}O_{80}]$

CRYSTAL DATA: *Ibm*2 (No. 46) **ba$\overline{\mathbf{c}}$** setting
$a = 13.472$ Å $b = 18.712$ Å $c = 8.4431$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.042$

REFERENCE: J. J. Pluth, J. V. Smith and J. W. Richardson, Jr., *J. Phys. Chem.* **92** 2734–2738 (1988).

Atom	x	y	z	B_{iso}	occ
Al 1	0.1390	0.0331	-0.203	3.553	1.034
Al 2	0.9501	0.1060	0.294	3.553	1.028
Al 3	0.8565	0.250	-0.208	2.921	1.010
P 1	0.1464	0.0365	0.170	3.324	0.913
P 2	0.9515	0.10846	-0.334	3.024	0.912
P 3	0.8621	0.250	0.163	2.661	0.904
O 1	0.1430	0.0364	0.000	9.396	1.0
O 2	0.9515	0.1120	0.491	10.185	1.0
O 3	0.8542	0.250	0.001	10.422	1.0
O 4	0.2455	0.0612	0.228	6.711	1.0
O 5	0.0690	0.0874	0.234	6.632	1.0
O 51	0.0564	0.0974	-0.277	6.79	1.0
O 6	0.1250	0.9611	0.232	7.106	1.0
O 61	0.1158	0.9498	-0.276	7.896	1.0
O 7	0.9175	0.1863	0.221	8.764	1.0
O 71	0.9169	0.1786	-0.267	8.922	1.0
O 8	0.7620	0.250	0.227	9.554	1.0
C 1	0.250	0.250	0.073	21.318	0.646
C 2	0.246	0.250	0.346	21.318	0.646
C 3	0.3449	0.250	0.457	13.738	1.292
C 4	0.161	0.250	0.448	17.371	1.292
N	0.301	0.206	0.242	17.371	0.323

REFINED COMPOSITION: $|(C_8N_8O_8)(H_2O)_8|\ [P_{24}Al_{24}O_{96}]$

CRYSTAL DATA: $P2_12_12_1$ (No. 19)
$a = 10.321$ Å $b = 13.631$ Å $c = 17.454$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement. $R_p = 0.140$, $R_{wp} = 0.182$, $R_{F^2} = 0.103$

REFERENCE: R. M. Kirchner, R. W. Grosse-Kunstleve, J. J. Pluth, S. T. Wilson, R. W. Broach and J. V. Smith,
Microporous and Mesoporous Materials **39** 319–332 (2000).

Atom	x	y	z	B_{iso}	occ
P 1	0.8718	0.0088	0.0463	1.05	1.0
P 2	0.1248	0.3179	0.1721	1.05	1.0
P 3	0.1135	0.8170	0.8271	1.05	1.0
P 4	0.8810	0.4973	0.9579	1.05	1.0
P 5	0.1237	0.7200	0.0851	1.05	1.0
P 6	0.1289	0.2104	0.9227	1.05	1.0
Al 1	0.1124	0.9905	0.9460	1.22	1.0
Al 2	0.8750	0.8123	0.1446	1.22	1.0
Al 3	0.1226	0.4884	0.0590	1.22	1.0
Al 4	0.8804	0.3091	0.8580	1.22	1.0
Al 5	0.9268	0.7311	0.9514	1.22	1.0
Al 6	0.9210	0.2354	0.0511	1.22	1.0
O 1	0.8514	0.2491	0.9560	0.83	1.0
O 2	0.8494	0.7656	0.0421	0.83	1.0
O 3	0.9414	0.1067	0.0646	0.83	1.0
O 4	0.9102	0.6021	0.9286	0.83	1.0
O 5	0.8696	0.4348	0.8842	0.83	1.0
O 6	0.8749	0.9373	0.1152	0.83	1.0
O 7	0.1273	0.6078	0.0976	0.83	1.0
O 8	0.0863	0.1051	0.9013	0.83	1.0
O 9	0.0864	0.2483	0.0029	0.83	1.0
O 10	0.9660	0.4661	0.0268	0.83	1.0
O 11	0.9946	0.2866	0.1359	0.83	1.0
O 12	0.9674	0.9566	0.9900	0.83	1.0
O 13	0.0440	0.7717	0.1486	0.83	1.0
O 14	0.2307	0.2390	0.1688	0.83	1.0
O 15	0.1777	0.4108	0.1322	0.83	1.0
O 16	0.9831	0.7730	0.8558	0.83	1.0
O 17	0.0876	0.7357	0.9998	0.83	1.0
O 18	0.0946	0.3485	0.2546	0.83	1.0
O 19	0.7355	0.0268	0.0144	0.83	1.0
O 20	0.2163	0.7365	0.8383	0.83	1.0
O 21	0.9102	0.3467	0.7561	0.83	1.0
O 22	0.2701	0.7347	0.0944	0.83	1.0
O 23	0.7596	0.2456	0.1026	0.83	1.0
O 24	0.0393	0.2626	0.8658	0.83	1.0
O 25	0.8490	0.4091	0.6274	0.83	1.0
O 26	0.7580	0.4987	0.4900	0.83	1.0
H_2O 1	0.7788	0.3736	0.2476	4.74	1.0
H_2O 2	0.7142	0.1702	0.2521	7.11	1.0

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Atom	x	y	z	B_{iso}	occ
N 1	0.0457	0.5689	0.2542	3.95	1.0
C 1	0.9121	0.5366	0.2338	3.95	1.0
N 2	0.4381	0.4467	0.2655	3.95	1.0
C 2	0.3506	0.5317	0.2604	3.95	1.0

REFINED COMPOSITION: $[Si_{72}O_{144}]$

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 33.2900$ Å $b = 14.7036$ Å $c = 8.3863$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.043$, $R_{F^2} = 0.077$

REFERENCE: J. W. Richardson, Jr. and E. T. C. Vogt,
Zeolites **12** 13–19 (1992).

Atom	x	y	z	B_{iso}	occ
Si 11	0.1904	0.416	0.066	-1.3	1.0
Si 12	0.0	0.132	-0.028	12.4	1.0
Si 21	0.0878	0.094	0.055	-0.1	1.0
Si 22	0.2740	0.404	-0.061	-0.1	1.0
Si 23	0.1573	0.226	-0.071	-0.1	1.0
O 11	0.1767	0.5	0.0	0.3	1.0
O 12	0.0	0.0	0.0	12.8	1.0
O 21	0.1772	0.402	0.25	-0.7	1.0
O 22	0.0	0.127	-0.25	12.5	1.0
O 31	0.0456	0.133	0.018	2.0	1.0
O 32	0.2317	0.394	0.020	3.0	1.0
O 33	0.1580	0.324	0.031	3.0	1.0
O 41	0.1993	0.175	0.017	3.0	1.0
O 42	0.0906	0.0	0.0	3.0	1.0
O 51	0.0847	0.096	0.25	6.6	1.0
O 52	0.2590	0.378	-0.25	6.6	1.0
O 53	0.1444	0.232	-0.25	6.6	1.0
O 61	0.1154	0.174	0.002	3.0	1.0
O 62	0.2865	0.5	0.0	3.0	1.0

Aluminophosphate material refined assuming SiO_2 composition
in a higher space group symmetry.

REFINED COMPOSITION: $|(Na_{10.134}K_{5.304}Ca_{9.332})((SO_4)_6Cl_{5.8}F_{0.18})|\ [Si_{24}Al_{24}O_{96}]$
Pitigliano, Tuscany, Italy

CRYSTAL DATA: $P31c$ (No. 159)
$a = 12.801$ Å $b = 12.801$ Å $c = 21.412$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_p = 0.045$, $R_{wp} = 0.102$

REFERENCE: P. Ballirano, E. Bonaccorsi, A. Maras and S. Merlino, *Eur. J. Mineral.* **9** 21–30 (1997).

Atom	x	y	z	B_{iso}	occ
Si 1	0.253	0.0	0.495	0.39	1.0
Al 1	0.7412	0.0	0.9952	0.92	1.0
Si 2	0.9234	0.5849	0.3687	0.72	1.0
Al 2	0.0784	0.4032	0.8684	0.69	1.0
Si 3	0.0056	0.257	0.2445	0.72	1.0
Al 3	0.004	0.7424	0.745	0.45	1.0
Si 4	0.9232	0.5851	0.1217	0.59	1.0
Al 4	0.0783	0.4035	0.622	0.55	1.0
O 1	0.342	0.333	0.6773	2.01	1.0
O 2	0.669	0.68	0.182	1.53	1.0
O 3	0.348	0.345	0.8062	1.27	1.0
O 4	0.663	0.668	0.302	1.53	1.0
O 5	0.122	0.887	0.7462	1.16	1.0
O 6	0.336	0.335	0.4281	2.1	1.0
O 7	0.674	0.677	0.9335	1.69	1.0
O 8	0.3516	0.3424	0.0554	1.21	1.0
O 9	0.658	0.669	0.5508	1.74	1.0
O 10	0.121	0.883	0.0028	2.45	1.0
O 11	0.117	0.887	0.4947	1.71	1.0
O 12	0.118	0.884	0.2491	1.76	1.0
O 13	0.458	0.5465	0.6257	2.31	1.0
O 14	0.4562	0.5482	0.875	1.59	1.0
O 15	0.2113	0.7732	0.6264	1.64	1.0
O 16	0.2128	0.7715	0.866	1.48	1.0
Ca 1	0.0	0.0	0.0	1.38	1.0
Ca 2	0.0	0.0	0.25	1.29	1.0
Ca 3	0.3333	0.6667	0.6296	1.03	0.9
Ca 31	0.3333	0.6667	0.66	1.03	0.1
Ca 4	0.3333	0.6667	0.8791	1.16	0.9
Ca 41	0.3333	0.6667	0.853	1.16	0.1
Cl 1	0.0	0.0	0.1237	5.53	1.0
Cl 2	0.0	0.0	0.3739	6.28	1.0
Cl 3	0.3333	0.6667	0.7527	9.14	0.9
F	0.4018	0.5995	0.7452	3.95	0.03
K 1	0.4432	0.2235	0.8651	3.06	0.218
Ca 1	0.4432	0.2235	0.8651	3.06	0.092
Na 1	0.4432	0.2235	0.8651	3.06	0.364
K 11	0.386	0.199	0.86	3.06	0.1
K 2	0.5054	0.5014	0.9912	2.98	0.243

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Atom	x	y	z	B_{iso}	occ
Ca 22	0.5054	0.5014	0.9912	2.98	0.103
Na 2	0.5054	0.5014	0.9912	2.98	0.423
K 3	0.5211	0.4845	0.7412	3.15	0.012
Ca 32	0.5211	0.4845	0.7412	3.15	0.005
Na 3	0.5211	0.4845	0.7412	3.15	0.573
K 4	0.423	0.21	0.6238	2.69	0.051
Ca 42	0.423	0.21	0.6238	2.69	0.022
Na 4	0.423	0.21	0.6238	2.69	0.329
K 41	0.456	0.236	0.6163	2.69	0.26
S 1	0.3333	0.6667	0.2475	3.39	1.0
S 2	0.3333	0.6667	0.4625	3.51	1.0
S 3	0.3333	0.6667	0.0301	4.2	1.0
O 17	0.444	0.744	0.278	7.26	0.3333
O 18	0.4	0.619	0.208	9.26	0.3333
O 19	0.4	0.64	0.296	10.95	0.3333
O 20	0.432	0.762	0.214	14.96	0.3333
O 21	0.3333	0.6667	0.5231	9.89	1.0
O 22	0.211	0.608	0.442	6.91	1.0
O 23	0.206	0.587	0.073	12.8	0.3333
O 24	0.215	0.608	0.042	9.88	0.6667
O 25	0.265	0.635	0.97	12.6	0.3333

REFINED COMPOSITION: $|C_{12}NF|\ [Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: *P*6*cc* (No. 184)
$a = 13.740$ Å $b = 13.740$ Å $c = 8.474$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.042$

REFERENCE: S. Qiu, W. Pang, H. Kessler and J. L. Guth, *Zeolites* **9** 440–444 (1989).

Atom	x	y	z	B_{iso}	occ
P	0.4529	0.3281	0.053	2.25	1.0
Al	0.4571	0.3382	0.425	1.89	1.0
O 1	0.4214	0.209	0.008	4.18	1.0
O 2	0.4550	0.3299	0.251	5.33	1.0
O 3	0.3658	0.3597	0.004	4.11	1.0
O 4	0.5742	0.4175	0.007	5.03	1.0
C 1	0.104	0.041	0.666	3.95	0.1667
C 2	0.125	0.979	0.750	3.95	0.1667
C 3	0.104	0.979	0.416	3.95	0.1667
C 4	0.000	0.895	0.500	3.95	0.1667
C 5	0.041	0.895	0.359	3.95	0.1667
C 6	0.082	0.957	0.221	3.95	0.1667
N	0.000	0.000	0.543	3.95	0.5
F	0.500	0.500	0.317	3.95	0.1667

REFINED COMPOSITION: $[Al_8P_8O_{32}]$

CRYSTAL DATA: $P\overline{1}$ (No. 2)
$a = 9.7041$ Å $b = 9.7361$ Å $c = 10.202$ Å
$\alpha = 77.811°$ $\beta = 77.504°$ $\gamma = 87.691°$
X-ray Rietveld refinement, $R_F = 0.059$, $R_P = 0.114$, $R_{wP} = 0.135$

REFERENCE: R. W. Broach, S. T. Wilson and R. M. Kirchner,
in *Proceedings of the 12th International Zeolite Conference*,
Ed. by M. M. J. Treacy, B. K. Marcus, J. B. Higgins and M. E. Bisher
(Materials Research Society: Warrendale) vol. **III** 1715–1722 (1999).

Atom	x	y	z	B_{iso}	occ
Al 1	0.2730	0.7425	0.8445	0.79	1.0
Al 2	0.4322	0.2004	0.9080	0.79	1.0
Al 3	0.8141	0.0506	0.6558	0.79	1.0
Al 4	0.0699	0.4732	0.2015	0.79	1.0
P 1	0.5246	0.9351	0.7996	1.03	1.0
P 2	0.2010	0.4282	0.9010	1.03	1.0
P 3	0.9511	0.1884	0.3437	1.03	1.0
P 4	0.7520	0.2740	0.8400	1.03	1.0
O 1	0.0766	0.4368	0.8348	0.79	1.0
O 2	0.3024	0.3126	0.8628	0.79	1.0
O 3	0.7757	0.2329	-0.0177	0.79	1.0
O 4	0.4396	0.6420	0.8307	0.79	1.0
O 5	0.4431	0.8367	0.7641	0.79	1.0
O 6	0.2989	0.5607	0.8480	0.79	1.0
O 7	0.0245	0.3297	0.3318	0.79	1.0
O 8	0.8582	0.1495	0.4864	0.79	1.0
O 9	0.9407	0.9216	0.6755	0.79	1.0
O 10	0.1609	0.4094	0.0595	0.79	1.0
O 11	0.8659	0.1898	0.2366	0.79	1.0
O 12	0.6009	0.2911	0.8439	0.79	1.0
O 13	0.8048	0.1556	0.7691	0.79	1.0
O 14	0.3519	0.0299	0.3184	0.79	1.0
O 15	0.4183	0.1391	0.0786	0.79	1.0
O 16	0.8210	0.4141	0.7623	0.79	1.0

REFINED COMPOSITION: $[Al_{10}P_{10}O_{40}]$

CRYSTAL DATA: $P112_1$ (No. 4) unique axis **c**
$a = 9.7179$ Å $b = 13.7915$ Å $c = 8.3591$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 110.6°$
X-ray Rietveld refinement, $R_{exp} = 0.023$, $R_{wp} = 0.164$, $R_F = 0.074$

REFERENCE: R. M. Kirchner and J. M. Bennett,
Zeolites **14** 523–528 (1994).

Atom	x	y	z	B_{iso}	occ
Al 1	0.562	0.122	0.638	1.97	1.0
Al 2	0.852	0.278	0.124	1.97	1.0
Al 3	0.725	0.443	0.627	1.97	1.0
Al 4	0.826	0.666	0.142	1.97	1.0
Al 5	0.580	0.743	0.672	1.97	1.0
P 1	0.548	0.096	0.022	1.97	1.0
P 2	0.859	0.284	0.499	1.97	1.0
P 3	0.713	0.440	0.008	1.97	1.0
P 4	0.828	0.671	0.518	1.97	1.0
P 5	0.561	0.716	0.016	1.97	1.0
O 1	0.449	0.138	0.146	3.0	1.0
O 2	0.543	0.127	0.839	3.0	1.0
O 3	0.708	0.156	0.042	3.0	1.0
O 4	0.518	0.976	0.048	3.0	1.0
O 5	0.835	0.385	0.548	3.0	1.0
O 6	-0.006	0.294	0.559	3.0	1.0
O 7	0.743	0.158	0.549	3.0	1.0
O 8	0.855	0.258	0.313	3.0	1.0
O 9	0.825	0.393	0.057	3.0	1.0
O 10	0.752	0.551	0.110	3.0	1.0
O 11	0.545	0.342	0.019	3.0	1.0
O 12	0.751	0.448	0.827	3.0	1.0
O 13	0.754	0.745	0.620	3.0	1.0
O 14	0.775	0.554	0.572	3.0	1.0
O 15	0.801	0.683	0.327	3.0	1.0
O 16	-0.022	0.730	0.555	3.0	1.0
O 17	0.744	0.742	0.061	3.0	1.0
O 18	0.534	0.679	0.834	3.0	1.0
O 19	0.546	0.806	0.089	3.0	1.0
O 20	0.464	0.605	0.089	3.0	1.0

REFINED COMPOSITION: $|((C_3H_7)_4N)_4|\ [Al_{32}P_{32}O_{128}]$

CRYSTAL DATA: *Pccn* (No. 56)
$a = 21.9443$ Å $b = 13.6911$ Å $c = 14.2486$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.149$, $R_{wp} = 0.161$, $R_F = 0.066$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
Microporous Materials **6** 51–54 (1996).

Atom	x	y	z	B_{iso}	occ
Al 1	0.0860	0.1417	0.2174	1.03	1.0
Al 2	0.1778	0.3624	0.0553	1.03	1.0
Al 3	-0.0119	0.3639	0.0615	1.03	1.0
Al 4	0.0833	0.0482	-0.0764	1.03	1.0
P 1	0.0858	0.3652	0.2198	1.03	1.0
P 2	0.1804	0.1295	0.0587	1.03	1.0
P 3	-0.0125	0.1420	0.0587	1.03	1.0
P 4	0.0836	0.4489	-0.0808	1.03	1.0
O 1	0.0954	0.2605	0.2514	0.79	1.0
O 2	0.1471	0.1050	0.1506	0.79	1.0
O 3	0.0207	0.1285	0.1529	0.79	1.0
O 4	0.0812	0.0682	0.3134	0.79	1.0
O 5	0.1372	0.3945	0.1554	0.79	1.0
O 6	0.0265	0.3770	0.1677	0.79	1.0
O 7	0.0857	0.4322	0.3036	0.79	1.0
O 8	0.1751	0.2388	0.0401	0.79	1.0
O 9	0.2525	0.4007	0.0687	0.79	1.0
O 10	0.1454	0.4190	-0.0410	0.79	1.0
O 11	0.1521	0.0719	-0.0229	0.79	1.0
O 12	-0.0369	0.2460	0.0526	0.79	1.0
O 13	0.0341	0.3867	-0.0342	0.79	1.0
O 14	-0.0741	0.4414	0.0607	0.79	1.0
O 15	0.0297	0.1238	-0.0260	0.79	1.0
O 16	-0.0659	0.0720	0.0550	0.79	1.0
N	0.25	-0.25	-0.0080	5.53	1.0
C 1	0.1994	-0.2871	0.0541	5.53	1.0
C 2	0.1726	-0.2012	0.1130	5.53	1.0
C 3	0.1186	-0.2388	0.1727	5.53	1.0
C 4	0.2243	-0.1690	-0.0669	5.53	1.0
C 5	0.2730	-0.1304	-0.1357	5.53	1.0
C 6	0.2487	-0.0377	-0.1838	5.53	1.0
H 11	0.1665	-0.3160	0.0142	0.0	1.0
H 12	0.2158	-0.3382	0.0972	0.0	1.0
H 21	0.1580	-0.1485	0.0698	0.0	1.0
H 22	0.2049	-0.1744	0.1552	0.0	1.0
H 31	0.1332	-0.2913	0.2160	0.0	1.0
H 32	0.0863	-0.2656	0.1304	0.0	1.0
H 33	0.1014	-0.1836	0.2103	0.0	1.0
H 41	0.2107	-0.1145	-0.0250	0.0	1.0
H 42	0.1886	-0.1940	-0.1032	0.0	1.0

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Atom	x	y	z	B_{iso}	occ
H 51	0.3111	-0.1145	-0.1004	0.0	1.0
H 52	0.2819	-0.1812	-0.1841	0.0	1.0
H 61	0.2307	0.0069	-0.1353	0.0	1.0
H 62	0.2165	-0.0559	-0.2303	0.0	1.0
H 63	0.2828	-0.0035	-0.2167	0.0	1.0

REFINED COMPOSITION: $|(C_4N)_6|$ $[Al_{28}P_{28}O_{112}]$

CRYSTAL DATA: $P3c1$ (No. 158)
$a = 13.2251$ Å $b = 13.2251$ Å $c = 26.8922$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.119$

REFERENCE: J. M. Bennett and B. K. Marcus,
in *Innovations in Zeolite Material Science* (*Stud. Surf. Sci. Catal. No. 37*)
Ed. by P. J. Grobet, W. J. Mortier, E. F. Vansant and G. Schulz-Ekloff
(Elsevier: Amsterdam) 269–279 (1988).
And J. M. Bennett, Private communication.

Atom	x	y	z	B_{iso}	occ
Al 1	0.00000	0.00000	0.06457	1.55	1.0
Al 2	0.46967	0.31584	0.13168	2.55	1.0
Al 3	0.19875	0.96524	0.18925	1.04	1.0
Al 4	0.46726	0.11576	0.30775	1.42	1.0
Al 5	0.19352	0.17290	0.36246	1.46	1.0
Al 6	0.66667	0.33333	0.43950	1.39	1.0
P 1	0.66667	0.33333	0.06039	1.22	1.0
P 2	0.19862	0.18082	0.13165	1.62	1.0
P 3	0.46965	0.10767	0.19050	1.02	1.0
P 4	0.20093	0.96592	0.30722	1.73	1.0
P 5	0.46960	0.31962	0.36555	1.16	1.0
P 6	0.00000	0.00000	0.43771	1.6	1.0
O 12	0.9846	0.1174	0.5852	1.75	1.0
O 16	0.0000	0.0000	0.9957	2.49	1.0
O 21	0.6875	0.2336	0.0819	1.36	1.0
O 22	0.7350	0.0649	0.1160	1.02	1.0
O 231	0.9192	0.4727	0.1661	2.29	1.0
O 23	0.7826	0.2713	0.1759	1.91	1.0
O 32	0.1515	0.2587	0.1616	2.65	1.0
O 321	0.1910	0.0927	0.1748	1.96	1.0
O 33	0.3389	0.9936	0.1796	2.58	1.0
O 34	0.1638	0.2199	0.7555	3.21	1.0
O 43	0.8976	0.5052	0.7477	1.74	1.0
O 44	0.3218	0.0036	0.3158	1.95	1.0
O 45	0.5189	0.4365	0.3483	1.15	1.0
O 451	0.4884	0.2442	0.3316	2.85	1.0
O 54	0.1405	0.2616	0.3398	1.76	1.0
O 541	0.1867	0.0777	0.3187	2.29	1.0
O 55	0.7279	0.0750	0.3741	2.09	1.0
O 56	0.9997	0.8889	0.4222	2.66	1.0
O 61	0.6666	0.3333	0.0081	2.85	1.0
O 65	0.7979	0.4676	0.4151	2.54	1.0
C 1	0.2968	0.1621	0.5117	4.0	1.0
C 11	0.0527	0.3242	0.4726	4.0	1.0
C 21	0.3242	0.4316	0.9472	4.0	1.0
C 2	0.9726	0.7011	0.5117	4.0	1.0
N	0.3242	0.0800	0.4863	4.0	1.0

REFINED COMPOSITION: $[Al_{36}P_{36}O_{144}]$

CRYSTAL DATA: $P\bar{3}1c$ (No. 163)
$a = 13.715$ Å $b = 13.715$ Å $c = 29.676$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.130$, $R_{wp} = 0.197$, $R_p = 0.173$

REFERENCE: N. K. McGuire, C. A. Bateman, C. S. Blackwell, S. T. Wilson and R. M. Kirchner, *Zeolites* **15** 460–469 (1995).

Atom	x	y	z	B_{iso}	occ
Al 1	0.231	0.000	0.198	1.97	1.0
Al 2	0.341	0.445	0.469	1.97	1.0
Al 3	0.435	0.326	0.635	1.97	1.0
P 1	0.225	0.223	0.202	1.97	1.0
P 2	0.339	0.448	0.368	1.97	1.0
P 3	0.435	0.329	0.534	1.97	1.0
O 1	0.267	0.007	0.253	1.97	1.0
O 2	0.234	0.125	0.182	1.97	1.0
O 3	0.097	-0.103	0.195	1.97	1.0
O 4	0.317	-0.026	0.163	1.97	1.0
O 5	0.344	0.413	0.414	1.97	1.0
O 6	0.362	0.354	0.503	1.97	1.0
O 7	0.445	0.581	0.477	1.97	1.0
O 8	0.223	0.453	0.487	1.97	1.0
O 9	0.302	0.323	0.170	1.97	1.0
O 10	0.472	0.224	0.648	1.97	1.0
O 11	0.550	0.452	0.651	1.97	1.0
O 12	0.394	0.318	0.580	1.97	1.0

REFINED COMPOSITION: $[Al_{24}P_{24}O_{96}]$

CRYSTAL DATA: $P\bar{3}1c$ (No. 163)
$a = 13.7617$ Å $b = 13.7617$ Å $c = 19.949$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.068$, $R_{wp} = 0.219$

REFERENCE: N. K. McGuire, C. S. Blackwell, C. A. Bateman, S. T. Wilson and R. M. Kirchner, *Microporous and Mesoporous Materials* **28** 125–137 (1999).

Atom	x	y	z	B_{iso}	occ
Al 1	0.001	0.225	0.077	1.185	1.0
Al 2	0.338	0.439	0.173	1.185	1.0
P 1	0.107	0.441	0.179	1.422	1.0
P 2	0.231	0.229	0.079	1.422	1.0
O 1	-0.126	0.112	0.104	1.974	1.0
O 2	0.105	0.189	0.093	1.974	1.0
O 3	0.024	0.348	0.119	1.974	1.0
O 4	0.013	0.277	-0.006	1.974	1.0
O 5	0.231	0.469	0.159	1.974	1.0
O 6	0.095	0.54	0.143	1.974	1.0
O 7	0.073	0.4	0.242	1.974	1.0
O 8	0.319	0.323	0.125	1.974	1.0

REFINED COMPOSITION: $|(C_4N)_6|\ [Al_6Co_2P_8O_{32}]$

CRYSTAL DATA: $P\overline{3}$ (No. 147)
$a = 12.7468$ Å $b = 12.7468$ Å $c = 9.0153$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.071$

REFERENCE: J. M. Bennett and B. K. Marcus,
in *Innovations in Zeolite Material Science* (*Stud. Surf. Sci. Catal. No. 37*)
Ed. by P. J. Grobet, W. J. Mortier, E. F. Vansant and G. Schulz-Ekloff
(Elsevier: Amsterdam) 269–279 (1988).
and J. M. Bennett, Private communication.

Atom	x	y	z	B_{iso}	occ
Al	0.85585	0.32535	0.40999	0.09	1.0
Co	0.33333	0.66667	0.18423	0.24	1.0
P 1	0.66667	0.33333	0.19314	0.23	1.0
P 2	0.32138	0.86415	0.38454	0.23	1.0
O 31	0.85934	0.44164	0.52440	0.29	1.0
O 32	0.39760	0.20587	0.52481	0.39	1.0
O 11	0.54705	0.23176	0.25047	0.45	1.0
O 12	0.20298	0.50794	0.24269	0.36	1.0
O 14	0.33333	0.66667	-0.02687	0.36	1.0
O 2	0.35660	0.99417	0.35229	0.44	1.0
C 1	0.40093	0.40351	0.07477	8.9	1.0
C 11	0.21931	0.21598	0.20291	10.03	1.0
C 2	0.46509	0.00622	0.04137	14.41	1.0
C 21	0.34138	0.32934	0.23073	17.57	1.0
N	0.28549	0.01616	0.90866	20.45	1.0

REFINED COMPOSITION: $|(H_2O)_4|$ $[Al_6P_6O_{24}]$

CRYSTAL DATA: $P112_1$ (No. 4) unique axis **c**
$a = 9.486$ Å $b = 9.914$ Å $c = 8.126$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 121.49°$
X-ray Rietveld refinement, $R_{wp} = 0.127$

REFERENCE: J. B. Higgins, R. M. Dessau, H-X. Li, M. E. Davis and J.M. Newsam, *American Crystallographic Association Abstracts* **K005** 39 (1993).

Atom	x	y	z	B_{iso}	occ
Al 1	0.0	0.215	0.139	1.263	1.0
Al 2	0.347	0.303	0.664	1.263	1.0
Al 3	0.348	0.037	0.134	1.263	1.0
P 1	0.007	0.094	0.526	1.263	1.0
P 2	0.366	0.349	0.064	1.263	1.0
P 3	0.373	0.038	0.537	1.263	1.0
O 1	0.014	0.067	0.013	2.052	1.0
O 2	0.0	0.116	0.337	2.052	1.0
O 3	0.229	0.347	0.165	2.052	1.0
O 4	0.419	0.234	0.112	2.052	1.0
O 5	0.352	0.333	0.876	2.052	1.0
O 6	0.512	0.523	0.067	2.052	1.0
O 7	0.16	0.254	0.576	2.052	1.0
O 8	-0.229	0.112	0.111	2.052	1.0
O 9	0.406	0.166	0.661	2.052	1.0
O 10	0.362	0.035	0.348	2.052	1.0
O 11	0.525	0.038	0.605	2.052	1.0
O 12	-0.138	0.097	0.608	2.052	1.0
H_2O 1	0.016	0.277	-0.097	1.815	0.5
H_2O 2	-0.045	0.384	0.196	1.815	0.5
H_2O 3	0.262	0.615	0.365	2.607	0.5
H_2O 4	0.752	0.408	0.265	2.607	0.5

REFINED COMPOSITION: $|Na_{16}(H_2O)_{16}|$ $[Si_{32}Al_{16}O_{96}]$
Cyclopean Islands, Greece

CRYSTAL DATA: $Ia\bar{3}d$ (No. 230)
$a = 13.73$ Å $b = 13.73$ Å $c = 13.73$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.04$

REFERENCE: G. Ferraris, D. W. Jones and J. Yerkess,
Z. Kristallogr. **135** 240–252 (1972).

Atom	x	y	z	B_{iso}	occ
Na	0.125	0.0	0.25	0.32	0.6667
Si	0.66208	-0.41208	0.125	0.14	0.6667
Al	0.66208	-0.41208	0.125	0.14	0.3333
O 1	0.10428	0.13440	0.71932	0.29	1.0
H 1	0.0791	0.0791	0.0791	1.05	0.25
H 2	0.1402	0.1006	0.0548	0.83	0.25
O 2	0.125	0.125	0.125	0.69	1.0

O1 z-coordinate changed from 0.21932 to 0.71932.

APC AlPO–C, Hydrated

REFINED COMPOSITION: $|(H_2O)_{16}O_8|\ [Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: *Pbca* (No. 61)
$a = 19.3525$ Å $b = 9.7272$ Å $c = 9.7621$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.033$

REFERENCE: J. J. Pluth and J. V. Smith,
Acta Cryst. **C42** 1118–1120 (1986).

Atom	x	y	z	B_{iso}	occ
Al 1	0.44808	0.08470	0.32419	0.23	1.0
Al 2	0.28207	0.33224	0.14654	0.21	1.0
P 1	0.44769	0.34071	0.13498	0.22	1.0
P 2	0.29050	0.06565	0.33879	0.21	1.0
O 1	0.37433	0.3765	0.1701	0.39	1.0
O 2	0.46047	0.1662	0.4804	0.45	1.0
O 3	0.49520	0.4497	0.1971	0.42	1.0
O 4	0.46889	0.2004	0.1942	0.34	1.0
O 5	0.27397	0.0582	0.4913	0.29	1.0
O 6	0.36522	0.0190	0.3136	0.42	1.0
O 7	0.28329	0.2158	0.2953	0.34	1.0
O 8	0.25855	0.4758	0.2592	0.29	1.0
H 1	0.15752	0.2988	0.0523	5.26	1.0
H 2	0.16096	0.2574	0.1883	3.95	1.0
H 3	0.28123	0.1025	0.0541	1.74	1.0
H 4	0.30108	0.1902	0.9490	1.42	1.0
O 9	0.18446	0.2831	0.1193	0.58	1.0
O 10	0.30512	0.1730	0.0340	0.39	1.0
O 11	0.11929	0.1440	0.3627	1.5	1.0

The third water molecule (O11) is missing hydrogen atoms.

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: *Pbca* (No. 61)
$a = 19.816$ Å $b = 10.047$ Å $c = 8.935$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.17$, $R_F = 0.051$; At $T = 100$°C.

REFERENCE: E. B. Keller, W. M. Meier and R. M. Kirchner,
Solid State Ionics **43** 93–102 (1990).

Atom	x	y	z	B_{iso}	occ
Al 1	0.455	0.160	0.360	0.3	1.0
Al 2	0.297	0.423	0.197	1.5	1.0
P 1	0.456	0.424	0.206	2.7	1.0
P 2	0.293	0.145	0.346	0.3	1.0
O 1	0.384	0.465	0.222	9.0	1.0
O 2	0.465	0.143	0.546	0.7	1.0
O 3	0.500	0.539	0.238	1.5	1.0
O 4	0.476	0.317	0.323	0.5	1.0
O 5	0.280	0.110	0.506	1.3	1.0
O 6	0.370	0.124	0.313	5.1	1.0
O 7	0.278	0.284	0.297	0.1	1.0
O 8	0.249	0.560	0.241	3.3	1.0

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: $Pca2_1$ (No. 29)
$a = 19.187$ Å $b = 8.576$ Å $c = 9.804$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.203$, $R_F = 0.115$; At $T = 100°C$.

REFERENCE: E. B. Keller, W. M. Meier and R. M. Kirchner,
Solid State Ionics **43** 93–102 (1990).

Atom	x	y	z	B_{iso}	occ
Al 11	0.531	0.065	0.133	9.1	1.0
Al 12	0.572	0.574	0.385	4.0	1.0
Al 21	0.721	0.074	0.320	0.2	1.0
Al 22	0.681	0.572	0.026	0.8	1.0
P 11	0.574	-0.031	0.421	6.9	1.0
P 12	0.529	0.473	0.107	2.5	1.0
P 21	0.680	-0.051	0.040	0.8	1.0
P 22	0.724	0.453	0.298	0.2	1.0
O 11	0.645	0.035	0.406	1.3	1.0
O 12	0.593	0.526	0.031	0.0	1.0
O 21	0.531	0.284	0.130	8.7	1.0
O 22	0.584	0.784	0.418	4.0	1.0
O 31	0.540	0.017	0.553	6.4	1.0
O 32	0.469	0.518	0.019	0.8	1.0
O 41	0.532	0.018	0.302	5.1	1.0
O 42	0.524	0.557	0.238	0.8	1.0
O 51	0.691	0.773	0.060	4.0	1.0
O 52	0.734	0.278	0.320	8.0	1.0
O 61	0.601	-0.015	0.045	0.7	1.0
O 62	0.655	0.498	0.361	9.4	1.0
O 71	0.716	0.025	0.154	0.8	1.0
O 72	0.724	0.478	0.150	0.8	1.0
O 81	0.789	-0.010	0.405	0.8	1.0
O 82	0.719	0.539	0.869	6.2	1.0

REFINED COMPOSITION: $|(C_7H_{13}N)_4|\ [Al_{20}P_{20}O_{80}]$

CRYSTAL DATA: $F23$ (No. 196)
$a = 13.3832$ Å $b = 13.3832$ Å $c = 13.3832$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.192$, $R_F = 0.106$

REFERENCE: J. M. Bennett and R. M. Kirchner,
Zeolites **11** 502–506 (1991).

Atom	x	y	z	B_{iso}	occ
Al 1	0.1186	0.1186	0.1186	6.4	1.0
P 1	-0.1116	0.1116	0.1116	5.2	1.0
P 2	0.2500	0.2500	0.2500	4.4	1.0
Al 2	-0.2500	0.2500	0.2500	2.5	1.0
O 1	-0.0078	0.1285	0.1495	3.0	1.0
O 2	0.1915	0.1915	0.1915	5.0	1.0
O 3	-0.1704	0.1704	0.1704	8.0	1.0
N	0.0560	0.4329	0.0424	6.0	0.0833
C 1	0.0056	0.3916	-0.0462	6.0	0.0833
C 2	-0.0601	0.4680	-0.0973	6.0	0.0833
C 3	0.1159	0.5193	0.0103	6.0	0.0833
C 4	0.0529	0.5988	-0.0393	6.0	0.0833
C 5	-0.0214	0.4689	0.1118	6.0	0.0833
C 6	-0.0878	0.5472	0.0646	6.0	0.0833
C 7	-0.0552	0.5662	-0.0418	6.0	0.0833
H 11	0.0566	0.3668	-0.0939	7.0	0.0833
H 12	-0.0351	0.3331	-0.0261	7.0	0.0833
H 21	-0.0382	0.4774	-0.1673	7.0	0.0833
H 22	-0.1300	0.4437	-0.0995	7.0	0.0833
H 31	0.1506	0.5481	0.0691	7.0	0.0833
H 32	0.1686	0.4965	-0.0364	7.0	0.0833
H 41	0.0592	0.6627	-0.0025	7.0	0.0833
H 42	0.0772	0.6110	-0.1081	7.0	0.0833
H 51	-0.0626	0.4116	0.1344	7.0	0.0833
H 52	0.0122	0.4970	0.1722	7.0	0.0833
H 61	-0.1583	0.5246	0.0658	7.0	0.0833
H 62	-0.0845	0.6099	0.1036	7.0	0.0833
H 7	-0.0978	0.6173	-0.0741	7.0	0.0833

AST Quinuclidinium fluoride octadecasil

REFINED COMPOSITION: $|C_{6.18}F_{0.07}|\ [Si_{20}O_{40}]$

CRYSTAL DATA: $I\,4/m$ (No. 87)
$a = 9.194$ Å $b = 9.194$ Å $c = 13.396$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.039$

REFERENCE: P. Caullet, J. L. Guth, J. Hazm, J. M. Lamblin and H. Gies, *Eur. J. Solid State Inorg. Chem.* **28** 345–361 (1991).

Atom	x	y	z	B_{iso}	occ
Si 1	0.2303	0.0387	0.1137	0.61	1.0
Si 2	0.5	0.0	0.25	0.47	1.0
O 1	0.3724	0.0659	0.1817	0.96	1.0
O 2	0.3308	0.6201	0.3583	1.27	1.0
O 3	0.2883	0.0502	0.0	1.36	1.0
C 1	0.05	0.14	0.5	11.91	0.151
C 2	0.13	0.06	0.41	14.5	0.184
C 3	0.00	0.07	0.37	3.87	0.049
C 4	0.14	0.13	0.16	6.15	0.078
F	0.0	0.0	0.0	2.91	0.037

REFINED COMPOSITION: $|(C_4N_2)(H_2O)_2|$ $[Ge_{20}O_{40}]$

CRYSTAL DATA: $P\,4/m\,cc$ (No. 124)
$a = 8.7795$ Å $b = 8.7795$ Å $c = 14.4696$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_F = 0.025$, $wR_{F2} = 0.053$; at -75 C.

REFERENCE: H. Li and O. M. Yaghi,
J. Am. Chem. Soc. **120** 10569–10570 (1998).

Atom	x	y	z	B_{iso}	occ
Ge 1	0.0	0.5000	0.2500	0.71	1.0
Ge 2	0.2565	0.4239	0.1086	0.71	1.0
O 1	0.1043	0.3755	0.1810	0.95	1.0
O 20	0.2010	0.3595	0.0	1.11	0.5
O 21	0.1764	0.4393	0.0	0.95	0.5
O 30	0.3257	0.5936	0.1557	1.18	0.5
O 31	0.3793	0.2692	0.1194	0.95	0.5
H_2O	0.5000	0.5000	0.0	2.53	1.0
C 1	0.0	0.0	0.1258	6.63	0.5
C 2	-0.0333	0.0537	0.2080	7.42	0.125
N	-0.0333	0.0537	0.2080	7.42	0.125

Framework oxygen atoms O2 and O3 are statistically disordered between two alternative sites in the lattice, O20 and O21, and O30 and O31, respectively.

REFINED COMPOSITION: $|C_{13.16}O_{0.168}|\ [Al_{7.512}P_{7.504}O_{32}]$

CRYSTAL DATA: $I\,4/m$ (No. 87)
$a = 13.2088$ Å $b = 13.2088$ Å $c = 5.2771$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.02$, $R_F = 0.093$

REFERENCE: W. H. Baur, W. Joswig, D. Kassner, A. Bieniok, G. Finger and J. Kornatowski, *Z. Kristallogr.* **214** 154–159 (1999).

Atom	x	y	z	B_{iso}	occ
P 1	0.21631	0.38206	0.0	2.4	0.898
P 2	0.1226	0.4167	0.0	1.2	0.04
Al 1	0.37846	0.20842	0.0	2.5	0.4495
Al^{3+} 1	0.37846	0.20842	0.0	2.5	0.4495
Al 2	0.4104	0.1156	0.0	1.6	0.02
Al^{3+} 2	0.4104	0.1156	0.0	1.6	0.02
O^- 1	0.31508	0.32477	0.0	4.6	0.959
O^- 2	0.15488	0.35625	0.2302	6.8	1.008
O^- 3	0.2418	0.49346	0.0	4.9	0.926
O^- 31	0.187	0.511	0.0	3.3	0.04
O^- 32	0.517	0.19	0.0	3.3	0.04
O^- 41	0.015	0.445	0.0	3.3	0.04
C 1	0.5	0.5	0.743	4.3	0.37
C 2	0.449	0.522	0.5	45.8	0.82
C 3	0.4857	0.513	0.0	23.7	0.259
C 4	0.4676	0.0389	0.0	10.5	0.381

The original refinement for the two Al sites used interpolated scattering factors for $Al^{+1.5}$, which we model as an equal mix of Al and Al^{3+}.

REFINED COMPOSITION: $|C_{14.76}|\ [Al_{17.71}P_{16.67}O_{72}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 20.839$ Å $b = 20.839$ Å $c = 5.041$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_{wF} = 0.018$, $R_F = 0.051$

REFERENCE: W. H. Baur, W. Joswig, D. Kassner and J. Kornatowski, *Acta Cryst.* **B50** 290–294 (1994).

Atom	x	y	z	B_{iso}	occ
Al	0.61736	0.08455	0.0381	1.89	0.984
P	0.47126	0.08774	0.1138	1.31	0.926
O 1	0.55134	0.10711	0.1317	3.0	1.0
O 2	0.42390	0.00893	0.0133	3.32	1.0
O 3	0.44586	0.09533	0.3880	3.32	1.0
O 4	0.46468	0.14061	0.9208	3.32	1.0
C 1	0.046	0.013	0.111	15.79	0.46
C 2	0.064	0.029	0.388	15.79	0.25
C 3	0.0	0.0	0.30	15.79	0.33

REFINED COMPOSITION: $[Si_{24}O_{48}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 13.1483$ Å $b = 21.5771$ Å $c = 5.1639$ Å
$\alpha = 90°$ $\beta = 91.84°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.112$, $R_{wp} = 0.135$, $R_F = 0.058$

REFERENCE: J. V. Smith, J. J. Pluth and K. J. Andries,
Zeolites **13** 166–169 (1993).

Atom	x	y	z	B_{iso}	occ
Si 1	0.619	0.041	0.767	0.92	1.0
Si 2	0.314	0.174	0.768	0.92	1.0
Si 3	0.617	0.243	0.223	0.92	1.0
O 1	0.690	0.101	0.773	1.237	1.0
O 2	0.500	0.048	0.750	1.237	1.0
O 3	0.622	0.212	0.934	1.237	1.0
O 4	0.354	0.189	0.069	1.237	1.0
O 5	0.500	0.265	0.250	1.237	1.0
O 6	0.645	0.001	0.022	1.237	1.0
O 7	0.811	0.195	0.748	1.237	1.0

REFINED COMPOSITION: $|(C_4NO)_4|\ [Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P2_12_12$ (No. 18)
$a = 10.3325$ Å $b = 14.6405$ Å $c = 9.5112$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.19$, $R_F = 0.17$

REFERENCE: P. R. Rudolf, C. Saldarriaga-Molina and A. Clearfield, *J. Phys. Chem.* **90** 6122–6125 (1986).

Atom	x	y	z	B_{iso}	occ
Al 1	0.354	0.608	0.387	3.0	1.0
Al 2	0.366	0.896	0.383	3.0	1.0
Al 3	0.349	0.249	0.139	3.0	1.0
P 1	0.339	0.770	0.157	4.8	1.0
P 2	0.354	0.112	0.368	4.8	1.0
P 3	0.343	0.415	0.369	4.8	1.0
O 1	0.338	0.696	0.272	4.3	1.0
O 2	0.311	0.864	0.218	4.3	1.0
O 3	0.482	0.758	0.086	4.3	1.0
O 4	0.249	0.764	0.018	4.3	1.0
O 5	0.318	0.137	0.210	4.3	1.0
O 6	0.370	0.012	0.381	4.3	1.0
O 7	0.485	0.168	0.412	4.3	1.0
O 8	0.244	0.143	0.466	4.3	1.0
O 9	0.300	0.506	0.317	4.3	1.0
O 10	0.337	0.349	0.242	4.3	1.0
O 11	0.482	0.412	0.425	4.3	1.0
O 12	0.254	0.381	0.488	4.3	1.0
C 1	-0.024	0.089	0.196	13.1	1.0
C 2	-0.131	-0.017	0.004	13.1	1.0
C 3	-0.018	0.587	0.249	13.1	1.0
C 4	-0.129	0.482	0.065	13.1	1.0
N 1	0.000	0.000	0.100	13.1	1.0
N 2	0.000	0.500	0.158	13.1	1.0
O 13	0.000	0.000	0.284	13.1	1.0
O 14	0.000	0.500	-0.024	13.1	1.0

REFINED COMPOSITION: $[Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: *Acmm* (No. 67) $\bar{\mathbf{c}}\mathbf{ba}$ setting
$a = 9.4489$ Å $b = 15.2028$ Å $c = 8.4084$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.041$, $R_{F^2} = 0.133$; At $T = 593$ K.

REFERENCE: J. W. Richardson, Jr., J. V. Smith and J. J. Pluth,
J. Phys. Chem. **94** 3365–3367 (1990).

Atom	x	y	z	B_{iso}	occ
Al 1	0.3535	0.0982	0.1987	2.63	0.5
Al 2	0.1566	0.2500	0.3142	0.92	0.5
P 1	0.3535	0.0982	0.1987	2.63	0.5
P 2	0.1566	0.2500	0.3142	0.92	0.5
O 1	0.3017	0.0000	0.2500	1.95	1.0
O 2	0.5000	0.1275	0.2500	2.08	1.0
O 3	0.2317	0.1625	0.2497	2.53	1.0
O 4	0.3308	0.0971	0.0000	2.95	1.0
O 5	0.0000	0.2500	0.2500	1.84	1.0
O 6	0.1076	0.2500	0.5000	5.76	1.0

REFINED COMPOSITION: $|N_{2.84}C_{13.41}O_4H_4|$ $[Al_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P1\,2_1/a\,1$ (No. 14) unique axis **b**, cell choice 3
$a = 10.3307$ Å $b = 17.5241$ Å $c = 8.6757$ Å
$\alpha = 90.0°$ $\beta = 123.369°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R = 0.046$, $R_w = 0.042$

REFERENCE: J. M. Bennett, J. M. Cohen, G. Artioli, J. J. Pluth and J. V. Smith, *Inorg. Chem.* **24** 188–193 (1985).

Atom	x	y	z	B_{iso}	occ
P 1	0.1335	0.0708	0.9738	0.58	1.0
P 2	0.0269	0.2112	0.3235	0.70	1.0
P 3	0.4967	0.1646	0.7462	0.65	1.0
Al 1	0.3082	0.1714	0.3192	0.76	1.0
Al 2	0.3372	0.3892	0.9739	0.61	1.0
Al 3	0.2057	0.2037	0.7707	0.63	1.0
O 1	0.3375	0.4885	0.0519	0.84	1.0
O 2	0.2331	0.0912	0.1807	1.16	1.0
O 3	0.421	0.2188	0.258	1.12	1.0
O 4	0.0904	0.1947	0.5237	1.29	1.0
O 5	0.0484	0.2523	0.7775	0.94	1.0
O 6	0.4254	0.1411	0.5439	1.46	1.0
O 7	0.4636	0.4153	0.9012	0.85	1.0
O 8	0.1819	0.1203	0.8696	1.08	1.0
O 9	0.3221	0.2905	0.8647	1.08	1.0
O 10	0.3759	0.1525	0.7924	1.01	1.0
O 11	0.1316	0.3898	0.8632	0.99	1.0
O 12	0.1589	0.2283	0.2955	1.33	1.0
O 13	0.4353	0.3575	0.2081	1.12	1.0
N	0.2155	0.4898	0.2852	3.06	0.71
C 1	0.3305	0.4857	0.4786	12.70	1.425
C 2	0.0868	0.4358	0.2039	7.39	1.295
C 3	0.177	0.4828	0.362	0.00	0.22
C 4	0.125	0.4639	0.477	7.11	0.412
H	0.381	0.286	0.854	2.02	1.0

REFINED COMPOSITION: $|P_2O_{8.48}(C_7N)_4|\ [Al_{24}P_{24}O_{96}]$

CRYSTAL DATA: $P\,4/n\,cc$ (No. 130) origin at centre $\overline{1}$
$a = 13.628$ Å $b = 13.628$ Å $c = 15.463$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.18$

REFERENCE: J. W. Richardson, Jr., J. J. Pluth and J. V. Smith, *Naturwiss.* **76** 467–469 (1989).
And J. J. Pluth, Private communication (1990).

Atom	x	y	z	B_{iso}	occ
Al 1	0.1360	0.8640	0.2500	0.63	1.0
Al 2	0.4660	-0.1419	0.4284	0.843	1.0
P 1	0.1354	0.8646	0.7500	0.737	1.0
P 2	0.6308	0.0185	0.4214	0.79	1.0
O 1	0.2565	-0.1166	0.2738	1.08	1.0
O 2	0.4998	-0.2584	0.4317	1.107	1.0
O 3	0.4258	-0.1044	0.3241	1.37	1.0
O 4	0.5794	-0.0795	0.4309	1.343	1.0
O 5	0.1060	-0.0629	0.1620	1.5	1.0
O 6	0.599	0.0912	0.4905	2.683	1.0
C 1	0.250	0.250	0.739	12.633	1.0
C 2	0.282	0.163	0.389	12.633	0.25
C 3	0.274	0.339	0.389	12.633	0.25
C 5	0.227	0.157	0.302	12.633	0.25
C 6	0.219	0.341	0.302	12.633	0.25
C 8	0.250	0.250	0.249	12.633	1.0
C 9	0.250	0.250	0.298	12.633	1.0
N	0.250	0.250	0.4389	12.633	1.0
P 3	0.250	0.750	0.000	0.87	0.5
O 7	0.164	0.787	0.936	0.71	0.5
O 8	0.276	0.0852	0.4213	5.267	0.03

Beta, Polymorph A SiO_2 Framework *BEA

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: $P4_122$ (No. 91)
$a = 12.661$ Å $b = 12.661$ Å $c = 26.406$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
DLS refinement.

REFERENCE: J. M. Newsam, M. M. J. Treacy, W. T. Koetsier and C. B. deGruyter, *Proc. Roy. Soc.* (London) **A420** 375–405 (1988).

Atom	x	y	z
Si 1	0.33694	0.79277	0.05619
Si 2	0.33711	0.54031	0.05606
Si 3	0.71647	0.79300	0.05872
Si 4	0.71656	0.54076	0.05884
Si 5	0.95425	0.79364	0.05555
Si 6	0.95434	0.54040	0.05556
Si 7	0.14278	0.85722	0.12500
Si 8	0.52836	0.85702	0.12552
Si 9	0.52842	0.47158	0.12500
O 10	0.33623	0.66652	0.06515
O 11	0.33454	0.81732	-0.00385
O 12	0.23433	0.84457	0.08279
O 13	0.44268	0.84276	0.08069
O 20	0.33456	0.51612	-0.00402
O 21	0.23464	0.48822	0.08264
O 22	0.44301	0.49038	0.08043
O 30	0.71891	0.66690	0.06809
O 31	0.83544	0.83902	0.06074
O 32	0.64609	0.84874	0.10222
O 40	0.83559	0.49490	0.06084
O 41	0.64627	0.48518	0.10242
O 50	1.00000	0.82149	0.00000
O 51	0.95304	0.66702	0.06321
O 52	1.02844	0.84708	0.09824
O 60	1.00000	0.51256	0.00000
O 61	1.02874	0.48708	0.09821

Zeolite beta is an intergrown material and *BEA represents the framework of a hypothetical end member. The $P4_322$ (No. 95) topology can be generated by the coordinate transformation $z \rightarrow -z$.

Beta, Polymorph B SiO_2 Framework

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 17.89654$ Å $b = 17.92002$ Å $c = 14.32815$ Å
$\alpha = 90°$ $\beta = 114.803°$ $\gamma = 90°$
DLS refinement

REFERENCE: J. M. Newsam, M. M. J. Treacy, W. T. Koetsier and C. B. deGruyter, *Proc. Roy. Soc.* (London) **A420** 375–405 (1988).

Atom	x	y	z
Si 1	0.60607	-0.02206	0.38112
Si 2	0.48332	-0.14331	0.37930
Si 3	0.79947	-0.21324	0.38677
Si 4	0.67495	-0.33750	0.38698
Si 5	0.91268	-0.33092	0.38275
Si 6	0.79042	-0.45237	0.38137
Si 7	0.50000	0.11084	0.25000
Si 8	0.69528	-0.08286	0.25183
Si 9	0.50000	-0.27723	0.25000
O 10	0.53355	-0.08379	0.34288
O 11	0.64810	-0.01901	0.50530
O 12	0.56790	0.05877	0.33609
O 13	0.67468	-0.04420	0.34022
O 20	0.52172	-0.14542	0.50343
O 21	0.38767	-0.11893	0.33454
O 22	0.49034	-0.22518	0.33637
O 30	0.73217	-0.27927	0.36034
O 31	0.88292	-0.24602	0.38479
O 32	0.76334	-0.14756	0.30231
O 33	0.81946	-0.18012	0.49966
O 40	0.70644	-0.42162	0.38400
O 41	0.58064	-0.32929	0.30322
O 51	0.83406	-0.38605	0.34599
O 52	0.95542	-0.33707	0.30360
O 60	0.76924	-0.52075	0.30078

Zeolite beta is an intergrown material. Polymorph B represents the framework of a hypothetical end member of the beta family.

REFINED COMPOSITION: $|Li_{1.86}(H_2O)_2|\ [Si_{3.89}Al_{2.13}O_{12}]$
Bikita, Zimbabwe

CRYSTAL DATA: $P1$ (No. 1)
$a = 8.6071$ Å $b = 4.9540$ Å $c = 7.5972$ Å
$\alpha = 89.900°$ $\beta = 114.437°$ $\gamma = 89.988°$
Neutron single crystal refinement, $R_w = 0.056$

REFERENCE: K. Ståhl, Å. Kvick and S. Ghose,
Zeolites **9** 303–311 (1989).

Atom	x	y	z	B_{iso}	occ
Li 1	0.3095	0.3657	0.1469	1.07	0.91
Li 2	0.6995	0.8655	0.8722	1.36	0.947
Si 11	0.1057	0.8645	0.0975	0.42	0.957
Si 12	0.1038	0.8006	0.5049	0.51	0.981
Si 22	0.8920	0.2984	0.4877	0.53	0.981
Si 23	0.6187	0.3748	0.0630	0.41	0.975
Al 13	0.3803	0.8749	0.9374	0.58	1.061
Al 21	0.8985	0.3639	0.9065	0.58	1.066
O 11	0.2641	0.7404	0.0569	0.85	1.0
O 12	0.0830	0.1853	0.0413	0.97	1.0
O 13	0.1584	0.8281	0.3279	1.49	1.0
O 14	0.0557	0.4868	0.5173	1.50	1.0
O 15	0.2612	0.8920	0.6947	1.34	1.0
O 16	0.4496	0.1940	0.0282	0.88	1.0
O 21	0.7311	0.2433	0.9552	0.85	1.0
O 22	0.9283	0.7021	0.9708	0.98	1.0
O 23	0.8414	0.3281	0.6655	1.52	1.0
O 24	0.9378	0.9872	0.4657	1.45	1.0
O 25	0.7318	0.3929	0.2966	1.29	1.0
O 26	0.5593	0.6797	0.9807	0.85	1.0
H 11	0.3230	0.2849	0.4786	5.96	1.0
H 12	0.4870	0.1784	0.4863	5.21	1.0
H 21	0.6853	0.7872	0.5420	6.35	1.0
H 22	0.5214	0.6763	0.5343	5.28	1.0
O 17	0.4083	0.3224	0.4347	2.35	1.0
O 27	0.5991	0.8225	0.5871	2.35	1.0

BOG Boggsite

REFINED COMPOSITION: $|(H_2O)_{137.04}|\ [Si_{77.76}Al_{18.24}O_{192}]$
Goble area, Oregon, U.S.A.

CRYSTAL DATA: *Imma* (No. 74)
$a = 20.236$ Å $b = 23.798$ Å $c = 12.798$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.094$

REFERENCE: J. J. Pluth and J. V. Smith,
American Mineralogist **75** 501–507 (1990).

Atom	x	y	z	B_{iso}	occ
Si 1	0.18881	0.18550	0.67190	1.38	0.81
Si 2	0.19006	0.02407	0.32970	1.54	0.81
Si 3	0.07689	0.18517	0.83570	1.29	0.81
Si 4	0.07768	0.022100	0.164300	.41	0.81
Si 5	0.22108	0.083000	0.537800	.35	0.81
Si 6	0.12270	0.083710	0.965600	.35	0.81
Al 1	0.18881	0.18550	0.67190	1.38	0.19
Al 2	0.19006	0.02407	0.32970	1.54	0.19
Al 3	0.07689	0.18517	0.83570	1.29	0.19
Al 4	0.07768	0.02210	0.16430	1.41	0.19
Al 5	0.22108	0.08300	0.53780	1.35	0.19
Al 6	0.12270	0.08371	0.96560	1.35	0.19
O 1	0.18820	0.250000	0.629100	.37	1.0
O 2	0.11940	0.170700	0.732200	.67	1.0
O 3	0.195000	0.145600	0.567900	.76	1.0
O 4	0.190000	0.070200	0.423600	.85	1.0
O 5	0.119400	0.031900	0.272200	.85	1.0
O 6	0.089300	0.250000	0.873100	.22	1.0
O 7	0.000000	0.173800	0.804300	.46	1.0
O 8	0.000000	0.026300	0.196800	.15	1.0
O 9	0.194400	0.037900	0.620400	.26	1.0
O 10	0.097800	0.146400	0.932700	.09	1.0
O 11	0.095900	0.072500	0.081300	.48	1.0
O 12	0.200700	0.080000	0.968200	.61	1.0
O 13	0.094900	0.039500	0.884700	.63	1.0
O 14	0.250000	0.175500	0.750000	.15	1.0
O 15	0.250000	-0.037500	0.750000	.39	1.0
H_2O 1	0.000000	0.173500	0.136000	5.26	1.85
H_2O 2	0.193600	0.170100	0.203000	7.89	1.35
H_2O 3	0.193000	0.250000	0.057000	9.74	0.92
H_2O 4	0.107400	0.175400	0.372000	3.96	1.16
H_2O 5	0.000000	0.175000	0.570000	13.7	3.2
H_2O 6	0.000000	0.028400	0.429000	6.07	0.91
H_2O 7	0.056200	0.114700	0.410000	9.74	0.63
H_2O 8	0.043100	0.081200	0.626000	1.33	0.77
H_2O 9	0.149000	0.250000	0.237000	4.22	0.5
H_2O 10	0.106000	0.250000	0.086000	5.0	0.61
H_2O 11	0.206000	0.250000	0.401000	4.74	1.32

REFINED COMPOSITION: $|Na_{8.36}K_{5.49}(H_2O)_{30.48}|\ [Be_{14}P_{14}O_{56}]$

CRYSTAL DATA: $P321$ (No. 150)
$a = 12.5815$ Å $b = 12.5815$ Å $c = 12.4508$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.192$, $R_F = 0.106$

REFERENCE: G. Harvey, Ch. Baerlocher and T. Wroblewski, *Z. Kristallogr.* **201** 113–123 (1992).

Atom	x	y	z	B_{iso}	occ
Na 1	0.3333	0.6667	0.502	1.02	1.0
Na 2	0.184	0.164	0.317	14.28	1.06
K 1	0.6260	0.0000	0.5000	1.02	1.0
K 2	0.5230	0.0000	0.0000	13.59	0.83
Be 1	0.6667	0.3333	0.1311	0.09	1.0
Be 2	0.3576	0.4981	0.2681	3.09	1.0
Be 3	0.6996	0.5607	0.3819	0.33	1.0
P 1	0.3333	0.6667	0.1199	0.08	1.0
P 2	0.4907	0.3534	0.2699	1.74	1.0
P 3	0.5609	0.6992	0.3793	1.11	1.0
O 1	0.5696	0.3736	0.1701	3.24	1.0
O 2	0.3333	0.6667	-0.0013	2.46	1.0
O 3	0.4332	0.5920	0.3659	0.09	1.0
O 4	0.4078	0.4054	0.2520	0.09	1.0
O 5	0.5869	0.8005	0.2973	3.72	1.0
O 6	0.4231	0.7992	0.1584	0.96	1.0
O 7	0.4102	0.2168	0.2954	0.09	1.0
O 8	0.5842	0.4242	0.3611	1.74	1.0
O 9	0.6548	0.6592	0.3646	2.85	1.0
O 10	0.5705	0.7509	0.4945	1.65	1.0
H_2O 1	0.406	0.282	-0.002	7.41	1.25
H_2O 2	0.079	-0.070	0.160	18.54	0.83
H_2O 3	0.045	0.237	-0.116	12.0	1.06
H_2O 4	0.044	0.168	0.515	9.09	1.02
H_2O 5	0.647	0.622	0.129	10.65	0.92

BRE Brewsterite

REFINED COMPOSITION: $|Ba_{0.52}Sr_{1.48}(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$
Strontian, Argyll, Scotland

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 6.793$ Å $b = 17.573$ Å $c = 7.759$ Å
$\alpha = 90°$ $\beta = 94.54°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: J. L. Schlenker, J. J. Pluth and J. V. Smith,
Acta Cryst. **B33** 2907–2910 (1977).

Atom	x	y	z	B_{iso}	occ
Ba	0.2501	0.2500	0.1780	1.19	0.26
Sr	0.2501	0.2500	0.1780	1.19	0.74
Si 1	0.3218	0.0812	0.8224	1.1	0.75
Si 2	0.4054	0.0566	0.2108	1.2	0.75
Si 3	0.5553	0.1582	0.5336	1.09	0.75
Si 4	0.9087	0.0528	0.6410	1.01	0.75
Al 1	0.3218	0.0812	0.8224	1.1	0.25
Al 2	0.4054	0.0566	0.2108	1.2	0.25
Al 3	0.5553	0.1582	0.5336	1.09	0.25
Al 4	0.9087	0.0528	0.6410	1.01	0.25
O 1	0.3501	0.1059	0.0283	1.78	1.0
O 2	0.4218	0.1240	0.3607	2.32	1.0
O 3	0.7825	0.1211	0.5454	1.93	1.0
O 4	0.4500	0.1408	0.7150	1.99	1.0
O 5	0.0850	0.0920	0.7615	2.33	1.0
O 6	0.2228	0.9966	0.2388	2.76	1.0
O 7	0.3851	0.9921	0.7952	1.83	1.0
O 8	0.0000	0.0000	0.5000	3.19	1.0
O 9	0.5718	0.2500	0.4994	2.81	1.0
H_2O 1	0.0598	0.2500	0.4699	4.14	1.0
H_2O 2	0.9286	0.1474	0.1518	5.6	1.0
H_2O 3	0.5996	0.2500	0.0241	4.39	1.0
H_2O 4	0.0665	0.2500	0.8660	4.25	1.0

REFINED COMPOSITION: $|Na_8(CO_3)_{1.2}(H_2O)_2|$ $[Si_6Al_6O_{24}]$
Synthetic crystal.

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 12.635$ Å $b = 12.635$ Å $c = 5.115$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.04$

REFERENCE: Y. I. Smolin, Y. F. Shepelev, I. K. Butikova and I. B. Kobyakov, *Kristallografiya* **26** 63–66 (1981).

Atom	x	y	z	B_{iso}	occ
Na 1	0.6667	0.3333	0.1354	1.86	1.0
Na 2	0.1254	0.2521	0.2943	1.21	1.0
Si	0.3300	0.4115	0.7500	0.32	1.0
Al	0.0772	0.4221	0.75	0.27	1.0
O 1	0.2019	0.4035	0.6586	0.56	1.0
O 2	0.1157	0.5619	0.7248	0.74	1.0
O 3	0.0329	0.3526	0.0588	0.69	1.0
O 4	0.3161	0.3582	0.0486	0.72	1.0
C	0.0	0.0	0.173	3.27	0.595
O 5	0.1179	0.0603	0.173	1.57	0.6
H_2O	0.378	0.701	0.179	5.28	0.333

REFINED COMPOSITION: $|Li_{2.9}Na_{1.7}K_2Ca_{0.7}O_6|$ $[Be_6P_6O_{24}]$
Tip Top Mine, Custer, S. Dakota, U.S.A.

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 11.655$ Å $b = 11.655$ Å $c = 4.692$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.048$

REFERENCE: D. R. Peacor, R. C. Rouse and J. H. Ahn, *American Mineralogist* **72** 816–820 (1987).

Atom	x	y	z	B_{iso}	occ
Li	0.2207	0.1137	0.7486	2.32	0.483
Na	0.2207	0.1137	0.7486	2.32	0.283
K	0.3333	0.6667	0.253	2.04	1.0
Ca	0.2207	0.1137	0.7486	2.32	0.1167
Be	0.338	0.418	0.746	0.63	1.0
P	0.0851	0.4167	0.7500	0.5	1.0
O 1	0.1902	0.3843	0.6518	0.97	1.0
O 2	0.1378	0.5647	0.7027	0.75	1.0
O 3	0.0547	0.3801	0.0688	0.95	1.0
O 4	0.3302	0.3747	0.0862	0.65	1.0
O 5	0.0000	0.0000	0.253	2.67	1.0
O 6	0.064	0.130	0.378	1.58	0.25
O 7	0.066	0.130	0.097	1.58	0.25
O 8	0.168	0.322	0.236	1.58	0.17

O5 represents a hydroxyl (OH) in the channel.
O6, O7 and 08 are non-framework oxygen atoms.

REFINED COMPOSITION: $|Cs_{3.26}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: *Ama*2 (No. 40)
$a = 16.776$ Å $b = 13.828$ Å $c = 5.021$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.0549$

REFERENCE: T. Araki,
Z. Kristallogr. **152** 207–213 (1980).

Atom	x	y	z	B_{iso}	occ
Cs	0.2500	0.20406	0.00000	4.665	0.814
Si 1	0.05281	0.74134	0.04651	1.469	1.0
Si 2	0.15709	0.42622	0.41971	1.404	1.0
Si 3	0.08952	0.02677	0.40524	1.444	1.0
O 1	0.00000	0.00000	0.31644	2.851	1.0
O 2	0.25000	0.41029	0.35466	4.888	1.0
O 3	0.12235	0.32339	0.51936	3.97	1.0
O 4	0.09931	0.14024	0.48097	3.014	1.0
O 5	0.02323	0.73969	0.35550	2.718	1.0
O 6	0.11123	0.45939	0.15344	4.334	1.0
O 7	0.14838	0.00661	0.15333	2.614	1.0

Coordinates converted from *Bbm*2 (**ba$\bar{\mathbf{c}}$**) setting.

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: *Imma* (No. 74)
$a = 13.695$ Å $b = 5.021$ Å $c = 25.497$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0875$, $R_{wp} = 0.1143$

REFERENCE: P. Wagner, M. Yoshikawa, M. Lavallo, K. Tsuji, M. Tsapatsis and M. E. Davis, *J. Chem. Soc., Chem. Commun.* 2179–2180 (1997).

Atom	x	y	z	B_{iso}	occ
Si 1	0.1160	0.2500	0.0317	3.32	1.0
Si 2	0.0000	0.7500	0.2788	6.47	1.0
Si 3	0.2820	0.7500	0.1887	3.95	1.0
Si 4	0.0000	0.2500	0.2177	1.58	1.0
Si 5	0.1936	0.2500	0.1479	3.24	1.0
O 1	0.0000	0.2500	0.0512	3.87	1.0
O 2	0.0853	0.2500	0.1737	1.18	1.0
O 3	0.0000	0.5776	0.2309	8.69	1.0
O 4	0.1303	0.0000	0.0000	42.56	1.0
O 5	0.1896	0.2500	0.0909	4.74	1.0
O 6	0.2500	0.7500	0.2500	6.79	1.0
O 7	0.0913	0.7500	0.3099	3.71	1.0
O 8	0.2640	0.4474	0.1665	5.53	1.0

REFINED COMPOSITION: $|C_{48}N_{16}|$ $[Co_{16}Ga_{20}P_{36}O_{144}]$

CRYSTAL DATA: $I1\,2/a\,1$ (No. 15) unique axis **b**, cell choice 3
$a = 15.002$ Å $b = 17.688$ Å $c = 15.751$ Å
$\alpha = 90°$ $\beta = 97.24°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.0704$, $R_w = 0.0850$

REFERENCE: A. M. Chippindale and A. R. Cowley,
Zeolites **18** 176–181 (1997).

Atom	x	y	z	B_{iso}	occ
Ga 1	0.75	0.29158	0.5	1.47	0.5556
Co 1	0.75	0.29158	0.5	1.47	0.4444
Ga 2	0.32984	0.16923	0.18415	1.63	0.5556
Co 2	0.32984	0.16923	0.18415	1.63	0.4444
Ga 3	0.42202	0.24028	0.41491	1.45	0.5556
Co 3	0.42202	0.24028	0.41491	1.45	0.4444
Ga 4	0.63514	0.18555	0.24494	1.63	0.5556
Co 4	0.63514	0.18555	0.24494	1.63	0.4444
Ga 5	0.52517	0.40972	0.18697	2.16	0.5556
Co 5	0.52517	0.40972	0.18697	2.16	0.4444
P 6	0.3610	0.3363	0.2520	1.71	1.0
P 7	0.5774	0.2711	0.0693	1.47	1.0
P 8	0.6822	0.3463	0.3219	2.04	1.0
P 9	0.4756	0.0936	0.3070	1.55	1.0
P 10	0.25	0.2890	0.5	1.98	1.0
O 1	0.8277	0.2249	0.4553	3.05	1.0
O 2	0.7114	0.3640	0.4163	2.79	1.0
O 3	0.4202	0.0985	0.2176	2.56	1.0
O 4	0.2386	0.1480	0.2461	3.96	1.0
O 5	0.3731	0.2661	0.1994	3.44	1.0
O 6	0.2983	0.1586	0.0673	2.83	1.0
O 7	0.4106	0.3250	0.3414	2.87	1.0
O 8	0.4355	0.1478	0.3661	2.98	1.0
O 9	0.5182	0.2648	0.4944	3.17	1.0
O 10	0.3135	0.2365	0.4613	3.71	1.0
O 11	0.5739	0.2161	0.1438	3.06	1.0
O 12	0.5731	0.1122	0.2980	3.34	1.0
O 13	0.6558	0.2632	0.3183	4.52	1.0
O 14	0.7439	0.1405	0.2334	4.74	1.0
O 15	0.6056	0.3974	0.2906	3.55	1.0
O 16	0.4009	0.4030	0.2099	2.23	1.0
O 17	0.5493	0.3499	0.0891	2.68	1.0
O 18	0.5272	0.5173	0.1552	2.59	1.0
N 1	0.8049	0.5046	0.0671	2.65	1.0
N 2	0.987	0.0584	0.0420	6.21	1.0
C 1	0.854	0.512	-0.009	4.69	0.5
C 2	0.740	0.569	0.066	4.23	0.5
C 3	0.753	0.4328	0.060	4.38	0.5
C 4	0.7130	0.519	0.088	5.0	0.5
C 6	0.807	0.4306	0.024	5.02	0.5

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Atom	x	y	z	B_{iso}	occ
C 5	0.831	0.564	0.010	5.01	0.5
C 7	0.993	0.074	-0.049	7.1	0.5
C 8	0.917	-0.001	0.049	4.87	0.5
C 9	1.075	0.027	0.081	13.81	0.5
C 10	1.018	-0.004	0.102	6.3	0.5
C 11	1.059	0.075	-0.011	5.74	0.5
C 12	0.907	0.031	-0.016	16.12	0.5

REFINED COMPOSITION: $|C_{28}N_4|$ $[Co_4Ga_{12}P_{16}O_{64}]$

CRYSTAL DATA: $P1\,2_1/c\,1$ (No. 14) unique axis **b**, cell choice 1
$a = 14.365$ Å $b = 16.305$ Å $c = 8.734$ Å
$\alpha = 90°$ $\beta = 90.243°$ $\gamma = 90°$
X-ray single crystal refinement. $R = 0.0310$, $R_w = 0.0365$

REFERENCE: A. R. Cowley and A. M. Chippindale,
Microporous and Mesoporous Materials **28** 163–172 (1999).

Atom	x	y	z	B_{iso}	occ
Ga 1	0.1365	0.0342	0.5716	1.0028	0.53
Ga 2	0.04238	0.2716	0.6324	1.1765	0.87
Ga 3	0.47446	-0.1263	0.5896	1.0659	0.88
Ga 4	0.36576	0.1616	0.8134	1.1133	0.72
Co 1	0.1365	0.0342	0.5716	1.0028	0.47
Co 2	0.04238	0.2716	0.6324	1.1765	0.13
Co 3	0.47446	-0.1263	0.5896	1.0659	0.12
Co 4	0.36576	0.1616	0.8134	1.1133	0.28
P 5	0.14798	0.1518	0.8485	1.3028	1.0
P 6	0.35984	0.0307	0.5527	0.9949	1.0
P 7	0.47275	0.2188	1.1099	0.9712	1.0
P 8	-0.02864	0.1324	0.4143	1.0106	1.0
O 1	0.4479	0.1630	0.9765	1.7134	1.0
O 2	0.464	-0.1709	0.7813	1.7528	1.0
O 3	-0.0339	0.1972	0.5409	2.3687	1.0
O 4	0.3701	-0.0628	0.5607	1.8634	1.0
O 5	-0.0364	0.1735	0.2574	2.2582	1.0
O 6	0.2498	0.1493	0.8965	2.8109	1.0
O 7	0.1352	0.2251	0.7428	2.7714	1.0
O 8	0.0883	0.1587	0.9916	2.9135	1.0
O 9	0.1184	0.0727	0.7705	2.5345	1.0
O 10	0.3842	0.253	0.6913	1.8239	1.0
O 11	0.4197	0.0638	0.4221	1.7134	1.0
O 12	0.0625	0.0856	0.4233	1.9187	1.0
O 13	0.2599	0.0521	0.5152	2.1792	1.0
O 14	0.392	0.0664	0.7056	2.0292	1.0
O 15	0.4704	-0.2072	0.4434	1.5554	1.0
O 16	0.1137	-0.0781	0.5674	1.8397	1.0
N 1	0.2511	0.9653	0.013	6.1665	0.483
N 2	0.2528	0.9332	0.236	8.1562	0.517
C 1	0.177	0.963	0.119	12.2067	0.483
C 2	0.167	0.882	0.189	11.9935	0.483
C 3	0.2399	0.9008	-0.099	4.3584	0.483
C 4	0.2491	0.8189	-0.028	4.6663	0.483
C 5	0.338	0.952	0.087	9.538	0.483
C 6	0.337	0.881	0.181	9.4038	0.483
C 7	0.254	0.8269	0.148	6.9245	0.483
C 8	0.254	0.8471	0.2510	7.6114	0.517
C 9	0.256	0.8053	0.0970	7.9588	0.517
C 10	0.3236	0.9609	0.1360	6.7666	0.517

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Atom	x	y	z	B_{iso}	occ
C 11	0.3053	0.9362	-0.0230	5.7165	0.517
C 12	0.1654	0.9564	0.1760	5.4717	0.517
C 13	0.139	0.9113	0.0390	4.1689	0.517
C 14	0.225	0.8699	-0.0280	5.3928	0.517

REFINED COMPOSITION: $|K_{4.16}(H_2O)_{7.23}|$ $[Si_{8.16}Al_{3.84}O_{24}]$
North East Azerbaijan, Iran

CRYSTAL DATA: $R\overline{3}m$ (No. 166) rhombohedral setting
$a = 9.459$ Å $b = 9.459$ Å $c = 9.459$ Å
$\alpha = 94.07°$ $\beta = 94.07°$ $\gamma = 94.07°$
X-ray single crystal refinement, $R = 0.05$

REFERENCE: M. Calligaris, G. Nardin and L. Randaccio, *Zeolites* **3** 205–208 (1983).

Atom	x	y	z	B_{iso}	occ
K 1	0.2222	0.2222	0.2222	0.529	0.97
K 2	0.5611	0.5611	0.2506	2.277	0.15
K 3	0.5255	0.5255	0.1064	2.5	0.22
Si	0.1033	0.3331	0.8743	0.223	0.68
Al	0.1033	0.3331	0.8743	0.223	0.32
O 1	0.2665	-0.2665	0.0	0.579	1.0
O 2	0.1506	-0.1506	0.5	0.52	1.0
O 3	0.2503	0.2503	0.8930	0.559	1.0
O 4	0.0204	0.0204	0.3193	0.406	1.0
H_2O 1	0.0	0.50	0.50	3.2	0.61
H_2O 2	0.7387	0.7387	0.4784	2.0	0.77
H_2O 3	0.4469	0.4469	0.2260	3.2	0.13

CHA Methylbutylamine SAPO–47

REFINED COMPOSITION: $|(C_5N)_{2.06}|\ [Al_{5.47}P_{5.37}O_{24}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) rhombohedral setting
$a = 9.3834$ Å $b = 9.3834$ Å $c = 9.3834$ Å
$\alpha = 94.085°$ $\beta = 94.085°$ $\gamma = 94.085°$
X-ray single crystal refinement, $R_w = 0.068$

REFERENCE: J. J. Pluth and J. V. Smith,
J. Phys. Chem. **93** 6516–6520 (1989).

Atom	x	y	z	B_{iso}	occ
Al	0.09888	0.33196	0.87510	1.2	0.912
P	0.33245	0.10847	0.87466	1.176	0.895
O 1	0.2580	-0.2704	-0.0127	2.763	1.0
O 2	0.1519	-0.1445	0.4911	2.424	1.0
O 3	0.2542	0.2460	0.8876	2.779	1.0
O 4	0.0291	0.0104	0.3178	3.008	1.0
C 1	-0.132	0.524	0.500	17.92	0.344
C 2	0.112	0.492	0.440	31.9	0.344
C 3	0.189	0.353	0.424	31.9	0.344
C 4	0.334	0.382	0.359	31.9	0.344
C 5	0.449	0.303	0.439	31.9	0.344
N	0.009	0.480	0.551	17.92	0.344

REFINED COMPOSITION: $|Ca_4Mn_4(H_2O)_8|\ [Si_{20}(BeOH)_8O_{52}]$
Val di San Giacomo, Chiavenna, Italy

CRYSTAL DATA: *Pnab* (No. 60) **c̄ba** setting
$a = 8.729$ Å $b = 31.326$ Å $c = 4.903$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.041$

REFERENCE: V. Tazzoli, M. C. Domeneghetti, F. Mazzi and E. Cannillo
Eur. J. Mineral. **7** 1339–1344 (1995).

Atom	x	y	z	B_{iso}	occ
Ca	0.25000	0.08789	0.00000	1.45	1.0
Mn	0.00000	0.00000	0.00000	1.20	1.0
Si 1	0.25000	0.00131	0.50000	0.98	1.0
Si 2	0.58376	0.23216	0.10475	1.46	1.0
Si 3	0.14247	-0.13511	0.24360	1.53	1.0
Be	-0.00037	0.05722	-0.42986	0.69	1.0
O 1	0.13917	-0.02785	0.31336	1.22	1.0
O 2	0.15170	0.03243	-0.29572	1.21	1.0
O 3	0.04143	0.23906	0.13475	3.23	1.0
O 4	0.25000	-0.24779	0.00000	2.25	1.0
O 5	0.25000	-0.11875	0.00000	6.10	1.0
O 6	0.25000	-0.13872	0.50000	0.28	1.0
O 7	0.07997	-0.18239	0.17734	2.70	1.0
O 8	0.00055	-0.10438	0.27050	1.63	1.0
OH	0.01254	0.05814	0.24296	1.63	1.0
H_2O	0.15815	0.14739	0.26022	2.93	1.0

The OH provide the terminal oxygens, where the framework is not fully connected.

REFINED COMPOSITION: $|F_{192}|$ $[Ga_{768}P_{768}O_{3168}]$

CRYSTAL DATA: $Fm\overline{3}c$ (No. 226)
$a = 51.7120$ Å $b = 51.7120$ Å $c = 51.7120$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.076$

REFERENCE: M. Estermann, L. B. McCusker, Ch. Baerlocher, A. Merrouche and H. Kessler, *Nature* **352** 320–322 (1991).

Atom	x	y	z	B_{iso}	occ
Ga 1	0.1341	0.3275	0.2780	1.098	1.0
Ga 2	0.0370	0.3507	0.3134	1.382	1.0
Ga 3	0.0958	0.3654	0.2236	1.105	1.0
Ga 4	0.0	0.3242	0.2140	1.184	1.0
Ga 5	0.0	0.3415	0.3801	2.487	1.0
P 1	0.0888	0.3656	0.2818	1.358	1.0
P 2	0.0	0.3226	0.2769	0.742	1.0
P 3	0.0	0.3876	0.3414	1.153	1.0
P 4	0.1336	0.3210	0.2180	0.616	1.0
P 5	0.0446	0.3097	0.3556	0.955	1.0
O 1	0.0800	0.3669	0.2542	2.771	1.0
O 2	0.1059	0.3885	0.2891	1.413	1.0
O 3	0.1036	0.3404	0.2866	2.448	1.0
O 4	0.0657	0.3679	0.2999	1.587	1.0
O 5	0.1360	0.3124	0.2458	3.995	1.0
O 6	0.1339	0.2970	0.2951	1.437	1.0
O 7	0.1631	0.3439	0.2914	4.572	1.0
O 8	0.0237	0.3376	0.2830	3.427	1.0
O 9	0.0	0.3158	0.2475	1.2	1.0
O 10	0.0	0.2979	0.2916	2.045	1.0
O 11	0.0521	0.3286	0.3360	4.24	1.0
O 12	0.0242	0.3795	0.3277	3.948	1.0
O 13	0.0	0.3738	0.3670	3.119	1.0
O 14	0.1091	0.3344	0.2142	3.206	1.0
O 15	0.0675	0.3692	0.2010	2.258	1.0
O 16	-0.0289	0.3436	0.2115	2.795	1.0
O 17	0.0283	0.3231	0.3764	3.119	1.0
O 18	0.0	0.4161	0.3461	1.169	1.0
O 19	0.0	0.3461	0.4150	5.993	1.0
F 1	0.1335	0.3664	0.25	1.729	1.0
F 2	0.0	0.3325	0.3297	2.037	1.0

O18 and O19 are terminal oxygens, where the framework is not fully connected.

REFINED COMPOSITION: $[Si_{56}O_{112}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 22.6242$ Å $b = 13.3503$ Å $c = 12.3642$ Å
$\alpha = 90°$ $\beta = 68.913°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.136$, $R_F = 0.106$

REFERENCE: R. F. Lobo and M. E. Davis,
J. Am. Chem. Soc. **117** 3766–3779 (1994).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0677	0.1102	0.4914	1.48	1.0
Si 2	0.1567	0.1889	0.2510	1.48	1.0
Si 3	0.0734	0.1204	0.7390	1.48	1.0
Si 4	0.2879	0.1171	0.1026	1.48	1.0
Si 5	0.2770	0.1141	0.8607	1.48	1.0
Si 6	0.0738	0.1195	0.1043	1.48	1.0
Si 7	0.1480	0.1898	0.8835	1.48	1.0
O 8	0.0763	0.0000	0.4256	1.42	1.0
O 9	0.0784	0.1380	0.6085	1.42	1.0
O 1	0.1205	0.1669	0.3814	1.42	1.0
O 2	0.0000	0.1458	0.5000	1.42	1.0
O 3	0.2185	0.1200	0.2009	1.42	1.0
O 4	0.1097	0.1569	0.1860	1.42	1.0
O 5	0.1728	0.3005	0.2109	1.42	1.0
O 6	0.0852	0.0000	0.7309	1.42	1.0
O 7	0.0003	0.1379	0.8223	1.42	1.0
O 8	0.1271	0.1859	0.7717	1.42	1.0
O 9	0.3045	0.0000	0.1272	1.42	1.0
O 10	0.2721	0.1330	0.9904	1.42	1.0
O 11	0.3442	0.1888	0.0983	1.42	1.0
O 12	0.2102	0.1217	0.8382	1.42	1.0
O 13	0.3046	0.0000	0.8219	1.42	1.0
O 14	0.0873	0.0000	0.1087	1.42	1.0
O 15	0.0837	0.1783	0.9900	1.42	1.0

SSZ-33/SSZ-26 family, Polymorph B SiO_2 framework.

SSZ-26/SSZ-33 family, Polymorph A SiO_2 framework

REFINED COMPOSITION: $[Si_{56}O_{112}]$

CRYSTAL DATA: *Pmna* (No. 53)

$a = 13.26$ Å	$b = 12.33$ Å	$c = 21.08$ Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$

REFERENCE: R. F. Lobo, M. Pan, I. Chan, H-X. Li, R. C. Medrud, S. I. Zones, P. A. Crozier and M. E. Davis, *Science* **262** 1543–1546 (1993).

Atom	x	y	z
Si 1	0.111	0.208	0.074
Si 2	0.114	0.158	0.927
Si 3	0.211	0.030	0.150
Si 4	0.113	0.463	0.072
Si 5	0.198	0.359	0.849
Si 6	0.112	0.960	0.271
Si 7	0.116	0.711	0.278
O 1	0.192	0.148	0.117
O 2	0.123	0.168	0.002
O 3	0.129	0.336	0.078
O 4	0.000	0.180	0.099
O 5	0.150	0.269	0.895
O 6	0.184	0.061	0.903
O 7	0.000	0.135	0.908
O 8	0.311	0.017	0.181
O 9	0.117	0.018	0.204
O 10	0.000	0.494	0.091
O 11	0.134	0.500	0.000
O 12	0.190	0.525	0.118
O 13	0.314	0.330	0.836
O 14	0.137	0.361	0.783
O 15	0.000	0.969	0.299
O 16	0.141	0.835	0.263
O 17	0.000	0.700	0.298

SSZ-33/SSZ-26 represents a family of intergrown materials. The polymorph A framework is a hypothetical end member of the family.

REFINED COMPOSITION: $|Na_{6.06}O_{9.12}|\ [Zn_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P6_122$ (No. 178)
$a = 10.4797$ Å $b = 10.4797$ Å $c = 15.089$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 120.0°$
X-ray single crystal refinement, $R = 0.0599$, $R_w = 0.0529$

REFERENCE: W. T. A. Harrison, T. E. Gier, G. D. Stucky, R. W. Broach and R. A. Bedard, *Chemistry of Materials* **8** 145–151 (1996).

Atom	x	y	z	B_{iso}	occ
Zn 1	0.8414	0.6827	0.25	1.44	1.0
Zn 2	0.5071	0.4929	0.41667	1.56	1.0
P	0.8324	0.5912	0.4409	1.6	1.0
O 1	0.805	0.5403	0.3439	1.82	1.0
O 2	1.0485	0.8019	0.2185	2.01	1.0
O 3	0.689	0.571	0.4808	2.59	1.0
O 4	0.873	0.489	0.4910	2.46	1.0
Na 1	0.668	0.336	0.25	2.92	0.53
Na 2	0.602	0.336	0.235	2.92	0.24
O 5	0.07	0.033	0.08333	2.92	0.10
O 6	0.410	0.302	0.161	2.92	0.29
O 7	0.076	0.0	0.0	2.92	0.24
O 8	0.425	0.247	0.117	2.92	0.30

CZP Chiral Sodium Zincophosphate, $P6_522$

REFINED COMPOSITION: $|Na_{2.04}O_{4.08}|\ [Zn_{12}P_{12}O_{48}]$

CRYSTAL DATA: $P6_522$ (No. 179)
$a = 10.412$ Å $b = 10.412$ Å $c = 15.184$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 120.0°$
X-ray single crystal refinement, $R = 0.0690$, $R_w = 0.0810$

REFERENCE: W. T. A. Harrison, T. E. Gier, G. D. Stucky, R. W. Broach and R. A. Bedard, *Chemistry of Materials* **8** 145–151 (1996).

Atom	x	y	z	B_{iso}	occ
Zn 1	0.84243	0.68486	0.75	1.8	1.0
Zn 2	0.49697	0.99393	0.75	2.46	1.0
P	0.17041	0.40605	0.06011	1.74	1.0
O 1	0.1976	0.4597	0.1566	2.68	1.0
O 2	0.0519	0.2464	0.0547	2.61	1.0
O 3	0.3130	0.4229	0.0201	2.37	1.0
O 4	0.1292	0.5030	0.0075	2.84	1.0
Na	0.6713	0.3425	0.75	8.76	0.34
O 5	0.5908	0.7113	0.3441	7.26	0.34

REFINED COMPOSITION: $|K_{0.62}Ca_{2.76}(H_2O)_{12}|\ [Si_{19.2}Al_{4.8}O_{48}]$
Elba, Italy

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 18.676$ Å $b = 7.518$ Å $c = 10.246$ Å
$\alpha = 90°$ $\beta = 107.87°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: G. Vezzalini,
Z. Kristallogr. **166** 63–71 (1984).

Atom	x	y	z	B_{iso}	occ
K	0.4544	0.0	0.4626	10.3	0.156
Ca	-0.0091	0.2598	0.1297	7.8	0.345
Si 11	0.2905	0.2084	0.1496	1.2	0.4
Si 12	0.2846	0.2053	0.1660	1.1	0.4
Si 21	0.1914	0.2901	0.3371	1.3	0.4
Si 22	0.1929	0.2978	0.3714	1.0	0.4
Si 3	0.0964	0.0	0.7007	1.1	0.8
Si 4	0.0816	0.0	0.3793	1.2	0.8
Al 11	0.2905	0.2084	0.1496	1.2	0.1
Al 12	0.2846	0.2053	0.1660	1.1	0.1
Al 21	0.1914	0.2901	0.3371	1.3	0.1
Al 22	0.1929	0.2978	0.3714	1.0	0.1
Al 3	0.0964	0.0	0.7007	1.1	0.2
Al 4	0.0816	0.0	0.3793	1.2	0.2
O 1	0.3636	0.3239	0.2168	3.3	1.0
O 2	0.1162	0.1770	0.3265	3.1	1.0
O 31	0.2188	0.2642	0.2070	2.4	0.5
O 32	0.2382	0.2370	0.2652	4.3	0.5
O 4	0.1002	0.0	0.5457	4.3	1.0
O 5	0.1688	0.5000	0.3487	4.0	1.0
O 6	0.3098	0.0	0.1759	3.5	1.0
O 7	0.2335	0.2452	0.0131	3.2	0.5
O 8	0.2427	0.2777	0.5249	2.9	0.5
O 9	0.0103	0.0	0.7080	1.9	1.0
H_2O 1	-0.0084	0.5	0.2668	5.4	1.0
H_2O 2	0.0884	0.0	0.0330	6.7	0.5
H_2O 3	0.0694	0.1037	0.0261	7.5	0.25
H_2O 4	0.0724	0.3931	0.0258	6.5	0.25
H_2O 5	0.0860	0.5000	0.0310	6.0	0.5

DDR N_2, 1-aminoadamantane Deca-Dodecasil 3R

REFINED COMPOSITION: $|C_{69}N_6|\ [Si_{120}O_{240}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.860$ Å $b = 13.860$ Å $c = 40.891$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.066$

REFERENCE: H. Gies,
Z. Kristallogr. **175** 93–104 (1986).

Atom	x	y	z	B_{iso}	occ
Si 1	0.7267	0.0511	0.0700	0.76	1.0
Si 2	0.1264	0.2527	0.1095	0.76	1.0
Si 3	0.2020	0.4039	0.1711	0.2	1.0
Si 4	0.1227	0.2454	0.2325	0.6	1.0
Si 5	0.2256	0.0000	0.0000	0.82	1.0
Si 6	0.0000	0.0000	0.2039	1.53	1.0
Si 7	0.0000	0.0000	0.1280	0.87	1.0
O 1	0.3576	0.3881	0.6358	2.37	1.0
O 2	0.2792	0.3749	0.5768	1.45	1.0
O 3	0.4067	0.2954	0.5889	1.96	1.0
O 4	0.2277	0.4554	0.6589	3.76	1.0
O 5	0.1767	0.3534	0.7447	2.24	1.0
O 6	0.3233	0.1616	0.5391	3.01	1.0
O 7	0.5401	0.2700	0.5494	3.7	1.0
O 8	0.2713	0.5426	0.5529	2.49	1.0
O 9	0.1780	0.3561	0.5230	3.33	1.0
O 10	0.1870	0.0000	0.5000	1.65	1.0
O 11	0.0000	0.0000	0.1661	4.47	1.0
C 512	0.5000	0.0000	0.5000	15.112	1.0
N 1	0.0000	0.0000	0.4455	40.908	0.9
C 1	0.0000	0.0000	0.4095	37.228	0.9
C 2	0.0596	0.1192	0.3954	14.915	0.9
C 3	0.0596	0.1192	0.3577	28.274	0.9
C 4	0.1192	0.0596	0.3438	14.654	0.9
N 11	0.0000	0.0000	0.2815	15.728	0.1
C 11	0.0000	0.0000	0.3175	23.237	0.1
C 21	0.0596	0.1192	0.3317	8.598	0.1
C 31	0.0596	0.1192	0.3694	4.461	0.1
C 41	0.1192	0.0596	0.3833	15.404	0.1

REFINED COMPOSITION: $|C_{23}|$ $[Si_{132}O_{264}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 22.351$ Å $b = 22.351$ Å $c = 21.693$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.122$

REFERENCE: P. A. Wright, R. H. Jones, S. Natarajan, R. G. Bell, J. Chen, M. B. Hursthouse and J. M. Thomas, *J. Chem. Soc., Chem. Comm.* 633–635 (1993).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0803	0.3024	0.50000	1.87	1.0
Si 2	0.1471	0.4356	0.1836	1.88	1.0
Si 3	0.0816	0.4710	0.2940	1.8	1.0
Si 4	0.0811	0.4703	0.0727	2.27	1.0
Si 5	0.1217	0.3812	0.3706	1.97	1.0
Si 6	0.0782	0.2904	0.2486	2.05	1.0
O 1	0.0993	0.3514	0.1995	3.71	1.0
O 2	0.0923	0.3520	0.4391	4.1	1.0
O 3	0.1063	0.4430	0.3533	3.48	1.0
O 4	0.1306	0.4517	0.1122	3.49	1.0
O 5	0.1298	0.4794	0.2351	4.37	1.0
O 6	0.0847	0.3203	0.3175	3.98	1.0
O 7	0.0	0.2363	0.5	3.29	1.0
O 8	0.1375	0.2750	0.5	4.37	1.0
O 9	0.0	0.2285	0.2361	2.88	1.0
O 10	0.0	0.4158	0.879	4.33	1.0
O 11	0.0	0.4188	0.2775	3.55	1.0
O 12	0.0953	0.4615	0.0	3.76	1.0
O 13	0.2295	0.4590	0.1903	3.45	1.0
O 14	0.0935	0.5468	0.3133	2.78	1.0
O 15	0.2050	0.4101	0.3678	2.8	1.0
O 16	0.1293	0.2586	0.2404	2.8	1.0
O 17	0.0974	0.5487	0.0867	4.36	1.0
C 1	0.5	0.0	0.5	11.84	1.0
C 2	0.4453	0.0246	0.5	11.84	0.3333
C 3	0.5197	0.0394	0.4403	11.84	0.3333
C 4	0.66667	0.33333	0.2688	11.84	1.0
C 5	0.6406	0.2811	0.3088	11.84	0.3333
C 6	0.5949	0.2974	0.3129	9.67	0.3333

Refined in higher symmetry space group ($P6/mmm$) with disordered T-sites.

REFINED COMPOSITION: $|C_{32}N_{32}|$ $[Mg_{32}P_{32}O_{128}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 20.9098$ Å $b = 17.8855$ Å $c = 14.7913$ Å
$\alpha = 90.0°$ $\beta = 134.842°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R = 0.1007, R_w = 0.0994$

REFERENCE: K. O. Kongshaug, H. Fjellvåg and K. P. Lillerud,
Chemistry of Materials **12** 1095–1099 (2000).

Atom	x	y	z	B_{iso}	occ
Mg 1	0.6337	0.5791	0.8697	0.71	1.0
Mg 2	0.1339	0.5828	0.8798	0.71	1.0
Mg 3	0.5134	0.6686	0.3938	0.63	1.0
Mg 4	0.0011	0.6701	0.3846	0.79	1.0
P 1	0.488	0.645	0.5859	0.71	1.0
P 2	0.8503	0.6002	0.1141	0.63	1.0
P 3	0.6496	0.3955	0.8964	0.71	1.0
P 4	-0.0044	0.6504	0.5961	0.63	1.0
O 1	0.5787	0.5965	0.9299	1.58	1.0
O 2	0.0369	0.7735	0.4253	1.18	1.0
O 3	0.5851	0.6279	0.7143	1.34	1.0
O 4	0.4803	0.6232	0.4771	0.87	1.0
O 5	0.9112	0.6126	0.0934	1.5	1.0
O 6	0.8792	0.651	0.2222	1.11	1.0
O 7	0.8516	0.5192	0.1478	0.87	1.0
O 8	0.7528	0.6233	-0.0102	1.11	1.0
O 9	0.6387	0.4745	0.8498	1.18	1.0
O 10	0.5918	0.3403	0.785	1.03	1.0
O 11	0.7491	0.3707	0.9848	0.87	1.0
O 12	0.6227	0.3894	0.9709	1.18	1.0
O 13	0.0852	0.6474	0.7371	1.26	1.0
O 14	-0.0463	0.7283	0.5554	0.87	1.0
O 15	0.9297	0.5921	0.571	1.26	1.0
O 16	0.014	0.6254	0.5161	0.79	1.0
N 1	0.1204	0.501	0.6262	1.03	1.0
N 2	0.6261	0.5053	0.6242	1.11	1.0
N 3	0.7586	0.2534	0.1335	1.03	1.0
N 4	0.7341	0.7513	0.1062	1.18	1.0
C 1	0.7169	0.4716	0.7168	1.11	1.0
C 2	0.2119	0.5328	0.7085	1.11	1.0
C 3	0.7604	0.2203	0.2269	0.87	1.0
C 4	0.7403	0.7825	0.204	1.03	1.0

REFINED COMPOSITION: $|C_{15.4}|$ $[Si_{34}O_{68}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 13.783$ Å $b = 13.783$ Å $c = 11.190$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.077$

REFERENCE: H. Gerke and H. Gies,
Z. Kristallogr. **166** 11–22 (1984).

Atom	x	y	z	B_{iso}	occ
Si 1	0.4186	0.2093	0.2252	2.12	1.0
Si 2	0.3868	0.0	0.3627	2.36	1.0
Si 3	0.2628	0.1314	0.0	1.63	1.0
Si 4	0.3333	0.6667	0.1384	1.95	1.0
O 1	0.1052	0.3933	0.3031	6.49	1.0
O 2	0.5429	0.2715	0.8164	5.56	1.0
O 3	0.3405	0.1702	0.1139	4.38	1.0
O 4	0.3601	0.0	0.5	4.49	1.0
O 5	0.1865	0.0	0.0	4.0	1.0
O 6	0.5	0.0	0.3451	7.25	1.0
O 7	0.3333	0.6667	0.0	10.14	1.0
C 1	0.333	0.667	0.356	10.26	0.1
C 2	0.381	0.762	0.402	10.26	0.1
C 3	0.309	0.618	0.436	10.26	0.1
C 4	0.230	0.760	0.500	10.26	0.1
C 5	0.0	0.5	0.036	10.26	0.1
C 6	0.092	0.636	0.0	10.26	0.1
C 7	0.122	0.531	0.0	10.26	0.1
C 8	0.0	0.431	0.0	10.26	0.1
C 9	0.140	0.570	0.122	10.26	0.1
C 10	0.0	0.0	0.296	10.26	0.1
C 11	0.038	0.010	0.380	10.26	0.1
C 12	0.040	0.080	0.458	10.26	0.1
C 13	0.041	0.082	0.316	10.26	0.1
C 14	0.085	0.0	0.398	10.26	0.1
C 15	0.0	0.0	0.049	10.26	0.1
C 16	0.199	0.398	0.462	10.26	0.1

Thermal parameter U_{33} for O1 was changed from 0.7570 to 0.0757 when computing B_{iso}.

REFINED COMPOSITION: $|Co_2C_{35}|$ $[Si_{64}O_{128}]$

CRYSTAL DATA: Pc (No. 7) unique axis **b**, cell choice 1
$a = 14.9701$ Å $b = 8.4761$ Å $c = 30.0278$ Å
$\alpha = 90°$ $\beta = 102.65°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_F = 0.041$, $R_{wp} = 0.134$

REFERENCE: T. Wessels, Ch. Baerlocher, L. B. McCusker and E. J. Creyghton, *J. Am. Chem. Soc.* **121** 6242–6247 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.096	0.180	0.1066	0.95	1.0
Si 2	0.076	0.313	0.1986	0.95	1.0
Si 3	0.124	0.180	0.2943	0.95	1.0
Si 4	0.240	0.305	0.3824	0.95	1.0
Si 5	0.410	0.176	0.4374	0.95	1.0
Si 6	0.608	0.306	0.4689	0.95	1.0
Si 7	0.793	0.183	0.4654	0.95	1.0
Si 8	0.912	0.307	0.3992	0.95	1.0
Si 9	0.929	0.182	0.3045	0.95	1.0
Si 10	0.868	0.309	0.2072	0.95	1.0
Si 11	0.769	0.176	0.1199	0.95	1.0
Si 12	0.585	0.308	0.0659	0.95	1.0
Si 13	0.398	0.190	0.040	0.95	1.0
Si 14	0.206	0.316	0.041	0.95	1.0
Si 15	0.902	0.318	0.0631	0.95	1.0
Si 16	0.108	0.180	0.4432	0.95	1.0
Si 17	0.081	0.816	0.1046	0.95	1.0
Si 18	0.076	0.675	0.1994	0.95	1.0
Si 19	0.127	0.807	0.2936	0.95	1.0
Si 20	0.239	0.678	0.3836	0.95	1.0
Si 21	0.418	0.808	0.4366	0.95	1.0
Si 22	0.604	0.687	0.4663	0.95	1.0
Si 23	0.798	0.810	0.4672	0.95	1.0
Si 24	0.914	0.679	0.4024	0.95	1.0
Si 25	0.931	0.797	0.3052	0.95	1.0
Si 26	0.867	0.670	0.2096	0.95	1.0
Si 27	0.762	0.809	0.1211	0.95	1.0
Si 28	0.587	0.313	0.5659	0.95	1.0
Si 29	0.386	0.181	0.5374	0.95	1.0
Si 30	0.194	0.685	0.040	0.95	1.0
Si 31	0.890	0.318	0.5625	0.95	1.0
Si 32	0.110	0.808	0.4458	0.95	1.0
O 1	0.169	0.278	0.0863	0.32	1.0
O 2	0.108	0.208	0.1608	0.32	1.0
O 3	0.131	0.265	0.2484	0.32	1.0
O 4	0.101	0.494	0.1903	0.32	1.0
O 5	0.209	0.230	0.3331	0.32	1.0
O 6	0.033	0.230	0.3097	0.32	1.0
O 7	0.125	0.995	0.287	0.32	1.0
O 8	0.348	0.283	0.3979	0.32	1.0

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Atom	x	y	z	B_{iso}	occ
O 9	0.191	0.220	0.4183	0.32	1.0
O 10	0.215	0.491	0.3798	0.32	1.0
O 11	0.513	0.230	0.443	0.32	1.0
O 12	0.375	0.202	0.4835	0.32	1.0
O 13	0.689	0.237	0.4472	0.32	1.0
O 14	0.624	0.264	0.5218	0.32	1.0
O 15	0.601	0.496	0.4626	0.32	1.0
O 16	0.851	0.210	0.4274	0.32	1.0
O 17	0.839	0.279	0.5109	0.32	1.0
O 18	0.890	0.251	0.3468	0.32	1.0
O 19	0.797	0.997	0.4778	0.32	1.0
O 20	0.887	0.494	0.402	0.32	1.0
O 21	0.870	0.253	0.2581	0.32	1.0
O 22	0.919	0.990	0.3025	0.32	1.0
O 23	0.797	0.197	0.1738	0.32	1.0
O 24	0.967	0.294	0.195	0.32	1.0
O 25	0.831	0.489	0.2009	0.32	1.0
O 26	0.664	0.227	0.1035	0.32	1.0
O 27	0.833	0.285	0.0962	0.32	1.0
O 28	0.489	0.247	0.0739	0.32	1.0
O 29	0.598	0.741	0.5166	0.32	1.0
O 30	0.590	0.502	0.5718	0.32	1.0
O 31	0.314	0.288	0.0503	0.32	1.0
O 32	0.382	0.996	0.5496	0.32	1.0
O 33	0.186	0.499	0.0267	0.32	1.0
O 34	0.112	0.995	0.0982	0.32	1.0
O 35	0.853	0.725	0.5119	0.32	1.0
O 36	0.994	0.221	0.0794	0.32	1.0
O 37	0.929	0.497	0.5648	0.32	1.0
O 38	0.019	0.282	0.4218	0.32	1.0
O 39	0.140	0.216	0.497	0.32	1.0
O 40	0.146	0.707	0.0822	0.32	1.0
O 41	0.095	0.780	0.1582	0.32	1.0
O 42	0.140	0.730	0.2469	0.32	1.0
O 43	0.212	0.756	0.334	0.32	1.0
O 44	0.034	0.750	0.3059	0.32	1.0
O 45	0.346	0.700	0.4027	0.32	1.0
O 46	0.185	0.760	0.4177	0.32	1.0
O 47	0.518	0.757	0.4306	0.32	1.0
O 48	0.406	0.218	0.988	0.32	1.0
O 49	0.401	0.992	0.4223	0.32	1.0
O 50	0.695	0.749	0.4535	0.32	1.0
O 51	0.848	0.780	0.4262	0.32	1.0
O 52	0.903	0.736	0.3507	0.32	1.0
O 53	0.864	0.721	0.2612	0.32	1.0
O 54	0.799	0.786	0.1748	0.32	1.0
O 55	0.969	0.689	0.2014	0.32	1.0
O 56	0.655	0.232	0.6092	0.32	1.0
O 57	0.817	0.305	0.5948	0.32	1.0
O 58	0.780	0.991	0.1064	0.32	1.0

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Atom	x	y	z	B_{iso}	occ
O 59	0.484	0.252	0.5629	0.32	1.0
O 60	0.303	0.269	0.5536	0.32	1.0
O 61	0.975	0.203	0.5788	0.32	1.0
O 62	0.153	0.211	0.9993	0.32	1.0
O 63	0.083	0.993	0.4353	0.32	1.0
O 64	0.019	0.702	0.4307	0.32	1.0
Co	0.502	0.258	0.2542	1.82	1.0
C 1	0.518	0.060	0.218	5.53	1.0
C 2	0.577	0.054	0.262	5.53	1.0
C 3	0.523	0.062	0.295	5.53	1.0
C 4	0.429	0.071	0.271	5.53	1.0
C 5	0.426	0.070	0.224	5.53	1.0
C 6	0.558	0.063	0.346	11.05	1.0
C 7	0.681	0.030	0.271	11.05	1.0
C 8	0.546	0.050	0.172	11.05	1.0
C 9	0.340	0.070	0.186	11.05	1.0
C 10	0.347	0.068	0.294	11.05	1.0
C 11	0.543	0.450	0.222	5.53	1.0
C 12	0.584	0.453	0.270	5.53	1.0
C 13	0.512	0.457	0.294	5.53	1.0
C 14	0.427	0.456	0.262	5.53	1.0
C 15	0.446	0.452	0.217	5.53	1.0
C 16	0.525	0.473	0.345	11.05	1.5
C 17	0.686	0.457	0.291	11.05	1.5
C 18	0.594	0.456	0.184	11.05	1.5
C 19	0.376	0.462	0.172	11.05	1.5
C 20	0.333	0.466	0.272	11.05	1.5

The occupancies of C16 – C20 were set to 1.5 to simulate a CH_3 group.

REFINED COMPOSITION: $|K_2Ca_6Sr_2(H_2O)_{30}|\ [Si_{18.45}Al_{17.55}O_{72}]$
Bellberg Volcano, Eifel, Germany

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.244$ Å $b = 13.244$ Å $c = 15.988$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.122$

REFERENCE: B. Rüdinger, E. Tillmanns and G. Hentschel, *Mineralogy and Petrology* **48** 147–152 (1993).

Atom	x	y	z	B_{iso}	occ
K	0.105	0.210	0.25	5.0	0.3333
Ca 1	0.0	0.0	0.0	0.5	1.0
Ca 2	0.33333	0.66667	0.130	6.9	1.0
Sr	0.33333	0.66667	0.9119	2.4	0.5
Si 1	0.4215	0.3313	0.1538	1.09	0.5125
Si 2	0.2476	0.0	0.0	0.36	0.5125
Al 1	0.4215	0.3313	0.1538	1.09	0.4875
Al 2	0.2476	0.0	0.0	0.36	0.4875
O 1	0.1127	0.225	0.003	0.5	1.0
O 2	0.6818	0.000	0.9158	1.2	1.0
O 3	0.958	0.327	0.25	2.1	1.0
O 4	0.2295	0.459	0.864	1.6	1.0
O 5	0.4590	0.918	0.862	1.8	1.0
H_2O 1	0.33333	0.66667	0.75	5.0	1.0
H_2O 2	0.413	0.826	0.25	3.5	1.0
H_2O 3	0.587	0.174	0.965	3.0	0.5
H_2O 4	0.218	0.436	0.159	3.6	1.0
H_2O 5	0.0	0.0	0.643	1.4	1.0

EAB (Na, Tetramethylammonium)-E

REFINED COMPOSITION: $|(H_2O)_{39.5}|\ [Si_{26.6}Al_{9.4}O_{72}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.28$ Å $b = 13.28$ Å $c = 15.21$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R = 0.19$

REFERENCE: W. M. Meier and M. Groner,
J. Solid State Chem. **37** 204–218 (1981).

Atom	x	y	z	B_{iso}	occ
Si 1	0.233	0.0	0.0	0.9	0.739
Si 2	0.425	0.093	0.146	2.4	0.739
Al 1	0.233	0.0	0.0	0.9	0.261
Al 2	0.425	0.093	0.146	2.4	0.261
O 1	0.309	-0.003	0.088	0.8	1.0
O 2	0.212	0.106	0.006	0.5	1.0
O 3	0.478	0.239	0.117	3.2	1.0
O 4	0.399	0.081	0.25	2.6	1.0
O 5	0.536	0.072	0.106	2.0	1.0
H_2O 1	0.6667	0.3333	-0.003	5.0	0.87
H_2O 2	0.461	-0.078	0.25	2.0	0.5
H_2O 3	0.454	0.227	-0.122	5.0	0.91
H_2O 4	0.0	0.0	-0.184	0.6	1.19
H_2O 5	0.068	0.136	0.75	0.9	0.7
H_2O 6	0.35	0.175	0.75	5.0	1.21
H_2O 7	0.708	0.354	-0.073	2.1	0.49

REFINED COMPOSITION: $|Ba_{1.95}(H_2O)_7|\ [Si_6Al_4O_{20}]$
Bathurst, New Brunswick, Canada

CRYSTAL DATA: $P2_12_12$ (No. 18)
$a = 9.537$ Å $b = 9.651$ Å $c = 6.509$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{wp} = 0.070$, $R_{F^2} = 0.055$

REFERENCE: Å. Kvick and J. V. Smith,
J. Chem. Phys. **79** 2356–2362 (1983).

Atom	x	y	z	B_{iso}	occ
Ba	0.5	0.0	0.63117	1.24	0.974
Si 1	0.0	0.0	0.01365	0.55	1.0
Si 2	-0.17568	0.09407	0.38762	0.57	1.0
Al	0.09245	0.17139	0.62657	0.42	1.0
O 1	0.17414	0.33126	0.63273	0.68	1.0
O 2	-0.05301	0.19639	0.46728	0.67	1.0
O 3	0.19836	0.03763	0.53741	0.78	1.0
O 4	0.03649	0.13362	0.87695	1.16	1.0
O 5	-0.13505	0.03586	0.15743	1.03	1.0
H 1	0.13081	0.26044	0.05620	3.03	0.844
H 2	0.23738	0.36941	0.06351	6.97	0.844
O 6	0.17627	0.32248	0.14994	1.73	0.844
H 3	0.30048	0.08839	0.04942	6.68	0.909
H 4	0.41511	0.20440	0.03767	4.22	0.909
O 7	0.37851	0.12200	-0.02375	3.2	0.909

EMT EMC-2, Calcined

REFINED COMPOSITION: $|Na_{8.3}(H_2O)_6|\ [Si_{76.03}Al_{19.97}O_{192}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 17.3864$ Å $b = 17.3864$ Å $c = 28.3459$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.181$, $R_{wp} = 0.206$, $R_F = 0.074$

REFERENCE: Ch. Baerlocher, L. B. McCusker and R. Chiappetta, *Microporous Materials* **2** 269–280 (1994).

Atom	x	y	z	B_{iso}	occ
Na 2	0.589	0.177	0.047	2.527	0.25
Na 3	0.66667	0.33333	0.627	2.527	0.325
Na 4	0.3571	0.179	0.388	2.527	0.333
Si 1	0.3734	0.0962	0.0167	0.869	0.792
Si 2	0.4275	0.034	0.1069	0.869	0.792
Si 3	0.4874	0.1546	-0.0730	0.869	0.792
Si 4	0.4867	0.1521	0.1961	0.869	0.792
Al 1	0.3734	0.0962	0.0167	0.869	0.208
Al 2	0.4275	0.034	0.1069	0.869	0.208
Al 3	0.4874	0.1546	-0.0730	0.869	0.208
Al 4	0.4867	0.1521	0.1961	0.869	0.208
O 1	0.457	0.130	-0.0187	1.5	1.0
O 2	0.292	0.0	0.0	1.5	1.0
O 3	0.340	0.170	0.018	1.5	1.0
O 4	0.403	0.093	0.0713	1.5	1.0
O 5	0.425	0.069	0.1601	1.5	1.0
O 6	0.356	-0.072	0.1103	1.5	1.0
O 7	0.528	0.056	0.094	1.5	1.0
O 8	0.478	0.239	-0.092	1.5	1.0
O 9	0.594	0.188	-0.074	1.5	1.0
O 10	0.472	0.236	0.181	1.5	1.0
O 11	0.591	0.1818	0.187	1.5	1.0
O 12	0.453	0.117	0.25	1.5	1.0
H_2O	0.709	0.291	0.080	2.527	0.5

REFINED COMPOSITION: $|Na_{20}C_{60}O_{24}(H_2O)_{22.6}|\ [Si_{76.03}Al_{19.97}O_{192}]$

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 17.3741$ Å $b = 17.3741$ Å $c = 28.3646$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.037$, $R_{wp} = 0.186$, $R_F = 0.068$

REFERENCE: Ch. Baerlocher, L. B. McCusker and R. Chiappetta, *Microporous Materials* **2** 269–280 (1994).

Atom	x	y	z	B_{iso}	occ
Si 1	0.370	0.096	0.018	1.34	0.792
Al 1	0.370	0.096	0.018	1.34	0.208
Si 2	0.429	0.037	0.108	1.34	0.792
Al 2	0.429	0.037	0.108	1.34	0.208
Si 3	0.488	0.155	-0.070	1.34	0.792
Al 3	0.488	0.155	-0.070	1.34	0.208
Si 4	0.489	0.154	0.195	1.34	0.792
Al 4	0.489	0.154	0.195	1.34	0.208
O 1	0.459	0.130	-0.015	1.11	1.0
O 2	0.288	0.0	0.0	1.11	1.0
O 3	0.333	0.167	0.015	1.11	1.0
O 4	0.396	0.088	0.073	1.11	1.0
O 5	0.427	0.069	0.162	1.11	1.0
O 6	0.361	-0.071	0.105	1.11	1.0
O 7	0.531	0.063	0.093	1.11	1.0
O 8	0.473	0.236	-0.087	1.11	1.0
O 9	0.594	0.188	-0.075	1.11	1.0
O 10	0.478	0.239	0.179	1.11	1.0
O 11	0.592	0.183	0.186	1.11	1.0
O 12	0.460	0.127	0.25	1.11	1.0
O 13	0.409	0.591	0.25	4.97	1.0
O 14	0.561	0.781	0.205	4.97	0.5
O 15	0.103	0.206	0.094	4.97	0.5
O 16	0.170	0.085	0.137	4.97	0.5
C 1	0.498	0.630	0.235	4.97	0.75
C 2	0.511	0.689	0.192	4.97	0.75
C 3	0.176	0.190	0.149	4.97	1.0
H_2O 1	0.717	0.283	0.073	4.97	0.667
H_2O 2	0.333	-0.333	0.003	4.97	0.65
H_2O 3	0.106	0.007	0.044	4.97	0.5
Na 1	0.333	0.667	0.111	3.0	0.5
Na 2	0.667	0.333	0.156	3.0	0.5
Na 3	0.344	0.172	0.110	3.0	0.5
Na 4	0.0	0.0	0.132	3.0	0.5
Na 5	0.333	0.667	0.25	3.0	1.0
Na 6	-0.404	0.192	0.034	3.0	0.5

EPI Epistilbite

REFINED COMPOSITION: $|Na_{1.04}Ca_{2.56}(H_2O)_{15.75}|\ [Si_{17.76}Al_{6.24}O_{48}]$
Teigarhorn, Iceland

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.08$ Å $b = 17.74$ Å $c = 10.25$ Å
$\alpha = 90°$ $\beta = 124.54°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.16$

REFERENCE: A. J. Perrotta,
Mineral. Mag. **36** 480–490 (1967).

Atom	x	y	z	B_{iso}	occ
Na	0.760	0.0	0.251	2.6	0.26
Ca	0.760	0.0	0.251	2.6	0.64
Si 1	0.001	0.088	0.161	0.6	0.74
Si 2	0.293	0.208	0.390	0.8	0.74
Si 3	0.707	0.197	0.097	1.1	0.74
Al 1	0.001	0.088	0.161	0.6	0.26
Al 2	0.293	0.208	0.390	0.8	0.26
Al 3	0.707	0.197	0.097	1.1	0.26
O 1	0.021	0.0	0.215	0.8	1.0
O 2	0.0	0.100	0.0	2.0	1.0
O 3	0.812	0.117	0.132	1.7	1.0
O 4	0.170	0.134	0.309	1.5	1.0
O 5	0.5	0.180	0.0	3.1	1.0
O 6	0.5	0.179	0.5	1.1	1.0
O 7	0.75	0.25	0.0	4.6	1.0
O 8	0.773	0.233	0.261	4.7	1.0
O 9	0.25	0.25	0.5	4.6	1.0
H_2O 1	0.724	0.0	0.502	4.9	0.875
H_2O 2	0.0	0.078	0.5	4.9	0.875
H_2O 3	0.559	0.082	0.281	4.0	0.875
H_2O 4	0.5	0.0	0.0	3.3	0.875

REFINED COMPOSITION: $|K_2Na_{1.86}Ca_{1.3}Mg_{0.7}(H_2O)_{6.12}|\ [Si_{27}Al_9O_{72}]$
Wenatchee, Washington, U.S.A.

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.27$ Å $b = 13.27$ Å $c = 15.05$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.15$

REFERENCE: J. A. Gard and J. M. Tait,
in *Proceedings of the Third International Conference on Molecular Sieves; Recent Progress Reports, Zurich*,
Ed. by J. B. Uytterhoeven (Leuven University Press) 94–99 (1973).

Atom	x	y	z	B_{iso}	occ
Na 1	0.3333	0.6667	0.14	3.0	0.30
Na 2	0.5	0.0	0.0	3.1	0.11
K	0.0	0.0	0.25	1.98	1.0
Mg	0.66667	0.33333	0.2030	3.0	0.175
Ca 1	0.3333	0.6667	0.14	3.0	0.07
Ca 2	0.5	0.0	0.0	3.1	0.04
Ca 3	0.66667	0.33333	0.0730	3.6	0.195
Si 1	0.00021	0.23350	0.10446	0.90	0.75
Si 2	0.0935	0.4245	0.2500	1.10	0.75
Al 1	0.00021	0.23350	0.10446	0.90	0.25
Al 2	0.0935	0.4245	0.2500	1.10	0.25
O 1	0.0267	0.3493	0.1610	2.42	1.0
O 2	0.0979	0.1957	0.1264	1.65	1.0
O 3	0.1258	0.2516	0.6339	1.90	1.0
O 4	0.2638	0.0	0.0	2.45	1.0
O 5	0.2293	0.4585	0.25	2.1	1.0
O 6	0.4603	0.9206	0.25	2.8	1.0
H_2O 1	0.4890	0.2450	0.25	4.6	0.34
H_2O 2	0.2490	0.4970	0.0160	1.9	0.11
H_2O 3	0.8950	0.4480	0.0950	4.2	0.23

REFINED COMPOSITION: $|C_{24}O_{4.14}|\ [Al_{18}P_{18}O_{72}]$

CRYSTAL DATA: $P6_3/m$ (No. 176)
$a = 13.2371$ Å $b = 13.2371$ Å $c = 14.7708$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.081$

REFERENCE: J. J. Pluth, J. V. Smith and J. M. Bennett,
Acta Cryst. **C42** 283–286 (1986).

Atom	x	y	z	B_{iso}	occ
Al 1	0.7708	0.9983	0.1180	2.76	1.0
Al 2	0.0999	0.4214	0.2500	1.9	1.0
P 1	0.9989	0.2369	0.0938	1.97	1.0
P 2	0.5675	0.9079	0.2500	1.42	1.0
O 1	0.0365	0.3435	0.1529	3.0	1.0
O 11	0.6373	0.9669	0.1649	2.13	1.0
O 2	0.0826	0.1910	0.1053	3.16	1.0
O 3	0.1432	0.2640	0.6244	3.16	1.0
O 4	0.2773	0.0030	0.9970	3.32	1.0
O 5	0.2468	0.4693	0.2500	2.6	1.0
O 6	0.4584	0.9171	0.2500	2.05	1.0
O 7	0.1721	0.1876	0.2500	3.47	0.69
C 1	0.3770	0.7930	0.9599	33.1	1.0
C 2	0.4590	0.7490	0.9920	33.1	1.0

REFINED COMPOSITION: $[Si_{48}O_{96}]$

CRYSTAL DATA: *Pnma* (No. 62)
$a = 9.7998$ Å $b = 12.4116$ Å $c = 22.8606$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.056$, $R_{wp} = 0.0611$

REFERENCE: R. Millini, G. Perego, L. Carluccio, G. Bellussi, D. E. Cox, B. J. Campbell and A. K. Cheetham, in *Proc. of the 12th International Zeolite Conference*, Ed. by M. M. J. Treacy, B. K. Marcus, J. B. Higgins and M. E. Bisher (Materials Research Society: Warrendale) vol. **I** 541–548 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.3402	0.8726	0.8634	1.97	1.0
Si 2	0.6431	0.8742	0.5312	1.97	1.0
Si 3	0.885	0.5148	0.9184	1.82	1.0
Si 4	0.1522	0.8753	0.6532	2.13	1.0
Si 5	0.9631	0.1242	0.809	1.34	1.0
Si 6	0.2262	0.4812	0.7616	1.5	1.0
O 1	0.3061	0.75	0.8436	2.92	1.0
O 2	0.2695	0.8974	0.9252	3.16	1.0
O 3	0.4999	0.8899	0.8714	3.32	1.0
O 4	0.2792	0.953	0.8154	6.08	1.0
O 5	0.639	0.75	0.5129	2.84	1.0
O 6	0.6641	0.9451	0.473	2.84	1.0
O 7	0.5035	0.902	0.5622	3.4	1.0
O 8	0.9441	0.4377	0.8693	4.26	1.0
O 9	0.7618	0.5839	0.8935	3.47	1.0
O 10	0.1818	0.75	0.669	4.97	1.0
O 11	0.1698	0.5614	0.7136	6.63	1.0
O 12	0.9527	0.25	0.8208	3.16	1.0
O 13	0.3481	0.4091	0.7358	3.87	1.0
O 14	0.1074	0.4034	0.7828	4.82	1.0

EUO EU-1, Calcined, Rehydrated

REFINED COMPOSITION: $|O_{36.16}|$ $[Si_{112}O_{224}]$

CRYSTAL DATA: *Cmme* (No. 67)
$a = 13.695$ Å $b = 22.326$ Å $c = 20.178$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld limited refinement. No R-factor reported.

REFERENCE: N. A. Briscoe, D. W. Johnson, M. D. Shannon, G. T. Kokotailo and L. B. McCusker, *Zeolites* **8** 74–76 (1988).

Atom	x	y	z	B_{iso}	occ
Si 1	0.115	0.2500	0.123	1.184	1.0
Si 2	0.187	0.3703	0.0630	1.184	1.0
Si 3	0.289	0.4315	0.185	1.184	1.0
Si 4	0.0000	0.448	0.053	1.184	1.0
Si 5	0.0000	0.528	0.181	1.184	1.0
Si 6	0.117	0.2500	0.277	1.184	1.0
Si 7	0.191	0.3739	0.308	1.184	1.0
Si 8	0.287	0.4302	0.431	1.184	1.0
Si 9	0.0000	0.450	0.308	1.184	1.0
Si 10	0.0000	0.534	0.432	1.184	1.0
O 1	0.0000	0.2500	0.113	2.369	1.0
O 2	0.158	0.3068	0.089	2.369	1.0
O 3	0.139	0.2500	0.199	2.369	1.0
O 4	0.2500	0.363	0.0000	2.369	1.0
O 5	0.245	0.405	0.118	2.369	1.0
O 6	0.094	0.407	0.044	2.369	1.0
O 7	0.2500	0.5000	0.196	2.369	1.0
O 8	0.405	0.431	0.176	2.369	1.0
O 9	0.260	0.389	0.246	2.369	1.0
O 10	0.0000	0.5000	0.0000	2.369	1.0
O 11	0.0000	0.477	0.126	2.369	1.0
O 12	0.0000	0.497	0.251	2.369	1.0
O 13	0.0000	0.2500	0.289	2.369	1.0
O 14	0.164	0.3065	0.309	2.369	1.0
O 15	0.094	0.409	0.303	2.369	1.0
O 16	0.244	0.391	0.374	2.369	1.0
O 17	0.2500	0.5000	0.424	2.369	1.0
O 18	0.2500	0.403	0.5000	2.369	1.0
O 19	0.404	0.425	0.427	2.369	1.0
O 20	0.0000	0.485	0.376	2.369	1.0
O 21	0.0000	0.5000	0.5000	2.369	1.0
O 51	0.2500	0.2000	0.5000	3.948	1.01
O 52	0.4000	0.2500	0.3820	3.948	1.27
O 53	0.5000	0.1250	0.067	3.948	0.53
O 54	0.5000	0.1860	0.2980	3.948	0.68
O 55	0.5000	0.2020	0.1760	3.948	0.63
O 56	0.0000	0.1830	0.4500	3.948	0.4

Extra-framework atoms O51–O56 were refined with oxygen scattering factors.
In editions of the *International Tables For Crystallography*
published after 1995, space group symbol *Cmme* replaces *Cmma*.

Faujasite FAU

REFINED COMPOSITION: $|Na_{16}Ca_{16}(H_2O)_{42.7}|\ [Si_{134.4}Al_{57.6}O_{384}]$
Kaiserstuhl, Germany

CRYSTAL DATA: $Fd\overline{3}m$ (No. 227) origin at centre ($\overline{3}m$)
$a = 24.74$ Å $b = 24.74$ Å $c = 24.74$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.13$

REFERENCE: W. H. Baur,
American Mineralogist **49** 697–704 (1964).

Atom	x	y	z	B_{iso}	occ
Na	0.0699	0.0699	0.0699	2.6	0.5
Ca	0.0699	0.0699	0.0699	2.6	0.5
Si	0.12544	0.94655	0.03626	1.2	0.7
Al	0.12544	0.94655	0.03626	1.2	0.3
O 1	0.1742	0.1742	0.9680	2.8	1.0
O 2	0.1773	0.1773	0.3232	2.5	1.0
O 3	0.2527	0.2527	0.1435	2.5	1.0
O 4	0.1053	0.8947	0.0	2.8	1.0
H_2O 1	0.1673	0.1673	0.1673	3.2	1.0
H_2O 2	0.272	0.272	0.272	3.9	0.333

FAU Na-X, Dehydrated

REFINED COMPOSITION: $|Na_{92.9}|\ [Si_{103.68}Al_{88.32}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 25.099$ Å $b = 25.099$ Å $c = 25.099$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.046$

REFERENCE: D. H. Olson,
Zeolites **15** 439–443 (1995).

Atom	x	y	z	B_{iso}	occ
Na 1	0.0	0.0	0.0	3.18	0.18
Na 2	0.0454	0.0454	0.0454	0.87	0.66
Na 3	0.056	0.056	0.056	1.26	0.25
Na 4	0.2292	0.2292	0.2292	2.53	0.97
Na 5	0.423	0.326	0.158	2.32	0.11
Na 6	0.432	0.280	0.164	1.68	0.11
Na 61	0.465	0.317	0.158	1.68	0.09
Si 1	-0.05381	0.12565	0.03508	1.41	1.0
Si 2	-0.05524	0.03639	0.12418	1.46	0.08
Al	-0.05524	0.03639	0.12418	1.46	0.92
O 1	-0.1099	0.0003	0.1056	2.47	1.0
O 2	-0.0011	-0.0028	0.1416	2.45	1.0
O 3	-0.0346	0.0758	0.0711	2.61	1.0
O 4	-0.0693	0.0726	0.1800	2.37	1.0

REFINED COMPOSITION: $|Na_{40.32}(H_2O)_{171.84}|\ [Si_{103.68}Al_{88.32}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 25.028$ Å $b = 25.028$ Å $c = 25.028$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.09$

REFERENCE: D. H. Olson,
J. Phys. Chem. **74** 2758–2764 (1970).

Atom	x	y	z	B_{iso}	occ
Na 1	0.0	0.0	0.0	2.53	0.54
Na 2	0.060	0.060	0.060	0.5	0.24
Na 3	0.230	0.230	0.230	0.5	0.39
Na 4	0.238	0.238	0.238	0.5	0.36
Si 1	-0.05291	0.12457	0.03509	1.16	1.0
Si 2	-0.05352	0.03671	0.12309	1.04	0.08
Al	-0.05352	0.03671	0.12309	1.04	0.92
O 1	-0.1099	0.0002	0.1054	2.2	1.0
O 2	-0.0025	-0.0041	0.1445	1.76	1.0
O 3	-0.0321	0.0730	0.0680	2.18	1.0
O 4	-0.0706	0.0772	0.1761	2.11	1.0
H_2O 1	0.074	0.074	0.074	0.61	0.36
H_2O 2	0.093	0.086	0.176	1.66	0.27
H_2O 3	0.245	0.245	0.245	0.87	0.24
H_2O 4	0.281	0.298	0.275	0.95	0.13
H_2O 5	0.353	0.345	0.186	3.58	0.31
H_2O 6	0.239	0.240	0.392	3.58	0.29
H_2O 7	0.174	0.204	0.422	1.55	0.18
H_2O 8	0.212	0.387	0.288	2.82	0.17
H_2O 9	0.312	0.381	0.200	1.92	0.10
H_2O 10	0.258	0.412	0.204	2.42	0.14

FAU Ultrastable Y, Dehydrated Dealuminated

REFINED COMPOSITION: $|Al_{5.6}O_{22.4}|\ [Si_{175.7}Al_{16.3}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}m$ (No. 227) origin at centre ($\overline{3}m$)
$a = 24.188$ Å $b = 24.188$ Å $c = 24.188$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{wp} = 0.1041$, $R_I = 0.0561$

REFERENCE: J. B. Parise, D. R. Corbin, L. Abrams and D. E. Cox, *Acta Cryst.* **C40** 1493–1497 (1984).

Atom	x	y	z	B_{iso}	occ
Si	0.1257	0.9460	0.0359	3.1	0.9153
Al 1	0.1257	0.9460	0.0359	3.1	0.0847
Al 2	0.1250	0.1250	0.1250	3.0	0.7
O 1	0.1076	-0.1076	0.0000	4.5	1.0
O 2	0.2539	0.2539	0.1406	4.5	1.0
O 3	0.1747	0.1747	0.9634	4.5	1.0
O 4	0.1798	0.1798	0.3217	4.5	1.0
O 5	0.085	0.085	0.085	3.0	0.7

Occupancy of Al2 was constrained to equal that of O5 so that the unit cell population of O5 is four times that of Al2.

REFINED COMPOSITION: $[Si_{188.16}O_{384}]$

CRYSTAL DATA: $Fd\bar{3}m$ (No. 227) origin at centre ($\bar{3}m$)
$a = 24.2576$ Å $b = 24.2576$ Å $c = 24.2576$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron Rietveld refinement, $R_{exp} = 0.022$, $R_{wp} = 0.031$

REFERENCE: J. J. Hriljac, M. M. Eddy, A. K. Cheetham, J. A. Donohue and G. J. Ray, *J. Solid State Chem.* **106** 66–72 (1993).

Atom	x	y	z	B_{iso}	occ
Si	-0.05392	0.12530	0.03589	0.37	0.98
O 1	0.0	-0.10623	0.10623	1.16	1.0
O 2	-0.00323	-0.00323	0.14066	1.42	1.0
O 3	0.07570	0.07570	-0.03577	1.33	1.0
O 4	0.07063	0.07063	0.32115	0.74	1.0

REFINED COMPOSITION: $|Li_{87.36}|\ [Si_{96}Al_{96}O_{384}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 25.6957$ Å $b = 25.6957$ Å $c = 25.6957$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray and neutron Rietveld refinement, $R_p = 0.057$, $R_{wp} = 0.069$

REFERENCE: M. Feuerstein and R. F. Lobo,
Chemistry of Materials 2197–2204 (1998).

Atom	x	y	z	B_{iso}	occ
Si	-0.0480	0.1246	0.0376	1.50	1.0
Al	-0.0511	0.0378	0.1224	1.50	1.0
O 1	-0.1045	0.0028	0.0972	2.13	1.0
O 2	0.0001	-0.0007	0.1533	2.13	1.0
O 3	-0.0220	0.0724	0.0702	2.13	1.0
O 4	-0.0742	0.0812	0.1711	2.13	1.0
Li 1	0.0466	0.0466	0.0466	4.58	0.978
Li 2	0.2232	0.2232	0.2232	2.92	1.047
Li 3	0.387	0.401	0.122	7.82	0.235

REFINED COMPOSITION: $|Na_{0.96}Mg_2(H_2O)_{12}|\ [Si_{30.24}Al_{5.76}O_{72}]$
Kamloops Lake, British Columbia, Canada

CRYSTAL DATA: *Immm* (No. 71)
$a = 19.156$ Å $b = 14.127$ Å $c = 7.489$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.11$

REFERENCE: P. A. Vaughan,
Acta Cryst. **21** 983–990 (1966).

Atom	x	y	z	B_{iso}	occ
Na	0.4285	0.0	0.0	3.0	0.24
Mg	0.0	0.0	0.500	3.29	1.0
Si 1	0.1548	0.0	0.0	1.74	0.84
Si 2	0.0841	0.2024	0.0	1.55	0.84
Si 3	0.2727	0.0	0.2905	2.0	0.84
Si 4	0.3232	0.2019	0.2067	2.08	0.84
Al 1	0.1548	0.0	0.0	1.74	0.16
Al 2	0.0841	0.2024	0.0	1.55	0.16
Al 3	0.2727	0.0	0.2905	2.0	0.16
Al 4	0.3232	0.2019	0.2067	2.08	0.16
O 1	0.0	0.2131	0.0	3.84	1.0
O 2	0.2528	0.0	0.5000	3.76	1.0
O 3	0.1025	0.0882	0.0	5.63	1.0
O 4	0.2039	0.0	0.1776	5.21	1.0
O 5	0.2500	0.2500	0.2500	4.5	1.0
O 6	0.1610	0.2833	0.5000	3.82	1.0
O 7	0.1155	0.2497	0.1796	4.42	1.0
O 8	0.3202	0.0907	0.2459	3.79	1.0
H_2O 1	0.0	0.0	0.2389	3.66	1.0
H_2O 2	0.0912	0.0691	0.5000	7.53	0.5
H_2O 3	0.0347	0.1403	0.5000	9.21	0.5

FER Ferrierite, Siliceous

REFINED COMPOSITION: $[Si_{36}O_{72}]$
Dealuminated, synthetic powder.

CRYSTAL DATA: *Pnnm* (No. 58)
$a = 14.07025$ Å $b = 7.41971$ Å $c = 18.7202$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Combined X-ray and neutron Rietveld refinement, $R_{wp} = 0.123$

REFERENCE: R. E. Morris, S. J. Weigel, N. J. Henson, L. M. Bull, M. T. Janicke, B. F. Chmelka and A. K. Cheetham,
J. Amer. Chem. Soc. **116** 11849–11855 (1994).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0	0.0	0.15462	0.95	1.0
Si 2	-0.0012	0.2905	0.27439	1.03	1.0
Si 3	0.19990	0.0037	0.08373	1.26	1.0
Si 4	0.2029	0.2255	0.33150	1.26	1.0
Si 5	0.7950	0.1894	0.68200	0.47	1.0
O 1	0.0	0.5	0.2479	1.97	1.0
O 2	0.0099	0.1788	0.2027	3.00	1.0
O 3	0.0899	0.0016	0.1039	2.29	1.0
O 4	0.7804	-0.0202	0.6560	1.89	1.0
O 5	0.2090	0.0377	0.0	0.87	1.0
O 6	0.2494	0.2851	0.2580	2.45	1.0
O 7	0.2403	0.1829	0.1248	1.66	1.0
O 8	0.7393	0.1675	0.8994	2.92	1.0
O 9	0.0879	0.2462	0.3291	2.21	1.0
O 10	0.9040	0.2477	0.6846	2.21	1.0

Coordinates converted from *Pmnn* (**cab**) setting.

REFINED COMPOSITION: $|Ca_{30.72}S_{22}O_{70}(H_2O)_6|$ $[Si_{30}Al_{30}O_{120}]$
Sacrofano, Latium, Italy

CRYSTAL DATA: $P321$ (No. 150)
$a = 12.916$ Å $b = 12.916$ Å $c = 26.543$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.0596$

REFERENCE: P. Ballirano, E. Bonaccorsi, A. Maras and S. Merlino, *Canadian Mineralogist* **38** 657–668 (2000).

Atom	x	y	z	B_{iso}	occ
Si 1	0.5834	0.6684	0.9018	1.25	1.0
Al 1	0.4190	0.3332	0.0978	1.07	1.0
Al 2	0.5866	0.6658	0.1963	1.50	1.0
Si 2	0.4158	0.3323	0.8038	0.96	1.0
Al 3	0.5927	0.6770	0.6028	0.95	1.0
Si 3	0.4162	0.3365	0.3964	1.10	1.0
Al 4	0.7511	0.7511	0.0000	1.42	1.0
Si 4	0.2472	0.2472	0.0000	1.03	1.0
Si 5	0.7486	0.7495	0.2976	1.03	1.0
Al 5	0.2540	0.2515	0.7026	1.18	1.0
Si 6	0.7485	0.7485	0.5000	1.11	1.0
Al 6	0.2544	0.2544	0.5000	0.95	1.0
O 1	0.4462	0.2180	0.1051	5.13	1.0
O 2	0.8750	0.7478	0.2876	2.21	1.0
O 3	0.2425	0.1159	0.5098	1.97	1.0
O 4	0.3220	0.0005	0.3468	2.21	1.0
O 5	0.6710	0.0020	0.6482	1.97	1.0
O 6	0.6590	0.6760	0.5470	1.74	1.0
O 7	0.3530	0.3302	0.4504	1.74	1.0
O 8	0.6690	0.6500	0.1495	3.87	1.0
O 9	0.3480	0.3510	0.8495	4.74	1.0
O 10	0.4501	0.2340	0.3901	1.74	1.0
O 11	0.6660	0.6860	0.9481	5.68	1.0
O 12	0.3270	0.3070	0.0468	6.63	1.0
O 13	0.4420	0.5490	0.1995	2.76	1.0
O 14	0.5410	0.0786	0.3940	2.05	1.0
O 15	0.6560	0.6730	0.2534	2.13	1.0
O 16	0.3440	0.3200	0.7537	4.18	1.0
O 17	0.8880	0.7821	0.6994	2.37	1.0
O 18	0.4275	0.2200	0.8161	2.92	1.0
O 19	0.9157	0.4540	0.0863	5.13	1.0
O 20	0.1200	0.2330	0.0106	5.84	1.0
S 1	0.3730	0.6760	0.0546	5.05	1.0
S 2	0.3430	0.7060	0.7415	6.16	1.0
S 3	0.0250	0.0230	0.1561	6.32	1.0
S 4	0.3333	0.6667	0.3199	2.31	1.0
S 5	0.3333	0.6667	0.4884	1.90	1.0
H_2O	0.0090	0.0390	0.6040	8.69	1.0
Ca 1	0.6667	0.3333	0.8189	2.92	1.0

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Atom	x	y	z	B_{iso}	occ
Ca 2	0.0000	0.0000	0.4900	15.79	0.50
Ca 3	0.0000	0.0000	0.7218	2.68	0.36
Ca 31	0.0000	0.0000	0.7477	2.68	0.18
Ca 32	0.0000	0.0000	0.7009	2.68	0.22
Ca 4	0.0000	0.0000	0.0318	4.74	0.27
Ca 41	0.0000	0.0000	0.0000	4.74	0.07
Ca 5	0.6667	0.3333	0.3733	2.18	1.0
Ca 6	0.6667	0.3333	0.0635	4.03	0.37
Ca 61	0.6667	0.3333	0.1339	4.03	0.25
Ca 1	0.5030	0.5030	0.0000	3.71	0.42
Ca 11	0.4500	0.5440	0.0150	3.71	0.14
Ca 2	0.7815	0.5649	0.5960	2.28	0.91
Ca 3	0.4909	0.5140	0.3017	3.13	0.66
Ca 4	0.5015	0.5015	0.5000	2.24	0.81
Ca 5	0.8490	0.6967	0.8973	3.24	0.29
Ca 51	0.8060	0.5860	0.9164	3.24	0.12
Ca 52	0.8730	0.7600	0.8870	3.24	0.15
Ca 53	0.8290	0.6500	0.9030	3.24	0.11
Ca 6	0.8340	0.6655	0.2001	2.68	0.33
Ca 61	0.7720	0.5560	0.2169	2.68	0.15
Ca 62	0.8730	0.7260	0.1849	2.68	0.13
Ca 63	0.7950	0.6050	0.2139	2.68	0.12
O 21	0.6170	0.3200	0.9054	9.47	1.0
O 22	0.3750	0.6030	0.0207	12.63	1.0
O 23	0.4880	0.7360	0.0760	12.63	1.0
O 24	0.4010	0.7860	0.7078	7.90	1.0
O 25	0.7300	0.4700	0.2250	5.53	1.0
O 26	0.7280	0.3990	0.2290	9.47	1.0
O 27	0.0460	0.1260	0.1310	6.32	1.0
O 28	0.1130	0.0780	0.1840	14.21	1.0
O 29	0.0450	0.0420	0.1130	10.26	1.0
O 30	0.3333	0.6667	0.2650	7.34	1.0
O 31	0.3960	0.7890	0.3390	4.18	1.0
O 32	0.3333	0.6667	0.5433	4.58	1.0
O 33	0.3970	0.7910	0.4698	3.32	1.0

The Ca cation sites are believed to be mixed with Na and K.
The Ca occupancies are adjusted in order to simulate the effective scattering from the site.

REFINED COMPOSITION: $|Ca_{3.68}(H_2O)_{17.28}|\ [Si_{8.8}Al_{7.2}O_{32}]$
Hohenberg, Buhne, Westfalia

CRYSTAL DATA: $P11\,2_1/a$ (No. 14) unique axis **c**, cell choice 1
$a = 9.843$ Å $b = 10.023$ Å $c = 10.616$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 92.417°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: K. F. Fischer and V. Schramm,
In *Molecular Sieve Zeolites - I* (*ACS Adv. Chem. Ser. No. 101*),
Ed. by E. M. Flanigen and L. B. Sand
(American Chemical Society: Washington, DC) 250–258 (1971).

Atom	x	y	z	B_{iso}	occ
Ca	0.3537	0.7192	0.0764	1.39	0.92
Si 1	0.18142	0.4147	0.11288	0.55	1.0
Si 2	0.16038	0.9082	0.87012	0.48	1.0
Si 3	0.16921	0.09656	0.11329	0.32	0.2
Al 1	0.16921	0.09656	0.11329	0.32	0.8
Al 2	0.149	0.59053	0.8669	0.52	1.0
O 1	0.9996	0.0787	0.1562	1.74	1.0
O 2	0.2125	0.2624	0.0763	1.85	1.0
O 3	0.0254	0.4361	0.1485	0.99	1.0
O 4	0.3037	0.245	0.4027	1.48	1.0
O 5	0.2136	0.9994	0.9861	0.85	1.0
O 6	0.2595	0.0449	0.2437	0.82	1.0
O 7	0.2777	0.4645	0.2288	0.91	1.0
O 8	0.2253	0.5107	0.9944	1.21	1.0
H_2O 1	0.5023	0.2596	0.1048	2.22	0.88
H_2O 2	0.5410	0.5914	0.1262	3.62	1.0
H_2O 3	0.5020	0.9113	0.1174	2.13	0.95
H_2O 4	0.2306	0.7732	0.2369	7.72	0.61
H_2O 5	0.4028	0.7407	0.3180	4.11	0.48
H_2O 6	0.1326	0.7620	0.1794	17.25	0.4

REFINED COMPOSITION: $|Na_{3.6}K_{3.76}(H_2O)_{9.86}|\ [Si_8Al_8O_{32}]$
Hoewenneg, Hegau, Germany

CRYSTAL DATA: $I121$ (No. 5) unique axis **b**, cell choice 3
$a = 10.226$ Å $b = 10.422$ Å $c = 9.884$ Å
$\alpha = 90°$ $\beta = 88.315°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.033$

REFERENCE: A. Alberti and G. Vezzalini,
Acta Cryst. **B35** 2866–2869 (1979).

Atom	x	y	z	B_{iso}	occ
Na	0.4312	0.2559	0.6716	2.53	0.9
K	0.3071	-0.0040	0.9692	2.09	0.94
Si 1	0.1523	-0.0133	0.3261	0.46	1.0
Si 2	0.1534	0.2615	0.8263	0.40	1.0
Al 1	0.1546	0.2491	0.1546	0.43	1.0
Al 2	0.1582	0.0027	0.6512	0.44	1.0
O 1	0.0010	-0.0471	0.3037	1.21	1.0
O 2	-0.0030	0.2956	0.2047	1.14	1.0
O 3	0.2031	0.1401	0.7354	0.96	1.0
O 4	0.1810	0.0304	0.4785	1.18	1.0
O 5	0.1712	0.2264	0.9833	1.13	1.0
O 6	0.1989	0.1018	0.2263	1.00	1.0
O 7	0.2620	0.3610	0.2184	1.09	1.0
O 8	0.7558	0.3812	0.2177	0.73	1.0
H_2O 1	0.3435	0.2507	0.4539	2.65	0.85
H_2O 2	0.4779	0.0682	0.2179	2.76	0.85
H_2O 3	0.0	0.3191	0.5	2.70	1.0
H_2O 4	0.5	0.4729	0.5	2.35	0.53

REFINED COMPOSITION: $|Na_{0.8}Ca_{2.82}(H_2O)_{12.08}|\ [Si_{10.4}Al_{5.6}O_{32}]$
Goble, Oregon, U.S.A.

CRYSTAL DATA: $I\bar{4}m2$ (No. 119)
$a = 9.9266$ Å $b = 9.9266$ Å $c = 10.3031$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.047$, $R_{wp} = 0.127$, $R_{F^2} = 0.111$

REFERENCE: G. Artioli,
American Mineralogist **77** 189–196 (1992).

Atom	x	y	z	B_{iso}	occ
Na	0.0	0.281	0.223	6.32	0.10
Ca 1	0.0	0.352	0.094	8.69	0.197
Ca 2	0.0	0.238	0.107	8.69	0.155
Si 1	0.1607	0.1607	0.5	3.08	0.65
Si 2	0.3421	0.1579	0.25	4.03	0.65
Al 1	0.1607	0.1607	0.5	3.08	0.35
Al 2	0.3421	0.1579	0.25	4.03	0.35
O 11	0.1746	0.0	0.5351	2.68	1.0
O 12	0.3078	0.0	0.2192	2.53	1.0
O 2	0.2922	0.2488	0.1244	6.71	1.0
H_2O 1	0.0	0.0	0.159	9.24	1.0
H_2O 21	0.105	0.395	0.25	2.05	0.14
H_2O 22	0.161	0.433	0.234	2.05	0.24
H_2O 3	0.0	0.173	0.981	16.58	0.39

REFINED COMPOSITION: $|Na_{2.6}K_{1.7}(H_2O)_{14.9}|\ [Si_{10}Al_6O_{32}]$
Antrim District, Northern Ireland

CRYSTAL DATA: $Pmn2_1$ (No. 31)
$a = 10.108$ Å $b = 9.766$ Å $c = 10.171$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.136$, $R_F = 0.126$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
Z. Kristallogr. **171** 281–289 (1985).

Atom	x	y	z	B_{iso}	occ
Na	0.247	0.228	0.284	9.16	0.65
K	0.500	-0.071	0.615	9.16	0.85
Si 1	0.156	0.432	-0.191	2.05	0.625
Si 2	0.154	0.110	-0.242	2.05	0.625
Si 3	0.345	0.073	0.000	2.05	0.625
Si 4	0.348	0.389	0.048	2.05	0.625
Al 1	0.156	0.432	-0.191	2.05	0.375
Al 2	0.154	0.110	-0.242	2.05	0.375
Al 3	0.345	0.073	0.000	2.05	0.375
Al 4	0.348	0.389	0.048	2.05	0.375
O 1	0.186	0.275	-0.241	1.82	1.0
O 2	0.000	0.441	-0.162	1.82	1.0
O 3	0.200	0.538	-0.309	1.82	1.0
O 4	0.254	0.459	-0.061	1.82	1.0
O 5	0.000	0.074	-0.197	1.82	1.0
O 6	0.198	0.048	-0.394	1.82	1.0
O 7	0.254	0.046	-0.138	1.82	1.0
O 8	0.312	0.226	0.059	1.82	1.0
O 9	0.500	0.073	-0.026	1.82	1.0
O 10	0.500	0.414	0.009	1.82	1.0
H_2O 1	0.500	0.243	0.321	9.16	1.1
H_2O 2	0.000	0.395	0.146	9.16	1.45
H_2O 3	0.000	0.314	0.306	9.16	0.9
H_2O 4	0.341	0.271	0.559	9.16	1.275
H_2O 5	0.500	0.338	0.600	9.16	1.45

REFINED COMPOSITION: $|(C_6H_{16}N)_2|\ [Al_8P_8O_{32}]$

CRYSTAL DATA: $I11\,2/b$ (No. 15) unique axis **c**, cell choice 3
$a = 10.2192$ Å $b = 10.2198$ Å $c = 10.0126$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90.987°$
X-ray single crystal refinement, $R_w = 0.049$

REFERENCE: J. J. Pluth, J. V. Smith and J. M. Bennett,
J. Am. Chem. Soc. **111** 1692–1698 (1989).

Atom	x	y	z	B_{iso}	occ
Al	0.14938	0.10057	0.12505	1.76	1.0
P	0.34269	0.09267	0.37490	1.72	1.0
O 1	0.1756	0.2667	0.0794	3.36	1.0
O 2	0.4833	0.0742	0.3297	3.37	1.0
O 3	0.2514	0.0604	0.2608	4.07	1.0
O 4	0.3101	0.0016	0.4896	4.07	1.0
N 1	0.001	-0.018	0.434	1.11	0.125
H 1	-0.077	-0.007	0.384	1.11	0.125
H 2	0.075	-0.001	0.378	1.11	0.125
C 1	0.009	-0.391	0.418	1.11	0.125
H 3	0.007	-0.451	0.345	1.11	0.125
H 4	-0.065	-0.408	0.474	1.11	0.125
H 5	0.087	-0.402	0.469	1.11	0.125
C 2	0.04	-0.250	0.366	1.03	0.125
H 6	0.078	-0.233	0.310	1.03	0.125
H 7	-0.074	-0.239	0.366	1.03	0.125
C 3	0.006	-0.154	0.484	3.24	0.125
H 8	0.084	-0.165	0.534	3.24	0.125
H 9	-0.068	-0.170	0.540	3.24	0.125
C 4	0.004	0.075	0.547	11.05	0.125
H 10	-0.070	0.058	0.603	11.05	0.125
H 11	0.082	0.063	0.597	11.05	0.125
C 5	-0.001	0.216	0.495	3.24	0.125
H 12	0.073	0.233	0.439	3.24	0.125
H 13	-0.079	0.227	0.445	3.24	0.125
C 6	0.001	0.312	0.613	10.26	0.125
H 14	-0.002	0.400	0.581	10.26	0.125
H 15	0.079	0.301	0.663	10.26	0.125
H 16	-0.073	0.295	0.669	10.26	0.125
N 2	0.232	0.754	0.319	11.05	0.125
H 17	0.246	0.679	0.373	11.05	0.125
H 18	0.247	0.831	0.370	11.05	0.125
C 7	-0.141	0.765	0.332	11.05	0.125
H 19	-0.200	0.771	0.405	11.05	0.125
H 20	-0.160	0.689	0.282	11.05	0.125
H 21	-0.150	0.840	0.277	11.05	0.125
C 8	0.000	0.760	0.386	12.63	0.125
H 22	0.009	0.685	0.441	12.63	0.125
H 23	0.019	0.837	0.436	12.63	0.125
C 9	0.097	0.752	0.268	3.08	0.125

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Atom	x	y	z	B_{iso}	occ
H 24	0.085	0.824	0.210	3.08	0.125
H 25	0.081	0.672	0.220	3.08	0.125
C 10	0.325	0.754	0.205	11.05	0.125
H 26	0.307	0.679	0.150	11.05	0.125
H 27	0.315	0.831	0.154	11.05	0.125
C 11	0.466	0.748	0.258	3.08	0.125
H 28	0.482	0.819	0.317	3.08	0.125
H 29	0.478	0.668	0.304	3.08	0.125
C 12	0.563	0.756	0.140	12.63	0.125
H 30	0.650	0.753	0.173	12.63	0.125
H 31	0.551	0.836	0.094	12.63	0.125
H 32	0.547	0.685	0.081	12.63	0.125

The x-coordinate for C2 has been changed from 0.004 to 0.04. Otherwise, C2 is too close to (0 -1/4 z).

REFINED COMPOSITION: $|Na_{5.92}(H_2O)_{11.28}|\ [Si_{9.92}Al_{6.08}O_{32}]$

CRYSTAL DATA: $I\bar{4}$ (No. 82)
$a = 10.043$ Å $b = 10.043$ Å $c = 10.043$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray twinned crystal refinement, $R = 0.05$

REFERENCE: Ch. Baerlocher and W. M. Meier,
Z. Kristallogr. **135** 339–354 (1972).

Atom	x	y	z	B_{iso}	occ
Na 4	0.0140	0.1895	0.4940	4.4	0.32
Na 5	0.3590	0.0825	0.2210	4.0	0.42
Si 1	0.1438	0.1692	-0.0181	1.1	0.62
Si 2	0.1683	0.3579	0.2329	0.9	0.62
Al 1	0.1438	0.1692	-0.0181	1.1	0.38
Al 2	0.1683	0.3579	0.2329	0.9	0.38
O 1	0.1890	0.0215	0.0410	0.5	1.0
O 2	0.1885	0.2895	0.0880	1.3	1.0
O 3	0.0090	0.3460	0.2985	2.5	1.0
O 4	0.2830	0.2845	0.3300	2.8	1.0
H_2O 1	0.0	0.0	0.3250	5.9	0.42
H_2O 2	0.2195	0.0240	0.3515	2.6	0.70
H_2O 3	0.2930	0.0020	0.3520	4.0	0.50

REFINED COMPOSITION: $|Ca_4(H_2O)_{26.4}|\ [Si_{16}Al_8O_{48}]$
Nova Scotia, Canada

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 13.75$ Å $b = 13.75$ Å $c = 10.05$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.17$

REFERENCE: K. Fischer,
Neues Jahrbuch für Mineralogie Monatshefte **1** 1–13 (1966).

Atom	x	y	z	B_{iso}	occ
Ca	0.3333	0.6667	0.073	6.0	1.0
Si	0.441	0.106	0.093	0.9	0.6667
Al	0.441	0.106	0.093	0.9	0.3333
O 1	-0.202	-0.404	0.063	2.0	1.0
O 2	0.575	0.150	0.064	2.3	1.0
O 3	0.411	0.067	0.250	2.3	1.0
O 4	0.354	0.0	0.0	2.3	1.0
H_2O 1	0.20	0.54	0.2500	3.5	0.25
H_2O 2	0.22	0.44	0.99	9.0	0.5
H_2O 3	0.43	0.86	0.97	9.0	0.5
H_2O 4	0.17	0.34	0.2500	5.0	0.5
H_2O 5	0.08	0.16	0.89	4.0	0.5
H_2O 6	0.10	0.20	0.06	6.5	0.2

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: $C222$ (No. 21)
$a = 16.4206$ Å $b = 20.0540$ Å $c = 5.0464$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray powder diffraction.

REFERENCE: J. Plevert, Y. Kubota, T. Honda, T. Okubo and Y. Sugi, *J. Chem. Soc., Chem. Commun.* 2363–2364 (2000).

Atom	x	y	z	B_{iso}	occ
Si 1	0.3074	0.1879	0.478	1.97	1.0
Si 2	0.1818	0.0767	0.527	1.97	1.0
Si 3	0.0937	0.1222	0.016	1.97	1.0
Si 4	0.0964	0.2819	-0.002	1.97	1.0
O 1	0.3549	0.1874	0.754	2.37	1.0
O 2	0.384	0.2092	0.307	2.37	1.0
O 3	0.25	0.25	0.522	2.37	1.0
O 4	0.2644	0.1170	0.477	2.37	1.0
O 5	0.1537	0.0785	0.834	2.37	1.0
O 6	0.212	0.0	0.5	2.37	1.0
O 7	0.1151	0.1023	0.317	2.37	1.0
O 8	0.0	0.1006	0.0	2.37	1.0
O 9	0.1021	0.2021	-0.013	2.37	1.0
O 10	0.0	0.297	0.0	2.37	1.0

REFINED COMPOSITION: $|Ca_2(H_2O)_{10}|\ [Si_{12}Al_4O_{32}]$
Loudon County, Virginia, U.S.A.

CRYSTAL DATA: $P12_11$ (No. 4) unique axis **b**
$a = 7.401$ Å $b = 17.439$ Å $c = 7.293$ Å
$\alpha = 90°$ $\beta = 105.44°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.049$

REFERENCE: R. C. Rouse and D. R. Peacor,
American Mineralogist **71** 1494–1501 (1986).

Atom	x	y	z	B_{iso}	occ
Ca	0.6557	0.2721	0.1969	1.78	1.0
Si 1	0.3374	0.4732	0.6282	1.18	1.0
Si 2	0.3168	0.1294	0.5997	1.12	1.0
Si 3	0.0219	0.2599	0.5249	1.03	1.0
Si 4	0.1044	0.0578	0.8612	1.08	1.0
Si 5	0.0892	0.3877	0.8325	1.07	1.0
Si 6	0.2394	0.0045	0.2768	1.06	1.0
Al 1	0.7482	0.1285	0.5887	1.0	1.0
Al 2	0.0682	0.3982	0.2632	1.02	1.0
O 1	0.7228	0.0612	0.4105	2.0	1.0
O 2	0.5336	0.1478	0.6346	1.87	1.0
O 3	0.8372	0.2097	0.5064	1.33	1.0
O 4	0.9065	0.1001	0.7936	1.78	1.0
O 5	0.2607	0.4392	0.8023	1.77	1.0
O 6	0.2666	0.4226	0.4408	1.51	1.0
O 7	0.5594	0.4662	0.7062	2.12	1.0
O 8	0.2017	0.2065	0.5155	1.6	1.0
O 9	0.2657	0.1069	0.7949	1.65	1.0
O 10	0.2515	0.0596	0.4581	1.86	1.0
O 11	0.0811	0.3051	0.7261	1.68	1.0
O 12	0.9698	0.3179	0.3431	1.58	1.0
O 13	0.9052	0.4718	0.2174	2.09	1.0
O 14	0.1728	0.0585	0.0904	1.98	1.0
O 15	0.1202	0.3741	0.0505	1.91	1.0
O 16	0.9022	0.4346	0.7315	2.06	1.0
H_2O 1	0.3512	0.2234	0.0964	4.83	1.0
H_2O 2	0.6565	0.2989	0.8717	4.81	1.0
H_2O 3	0.5102	0.3063	0.4504	3.5	1.0
H_2O 4	0.7574	0.1530	0.1048	3.92	1.0
H_2O 5	0.5650	0.4074	0.1595	3.73	1.0

REFINED COMPOSITION: $|K_{8.48}(H_2O)_{18}|$ $[Si_{26.64}Al_{9.36}O_{72}]$
Mossyrock Dam, Washington, U.S.A.

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 17.767$ Å $b = 17.958$ Å $c = 7.431$ Å
$\alpha = 90°$ $\beta = 115.93°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.07$

REFERENCE: E. Galli, G. Gottardi, H. Mayer, A. Preisinger and E. Passaglia, *Acta Cryst.* **B39** 189–197 (1983).

Atom	x	y	z	B_{iso}	occ
K 1	0.079	0.0	0.281	19.1	0.34
K 2	0.071	0.0	0.110	10.6	0.36
K 3	0.241	0.500	0.061	3.4	0.74
K 4	0.210	0.500	-0.033	4.6	0.19
K 5	0.032	0.500	0.190	9.6	0.49
Si 1	0.1794	0.1686	0.0978	1.0	0.74
Si 2	0.2146	0.4108	0.5063	1.1	0.74
Si 3	0.2083	0.1912	0.7161	1.0	0.74
Si 4	0.0668	0.2983	0.4176	1.1	0.74
Si 5	0.0	0.2173	0.0	1.3	0.74
Al 1	0.1794	0.1686	0.0978	1.0	0.26
Al 2	0.2146	0.4108	0.5063	1.1	0.26
Al 3	0.2083	0.1912	0.7161	1.0	0.26
Al 4	0.0668	0.2983	0.4176	1.1	0.26
Al 5	0.0	0.2173	0.0	1.3	0.26
O 1	0.1981	0.5000	0.4565	2.3	1.0
O 2	0.2330	0.1213	0.6144	2.7	1.0
O 3	0.1882	0.1535	0.8902	3.0	1.0
O 4	0.2304	0.1008	0.2473	2.5	1.0
O 5	0.0	0.3257	0.5000	3.2	1.0
O 6	0.0805	0.1614	0.0499	2.6	1.0
O 7	0.1226	0.2296	0.5515	3.2	1.0
O 8	0.0142	0.2709	0.1891	3.4	1.0
O 9	0.2153	0.2492	0.1928	2.4	1.0
O 10	0.1208	0.3708	0.4225	2.8	1.0
H_2O 1	0.408	0.092	0.049	9.7	1.0
H_2O 2	0.008	0.099	0.414	8.0	0.5
H_2O 3	0.365	0.500	0.334	6.7	0.45
H_2O 4	0.419	0.500	0.207	10.3	0.55
H_2O 5	0.0	0.500	0.500	10.9	1.0

HEU Clinoptilolite

REFINED COMPOSITION: $|Na_{1.84}K_{1.76}Mg_{0.2}Ca_{1.24}(H_2O)_{21.36}|\ [Si_{29.84}Al_{6.16}O_{72}]$
Agoura, California, U.S.A.

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 17.662$ Å $b = 17.911$ Å $c = 7.407$ Å
$\alpha = 90°$ $\beta = 116.40°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.088$

REFERENCE: K. Koyama and Y. Takeuchi,
Z. Kristallogr. **145** 216–239 (1977).

Atom	x	y	z	B_{iso}	occ
Na 1	0.1428	0.0	0.667	5.49	0.36
Na 2	0.0393	0.5	0.210	3.13	0.10
K	0.2413	0.5	0.049	5.1	0.44
Mg	0.0	0.0	0.5	1.1	0.10
Ca 1	0.1428	0.0	0.667	5.49	0.06
Ca 2	0.0393	0.5	0.210	3.13	0.25
Si 1	0.17906	0.16943	0.0963	1.07	0.83
Si 2	0.21334	0.41099	0.5040	1.1	0.69
Si 3	0.20846	0.19034	0.7153	1.01	0.87
Si 4	0.06623	0.29837	0.4148	1.09	0.89
Si 5	0.0	0.21651	0.0	1.11	0.9
Al 1	0.17906	0.16943	0.0963	1.07	0.17
Al 2	0.21334	0.41099	0.5040	1.1	0.31
Al 3	0.20846	0.19034	0.7153	1.01	0.13
Al 4	0.06623	0.29837	0.4148	1.09	0.11
Al 5	0.0	0.21651	0.0	1.11	0.1
O 1	0.1959	0.5	0.4574	2.39	1.0
O 2	0.2336	0.1204	0.6144	2.47	1.0
O 3	0.1850	0.1551	0.8559	2.64	1.0
O 4	0.2333	0.1041	0.2509	2.37	1.0
O 5	0.0	0.3232	0.5	2.64	1.0
O 6	0.0808	0.1627	0.0555	1.96	1.0
O 7	0.1268	0.2317	0.5492	3.05	1.0
O 8	0.0122	0.2702	0.1856	2.48	1.0
O 9	0.2123	0.2520	0.1860	2.31	1.0
O 10	0.1188	0.3718	0.4148	2.42	1.0
H_2O 1	0.211	0.500	-0.033	6.2	0.38
H_2O 2	0.084	0.0	0.888	14.6	0.44
H_2O 3	0.0777	0.4206	0.964	9.5	1.0
H_2O 4	0.0	0.5	0.5	7.4	1.0
H_2O 5	0.0	0.095	0.5	22.1	0.76
H_2O 6	0.073	0.0	0.249	19.1	0.84
H_2O 7	0.096	0.0	0.756	10.2	0.42

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: $I1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 3
$a = 18.65243$ Å $b = 13.49597$ Å $c = 7.63109$ Å
$\alpha = 90.0°$ $\beta = 101.9781°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_{wp} = 0.0767$, $R_p = 0.0558$, $R_b = 0.0644$

REFERENCE: P. A. Barrett, M. A. Camblor, A. Corma, R. H. Jones and L. A. Villaescusa, *Chemistry of Materials* **9** 1713–1715 (1997).

Atom	x	y	z	B_{iso}	occ
Si 1	-0.01265	0.11371	0.2918	1.60	1.0
Si 2	0.249813	0.11336	0.6215	1.78	1.0
Si 3	0.14687	0.11588	0.2469	1.38	1.0
Si 4	0.16169	0.20243	-0.1058	1.84	1.0
O 5	0.31979	0.17940	0.6417	1.30	1.0
O 6	-0.07340	0.18435	0.1910	1.30	1.0
O 7	0.0	0.12865	0.5	1.30	1.0
O 8	0.06025	0.13926	0.2230	1.30	1.0
O 9	0.15762	0.0	0.2024	1.30	1.0
O 10	0.18823	0.13830	0.4442	1.30	1.0
O 11	-0.03438	0.0	0.2395	1.30	1.0
O 12	0.21031	0.13257	0.7932	1.30	1.0
O 13	0.27006	0.0	0.6233	1.30	1.0
O 14	0.17722	0.17880	0.0971	1.30	1.0

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: $P\,4_2/m\,mc$ (No. 131)
$a = 12.8528$ Å $b = 12.8528$ Å $c = 25.2136$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0827$, $R_{wp} = 0.1076$, $R_b = 0.0.0626$

REFERENCE: L. A. Villaescusa, P. A. Barrett and M. A. Camblor,
Angew. Chem., Int. ed. **38** 1997–2000 (1999).

Atom	x	y	z
Si 1	0.1192	0.1146	0.06251
Si 2	0.3062	0.2511	0.90459
Si 3	0.5	0.1167	0.06146
Si 4	0.3822	0.3849	0.18813
Si 5	0.3793	0.388	0.0
O 1	0.1426	0.1313	0.0
O 2	0.1512	0.0	0.0788
O 3	0.0	0.1379	0.0742
O 4	0.2002	0.1888	0.087
O 5	0.3996	0.1685	0.9116
O 6	0.3197	0.3334	0.9486
O 7	0.3205	0.3027	0.8453
O 8	0.5	0.0	0.0759
O 9	0.5	0.1373	0.0
O 10	0.5	0.3733	0.0
O 11	0.3327	0.5	0.0
O 12	0.3584	0.3584	0.25
O 13	0.5	0.3626	0.1782
O 14	0.3552	0.5	0.1725

REFINED COMPOSITION: $[Si_{64}O_{128}]$

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 20.622$ Å $b = 9.7242$ Å $c = 19.623$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_{wp} = 0.086$, $R_p = 0.062$

REFERENCE: M.A. Camblor, A. Corma, P. Lightfoot, L.A. Villaescusa and P.A. Wright, *Angew. Chem., Int. ed.* **36** 2659–2661 (1997).

Atom	x	y	z	B_{iso}	occ
Si 1	0.32018	-0.0430	0.1701	1.10	1.0
Si 2	0.07561	0.4067	0.0561	1.10	1.0
Si 3	0.2641	0.2255	0.1121	1.10	1.0
Si 4	0.15302	0.1551	0.0036	1.10	1.0
O 1	0.3427	-0.0581	0.2500	0.40	1.0
O 2	0.2675	-0.1485	0.1491	0.40	1.0
O 3	0.0996	0.5000	0.0000	0.40	1.0
O 4	0.0978	0.2516	0.0287	0.40	1.0
O 5	0.0000	0.4105	0.0718	0.40	1.0
O 6	0.2148	0.1587	0.0569	0.40	1.0
O 7	0.3870	-0.0628	0.1288	0.40	1.0
O 8	0.2913	0.1093	0.1625	0.40	1.0
O 9	0.3275	0.2871	0.0695	0.40	1.0
O 10	0.1308	0.0000	0.0000	0.40	1.0

REFINED COMPOSITION: $|Na_3H_2O|\ [Si_3Al_3O_{12}]$

CRYSTAL DATA: $Pmc2_1$ (No. 26)
$a = 7.503$ Å $b = 8.233$ Å $c = 5.230$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.039$

REFERENCE: A. Rheinhardt, E. Hellner and H. Ahsbahs, *Fortsch. der Mineralogie* **60** 175–176 (1982).

Atom	x	y	z	B_{iso}	occ
Na 1	0.5000	0.1774	0.466	1.9	1.0
Na 2	0.0000	0.419	0.106	4.9	0.5
Si 1	0.5000	0.3942	-0.015	0.9	0.5
Si 2	0.2173	0.1060	0.000	0.9	0.5
Al 1	0.5000	0.3942	-0.015	0.9	0.5
Al 3	0.2173	0.1060	0.000	0.9	0.5
O 1	0.0000	0.1420	0.014	1.8	1.0
O 2	0.5000	0.5628	0.170	1.8	1.0
O 3	0.2849	0.0326	0.718	2.0	1.0
O 4	0.3204	0.1833	0.061	1.8	1.0
H_2O 1	0.0000	0.330	0.514	2.9	0.25
H_2O 2	0.0000	0.470	0.538	3.9	0.25

(Cs,K) ZK5, Dehydrated KFI

REFINED COMPOSITION: $|Cs_{9.72}K_{12.88}|\ [Si_{72.96}Al_{23.04}O_{192}]$

CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 18.671$ Å $b = 18.671$ Å $c = 18.671$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.09$

REFERENCE: J. B. Parise, R. D. Shannon, E. Prince and D. E. Cox, *Z. Kristallogr.* **165** 175–190 (1983).

Atom	x	y	z	B_{iso}	occ
K 1	0.0	0.2500	0.5000	3.9	0.78
K 2	0.150	0.150	0.150	3.9	0.22
Cs	0.0	0.0	0.314	4.7	0.81
Si	0.0825	0.2023	0.3211	1.1	0.76
Al	0.0825	0.2023	0.3211	1.1	0.24
O 1	0.1280	0.1280	0.3145	2.0	1.0
O 2	0.2522	0.2522	0.4081	1.3	1.0
O 3	0.0	0.1783	0.3369	1.7	1.0
O 4	0.2500	0.1085	0.3915	1.7	1.0

REFINED COMPOSITION: $|Ca_4(H_2O)_{18}|\ [Si_{16}Al_8O_{48}]$
Nasik, India

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.8538$ Å $b = 13.1695$ Å $c = 7.5421$ Å
$\alpha = 90°$ $\beta = 110.323°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.115$, $R_p = 0.090$, $R_{F^2} = 0.046$

REFERENCE: G. Artioli and K. Ståhl,
Zeolites **13** 249–255 (1993).

Atom	x	y	z	B_{iso}	occ
Ca	0.2601	0.5	0.737	3.4	1.0
Si 1	0.2368	0.3838	0.156	1.89	1.0
Si 2	0.0763	0.3834	0.325	2.13	1.0
Al	0.1315	0.3080	0.737	2.61	1.0
O 1	0.260	0.5	0.219	0.79	1.0
O 2	0.2084	0.3744	0.919	1.66	1.0
O 3	0.1384	0.3838	0.552	0.55	1.0
O 4	0.146	0.3454	0.203	2.92	1.0
O 5	0.3205	0.3185	0.248	0.79	1.0
O 6	0.043	0.5	0.267	0.71	1.0
O 7	0.013	0.3083	0.743	2.53	1.0
H_2O 1	0.029	0.171	0.0	2.45	0.5
H_2O 2	0.401	0.5	0.026	5.92	1.0
H_2O 5	0.5	0.467	0.5	3.16	0.5
H_2O 8	0.1426	0.129	0.332	4.03	1.0

REFINED COMPOSITION: $|Ca_4H_{25.184}O_{13.36}|$ $[Si_{16.4}Al_{7.6}O_{48}]$
Teigahorn, Berufjördur, Iceland

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.690$ Å $b = 13.061$ Å $c = 7.574$ Å
$\alpha = 90°$ $\beta = 112.01°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{F^2} = 0.084$; At T = 15K.

REFERENCE: G. Artioli, J. V. Smith and Å. Kvick,
Zeolites **9** 377–391 (1989).

Atom	x	y	z	B_{iso}	occ
Si 1	0.23810	0.38177	0.15515	0.74	1.0
Si 2	0.08281	0.38285	0.32651	0.71	1.0
Si 3	0.12982	0.30997	0.73198	0.76	0.05
Al	0.12982	0.30997	0.73198	0.76	0.95
O 1	0.25981	0.5	0.22658	0.9	1.0
O 2	0.21108	0.37669	0.92717	0.96	1.0
O 3	0.14973	0.38130	0.55330	1.01	1.0
O 4	0.14659	0.33896	0.20664	0.94	1.0
O 5	0.33598	0.31686	0.26834	0.94	1.0
O 6	0.05002	0.5	0.26109	0.9	1.0
O 7	0.01051	0.31005	0.71791	1.06	1.0
Ca	0.27540	0.5	0.75776	1.06	1.0
O 11	0.41286	0.5	0.03570	2.64	0.130
O 12	0.41489	0.45514	0.05147	1.78	0.311
O 13	0.5	0.43199	0.5	1.97	0.450
O 14	0.38445	0.42560	0.62407	1.57	0.327
O 15	0.37628	0.38162	0.65890	2.39	0.200
O 16	0.39527	0.37909	0.77087	2.91	0.286
O 17	0.40290	0.38065	0.84035	1.38	0.143
O 18	0.41917	0.37517	0.98301	1.55	0.113
H 1	0.47394	0.43341	0.03731	3.13	0.224
H 2	0.47076	0.5	0.05896	3.65	0.080
H 3	0.45425	0.47073	0.11239	3.86	0.123
H 4	0.40834	0.38935	0.12684	4.03	0.132
H 5	0.41832	0.42092	0.16151	3.55	0.224
H 6	0.44714	0.38924	0.41741	2.73	0.433
H 7	0.37143	0.37046	0.52675	3.45	0.456
H 8	0.36681	0.39410	0.53068	3.72	0.089
H 9	0.42706	0.47454	0.59007	2.47	0.314
H 10	0.42967	0.39404	0.66218	2.15	0.140
H 11	0.41716	0.33596	0.73197	2.36	0.145
H 12	0.44065	0.37303	0.73626	3.32	0.155
H 13	0.38262	0.30594	0.74108	4.21	0.126
H 14	0.37938	0.29567	0.81611	2.59	0.215
H 15	0.40073	0.33226	0.82437	3.38	0.090
H 16	0.47481	0.39229	0.89948	3.75	0.101
H 17	0.41649	0.31170	0.90170	3.35	0.141

LAU Cobalt Gallophosphate

REFINED COMPOSITION: $|(C_5H_6N)_8|$ $[Co_8Ga_{16}P_{24}O_{96}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 15.058$ Å $b = 13.197$ Å $c = 15.273$ Å
$\alpha = 90°$ $\beta = 112.20°$ $\gamma = 90°$

REFERENCE: A. M. Chippindale and R. I. Walton,
J. Chem. Soc., Chem. Commun. 2453–2454 (1994).

Atom	x	y	z	B_{iso}	occ
Ga 1	0.56738	0.10568	0.65382	2.07	0.6667
Co 1	0.56738	0.10568	0.65382	2.07	0.3333
Ga 2	0.73158	-0.12692	0.57730	2.04	0.6667
Co 2	0.73158	-0.12692	0.57730	2.04	0.3333
Ga 3	0.63532	0.19004	0.36767	2.1	0.6667
Co 3	0.63532	0.19004	0.36767	2.1	0.3333
P 1	0.5716	-0.1306	0.6573	2.17	1.0
P 2	0.7317	0.1144	0.5759	2.1	1.0
P 3	0.6368	0.1869	0.8647	2.2	1.0
O 1	0.6270	-0.1711	0.6002	3.61	1.0
O 2	0.7156	0.1423	0.9528	2.53	1.0
O 3	0.5295	-0.0264	0.6227	3.46	1.0
O 4	0.7126	0.1169	0.4706	3.28	1.0
O 5	0.7572	0.0068	0.6151	2.48	1.0
O 6	0.8178	0.1799	0.6299	3.25	1.0
O 7	0.4905	-0.2056	0.6435	2.68	1.0
O 8	0.6349	0.1218	0.7831	3.3	1.0
O 9	0.6598	0.2974	0.8514	3.2	1.0
O 10	0.6379	-0.1243	0.7616	3.44	1.0
O 11	0.4594	0.1869	0.6233	3.38	1.0
O 12	0.6437	0.1546	0.5907	3.41	1.0
C 1	0.170	0.0043	0.139	5.7	1.0
N	0.124	-0.080	0.144	9.07	1.0
C 2	0.124	0.096	0.130	7.49	1.0
C 3	0.031	0.100	0.123	7.94	1.0
C 4	-0.012	0.010	0.135	10.94	1.0
C 5	0.035	-0.081	0.144	8.69	1.0
H 11	0.2373	0.0011	0.1413	6.47	1.0
H 111	0.1579	-0.1462	0.1486	9.19	1.0
H 21	0.1594	0.1600	0.1290	8.35	1.0
H 31	-0.0055	0.1653	0.1099	7.82	1.0
H 41	-0.0774	0.0124	0.1370	11.99	1.0
H 51	0.0042	-0.1460	0.1501	9.69	1.0

REFINED COMPOSITION: $|Ca_{7.8}Na_{2.16}K_{0.72}(H_2O)_{46.08}|\ [Si_{35.1}Al_{18.9}O_{108}]$
Nurri, Nuoro, Sardinia, Italy

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.338$ Å $b = 13.338$ Å $c = 23.014$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: S. Merlino, E. Galli and A. Alberti,
Tschermaks Mineral. Petrogr. Mitt. **22** 117–129 (1975).

Atom	x	y	z	B_{iso}	occ
Na 2	0.0	0.0	0.2782	3.4	0.12
Na 3	0.0	0.0	0.4095	9.4	0.12
Na 4	0.0	0.0	0.4498	0.7	0.06
Na 5	0.0	0.0	0.5	0.7	0.12
K 2	0.0	0.0	0.2782	3.4	0.06
K 3	0.0	0.0	0.4095	9.4	0.06
Ca 1	0.0	0.0	0.1389	3.48	1.0
Ca 2	0.0	0.0	0.2782	3.4	0.12
Ca 3	0.0	0.0	0.4095	9.4	0.12
Ca 4	0.0	0.0	0.4498	0.7	0.06
Si 1	0.0001	0.2322	0.0697	1.39	0.65
Si 2	0.2396	0.0	0.5	1.32	0.65
Al 1	0.0001	0.2322	0.0697	1.39	0.35
Al 2	0.2396	0.0	0.5	1.32	0.35
O 1	0.0339	0.3493	0.1079	2.72	1.0
O 2	0.0920	-0.0920	0.0827	2.98	1.0
O 3	0.1275	-0.1275	-0.0910	3.45	1.0
O 4	0.2643	0.0	0.0	3.83	1.0
O 5	0.2219	-0.2219	0.1793	2.98	1.0
H_2O 1	0.2567	-0.2567	-0.1241	4.8	1.0
H_2O 2	0.1222	-0.1222	0.2852	8.0	0.74
H_2O 3	0.2547	-0.2547	0.0187	6.5	0.54
H_2O 4	0.5429	-0.5429	-0.0445	5.7	0.28

LEV 1-aminoadamantane NU-3

REFINED COMPOSITION: $|(C_{10}N)_6|\ [Si_{54}O_{108}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) hexagonal setting
$a = 13.2251$ Å $b = 13.2251$ Å $c = 22.2916$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.104$, $R_F = 0.060$

REFERENCE: L. B. McCusker,
Mat. Sci. Forum Vol. **133-136** 423–434 (1993).
And L. B. McCusker, Private communication (1995).

Atom	x	y	z	B_{iso}	occ
Si 1	0.2327	0.0006	0.0694	0.95	1.0
Si 2	0.33333	-0.0943	0.16667	0.95	1.0
O 1	0.2641	0.0	0.0	1.18	1.0
O 2	0.0956	-0.0956	0.0795	1.82	1.0
O 3	0.2492	0.1246	0.0890	1.26	1.0
O 4	0.4460	-0.1080	0.1544	1.11	1.0
O 5	0.3121	-0.0340	0.1078	1.03	1.0
C 1	0.0	0.0	0.2190	5.37	1.0
C 2	0.0635	0.1270	0.2449	5.37	1.0
C 3	0.0651	0.1302	0.3130	5.37	1.0
C 4	0.1248	0.0624	0.3386	5.37	1.0
N	0.1254	0.2508	0.3320	5.37	0.333

The y-value of O4 has been corrected to $2x - 1$, rather than $1 - 2x$.

REFINED COMPOSITION: $|K_{13.788}Ca_6(SO_4)_5Cl_{3.5}F_{0.5}|$ $[Si_{18}Al_{18}O_{72}]$
Pitigliano, Tuscany, Italy

CRYSTAL DATA: $P\overline{6}$ (No. 174)
$a = 12.8701$ Å $b = 12.8701$ Å $c = 16.096$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_p = 0.0365$, $R_{wp} = 0.0829$

REFERENCE: P. Ballirano, S. Merlino and E. Bonaccorsi, *Canadian Mineralogist* **34** 1021–1030 (1996).

Atom	x	y	z	B_{iso}	occ
Si 1	0.9954	0.7437	0.0	0.61	1.0
Al 1	0.3339	0.4088	0.833	0.64	1.0
Si 2	0.6718	0.0822	0.6637	0.59	1.0
Al 2	0.3364	0.4097	0.5	0.56	1.0
Si 3	0.5852	0.6661	0.8329	0.61	1.0
Al 3	0.7378	0.7488	0.0	0.6	1.0
Si 4	0.5873	0.67	0.5	0.57	1.0
Al 4	0.9282	0.3431	0.6635	0.62	1.0
O 1	0.8771	0.1258	0.0	1.97	1.0
O 2	0.1025	0.8798	0.0	1.63	1.0
O 3	0.9943	0.6706	0.9182	1.5	1.0
O 4	0.6631	0.6698	0.9119	1.6	1.0
O 5	0.2179	0.7886	0.8253	1.65	1.0
O 6	0.4501	0.5552	0.8386	1.65	1.0
O 7	0.3463	0.331	0.7491	1.41	1.0
O 8	0.6574	0.656	0.7543	1.52	1.0
O 9	0.5464	0.4367	0.6545	1.34	1.0
O 10	0.7933	0.2105	0.6632	2.1	1.0
O 11	0.6772	0.0062	0.5856	1.41	1.0
O 12	0.6659	0.6735	0.5794	1.4	1.0
O 13	0.2173	0.7836	0.5	1.56	1.0
O 14	0.454	0.5557	0.5	1.17	1.0
Ca 1	0.3333	0.6667	0.5	1.28	1.0
Ca 2	0.3333	0.6667	0.833	1.36	1.0
Ca 3	0.0	0.0	0.9783	1.73	0.5
Ca 4	0.6667	0.3333	0.3915	1.51	0.5
Ca 5	0.6667	0.3333	0.3436	2.32	0.5
K 1	0.8463	0.1651	0.5	1.34	0.572
K 11	0.857	0.143	0.5	1.34	0.182
K 2	0.1125	0.8864	0.6651	3.1	0.684
K 22	0.145	0.851	0.675	3.1	0.074
K 3	0.8364	0.1722	0.8313	1.96	0.694
K 33	0.816	0.191	0.847	1.96	0.058
K 4	0.5543	0.4458	0.0	2.67	0.822
F	0.7476	0.27	0.5	2.02	0.167
Cl 1	0.3333	0.6667	0.0	5.78	1.0
Cl 2	0.6667	0.3333	0.5	12.7	0.5
Cl 3	0.3333	0.6667	0.3335	5.86	1.0
S 1	0.0	0.0	0.7971	1.36	0.5

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Atom	x	y	z	B_{iso}	occ
S 11	0.977	0.013	0.7874	2.67	0.167
S 2	0.0357	0.017	0.5	2.75	0.333
S 3	0.6667	0.3333	0.8568	3.24	1.0
O 21	0.0	0.0	0.886	7.94	0.5
O 22	0.1213	0.0582	0.7676	5.83	0.667
O 23	0.056	0.094	0.723	9.11	0.167
O 24	0.119	0.054	0.845	6.82	0.333
O 25	0.119	0.058	0.426	5.12	0.333
O 26	0.11	0.051	0.479	10.65	0.333
O 27	0.6667	0.3333	0.2409	2.76	0.5
O 28	0.7285	0.4595	0.8789	2.89	0.667
O 29	0.692	0.298	0.211	7.35	0.167
O 30	0.728	0.288	0.913	10.11	0.333

REFINED COMPOSITION: $|Na_{12.5}(H_2O)_{14.32}|\ [Si_{12}Al_{12}O_{48}]$
Synthetic material

CRYSTAL DATA: $P6_3mc$ (No. 186)
$a = 12.906$ Å $b = 12.906$ Å $c = 10.541$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{wp} = 0.154$, $R_F = 0.084$, $R_{exp} = 0.136$

REFERENCE: P. A. Schicker,
Ph.D. Thesis No. 8494, ETH Zurich (1988).

Atom	x	y	z	B_{iso}	occ
Na 1	0.897	0.449	-0.018	11.2	0.98
Na 2	0.846	0.1539	-0.24	5.5	0.73
Na 3	0.0	0.0	-0.45	0.0	0.52
Na 4	0.6667	0.3333	-0.66	1.5	0.60
Si 1	0.250	-0.002	0.0	1.5	0.5
Al 1	0.250	-0.002	0.0	1.5	0.5
Si 2	0.414	0.084	0.248	1.9	0.5
Al 2	0.414	0.084	0.248	1.9	0.5
O 1	0.220	0.110	-0.006	4.4	1.0
O 2	0.358	0.025	0.102	2.1	1.0
O 3	0.458	0.229	0.257	5.8	1.0
O 4	0.529	0.058	0.267	4.1	1.0
O 5	0.125	-0.125	0.035	14.3	1.0
O 6	0.312	0.007	0.354	3.5	1.0
H_2O 1	0.749	0.251	-0.22	12.9	0.87
H_2O 2	0.774	0.387	-0.442	13.7	0.88
H_2O 3	0.0	0.0	-0.61	0.5	0.53
H_2O 4	0.0	0.0	-0.24	0.0	0.52
H_2O 5	0.6667	0.3333	0.06	11.5	0.86

LOV Lovdarite

REFINED COMPOSITION: $|Na_{12}K_4(H_2O)_{18}|\ [Si_{28}Be_8O_{72}]$
Mt. Karnasurt, Lovezero Pluton, Russia

CRYSTAL DATA: $Pma2$ (No. 28)
$a = 39.576$ Å $b = 6.9308$ Å $c = 7.1526$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.09$

REFERENCE: S. Merlino,
Eur. J. Mineral. **2** 809–817 (1990).

Atom	x	y	z	B_{iso}	occ
Na 1	0.25	0.6098	0.2437	1.95	1.0
Na 2	0.25	0.6217	0.7683	1.97	1.0
Na 3	0.1283	0.8542	0.6990	2.18	1.0
Na 4	0.0069	0.2840	0.8652	6.10	1.0
K	0.3860	0.0417	0.1828	1.98	1.0
Si 1	0.2113	0.0504	0.2770	0.73	1.0
Si 2	0.2113	0.0497	0.7179	0.84	1.0
Si 3	0.1952	0.3671	-0.0008	0.77	1.0
Si 4	0.1248	0.5026	-0.0269	0.89	1.0
Si 5	0.0582	0.5267	0.1399	0.92	1.0
Si 6	0.0333	0.2593	0.4469	0.79	1.0
Si 7	0.0458	0.8202	0.4588	0.87	1.0
Be 1	0.1805	0.7820	0.0050	0.47	1.0
Be 2	0.0670	0.5415	0.7334	1.00	1.0
O 1	0.25	-0.0319	0.2723	0.61	1.0
O 2	0.2103	0.2603	0.1857	1.35	1.0
O 3	0.1858	-0.0960	0.1901	1.12	1.0
O 4	0.2023	0.0905	0.5007	1.33	1.0
O 5	0.25	-0.0324	0.7287	1.20	1.0
O 6	0.2106	0.2624	0.8147	1.14	1.0
O 7	0.1858	-0.1014	0.8030	1.15	1.0
O 8	0.2065	0.5870	0.0011	0.77	1.0
O 9	0.1540	0.3356	0.0027	1.33	1.0
O 10	0.1409	0.7122	-0.0041	1.25	1.0
O 11	0.0979	0.4563	0.1463	1.00	1.0
O 12	0.1057	0.4735	0.7794	1.34	1.0
O 13	0.0355	0.3608	0.2493	1.22	1.0
O 14	0.0563	0.7205	0.2606	1.89	1.0
O 15	0.0448	0.5539	-0.0671	1.40	1.0
O 16	0.0514	0.0501	0.4226	1.13	1.0
O 17	0.0493	0.3782	0.6145	1.51	1.0
O 18	-0.0060	0.2198	0.5039	1.43	1.0
O 19	0.0678	-0.2501	0.6341	0.88	1.0
H_2O 1	0.2115	0.5643	0.5123	2.17	1.0
H_2O 2	0.1438	0.6958	0.4247	2.38	1.0
H_2O 3	0.1290	0.1820	0.5459	2.70	1.0
H_2O 4	0.0744	0.0616	0.8790	3.91	1.0
H_2O 5	0.0	0.0	0.0134	8.03	1.0

Linde Type A, Hydrated LTA

REFINED COMPOSITION: $|Na_{64}(H_2O)_{326.71}|\ [Si_{96}Al_{96}O_{384}]$

CRYSTAL DATA: $Fm\overline{3}c$ (No. 226)
$a = 24.61$ Å $b = 24.61$ Å $c = 24.61$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: V. Gramlich and W. M. Meier,
Z. Kristallogr. **133** 134–149 (1971).

Atom	x	y	z	B_{iso}	occ
Na	0.1064	0.1064	0.1064	7.74	1.0
Si	0.0	0.0929	0.1844	1.16	1.0
Al	0.0	0.1864	0.0902	1.0	1.0
O 1	0.0	0.1116	0.2473	2.55	1.0
O 2	0.0	0.1463	0.1476	2.08	1.0
O 3	0.0538	0.0583	0.1704	2.45	1.0
O 4	0.02	0.03	0.064	25.0	0.115
O 5	0.03	0.02	0.064	25.0	0.115
O 6	0.1598	0.1598	0.1598	18.16	0.91
O 7	0.1155	0.167	0.262	33.43	0.325
O 8	0.167	0.1155	0.262	33.43	0.325
O 9	0.041	0.210	0.235	34.74	0.22
O 10	0.210	0.041	0.235	34.74	0.22
O 11	0.25	0.25	0.25	61.59	1.88

Extra-framework atoms O5–O11 were assumed to have oxygen scattering factors.

LTA Linde Type A, Dehydrated

REFINED COMPOSITION: $|Na_{91.78}|\ [Si_{96}Al_{96}O_{384}]$

CRYSTAL DATA: $Fm\overline{3}c$ (No. 226)
$a = 24.555$ Å $b = 24.555$ Å $c = 24.555$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.023$

REFERENCE: J. J. Pluth and J. V. Smith,
J. Am. Chem. Soc. **102** 4704–4708 (1980).

Atom	x	y	z	B_{iso}	occ
Na 1	0.09960	0.09960	0.09960	3.79	0.972
Na 2	0.0	0.2165	0.2111	6.35	0.242
Na 3	0.2500	0.1060	0.1060	4.34	0.066
Si	0.0	0.09316	0.18499	1.89	1.0
Al	0.0	0.18715	0.09042	1.98	1.0
O 1	0.0	0.11367	0.24663	3.17	1.0
O 2	0.0	0.14459	0.14591	3.68	1.0
O 3	0.05379	0.05865	0.17152	2.98	1.0

REFINED COMPOSITION: $|K_{7.56}Tl_{3.8}(H_2O)_{22.46}|\ [Si_{24}Al_{12}O_{72}]$
Murun Massif, Russia

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 18.5432$ Å $b = 18.5432$ Å $c = 7.5310$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R_{wp} = 0.20$, $R_p = 0.17$

REFERENCE: G. Artioli and Å. Kvick,
Eur. J. Mineral. **2** 749–759 (1990).

Atom	x	y	z	B_{iso}	occ
K 1	0.33333	0.66667	0.0	5.53	0.18
K 2	0.33333	0.66667	0.5	1.18	0.38
K 21	0.33333	0.66667	0.427	1.18	0.31
K 3	0.297	0.0	0.0	3.63	0.517
Tl 3	0.315	0.0	0.0	3.63	0.483
K 4	0.5	0.0	0.5	3.24	0.699
Tl 4	0.5	0.0	0.5	3.24	0.301
Si 1	0.0924	0.3546	0.5	2.53	0.667
Si 2	0.1672	0.4975	0.215	4.9	0.667
Al 1	0.0924	0.3546	0.5	2.53	0.333
Al 2	0.1672	0.4975	0.215	4.9	0.333
O 1	0.0	0.272	0.5	0.79	1.0
O 2	0.158	0.316	0.5	4.74	1.0
O 3	0.260	0.520	0.288	5.53	1.0
O 4	0.1038	0.4125	0.326	1.82	1.0
O 5	0.4092	0.818	0.213	4.74	1.0
O 6	0.156	0.483	0.0	1.18	1.0
H_2O 1	0.11	0.0	0.0	7.11	0.40
H_2O 2	0.134	0.0	0.37	7.11	0.91
H_2O 3	0.28	0.14	0.0	2.37	0.25
H_2O 4	0.28	0.14	0.26	7.9	0.19
H_2O 5	0.0	0.0	0.172	7.9	0.70
H_2O 6	0.560	0.280	0.0	7.9	0.66

The presence of thallium atoms at the K3 and K4 sites in the larger cavities of the zeolite framework is considered to be an artifact of heavy liquid separation.

LTL Linde Type L

REFINED COMPOSITION: $|Na_5K_{4.7}(H_2O)_{20.8}|\ [Si_{27}Al_9O_{72}]$
Synthetic material

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 18.40$ Å $b = 18.40$ Å $c = 7.52$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray powder refinement, $R_F = 0.13$

REFERENCE: R. M. Barrer and H. Villiger,
Z. Kristallogr. **128** 352–270 (1969).

Atom	x	y	z	B_{iso}	occ
Na 1	0.3333	0.6667	0.0	4.0	0.7
Na 2	0.0	0.303	0.0	2.0	0.6
K 1	0.3333	0.6667	0.5	1.0	1.0
K 2	0.0	0.5	0.5	3.0	0.9
Si 1	0.0946	0.3595	0.5	1.2	0.75
Si 2	0.1662	0.4989	0.2137	0.6	0.75
Al 1	0.0946	0.3595	0.5	1.2	0.25
Al 2	0.1662	0.4989	0.2137	0.6	0.25
O 1	0.0	0.2674	0.5	1.0	1.0
O 2	0.1646	0.3292	0.5	1.0	1.0
O 3	0.2620	0.5240	0.260	2.5	1.0
O 4	0.1004	0.4078	0.330	1.0	1.0
O 5	0.4261	0.8522	0.275	1.3	1.0
O 6	0.1360	0.4691	0.0	0.8	1.0
H_2O 1	0.0700	0.1400	0.5	4.0	0.7
H_2O 2	0.0	0.09	0.5	7.0	0.25
H_2O 3	0.0	0.0	0.5	15.0	0.5
H_2O 4	0.0	0.135	0.243	4.0	0.25
H_2O 5	0.092	0.184	0.203	5.0	0.25
H_2O 6	0.0	0.0	0.189	10.0	0.7
H_2O 7	0.116	0.232	0.0	6.0	0.7
H_2O 8	0.0	0.195	0.0	5.0	0.5

REFINED COMPOSITION: $|Na_{426.6}(H_2O)_{393.6}|\ [Si_{384}Al_{384}O_{1536}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre $(\overline{3})$
$a = 36.95$ Å $b = 36.95$ Å $c = 36.95$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.051$

REFERENCE: Y. F. Shepelev, Y. I. Smolin, I. K. Butikova and V. I. Tarasov, *Doklady Akad. Nauk SSSR* **272** 1133–1137 (1975).

Atom	x	y	z	B_{iso}	occ
Na 1	0.0420	0.0420	0.0420	3.0	1.0
Na 2	0.2312	0.2132	0.2132	0.8	0.56
Na 3	0.2337	0.2337	0.2337	3.0	0.26
Na 4	0.6964	0.6964	0.6964	2.4	0.77
Na 5	0.4184	0.4184	0.4184	3.0	0.53
Na 6	0.4322	0.4322	0.4322	3.5	0.21
Na 7	0.4564	0.4564	0.4564	3.3	0.09
Na 8	0.1770	0.0742	0.8278	2.1	0.46
Na 9	0.1895	0.0621	0.8156	2.4	0.24
Na 10	0.2006	0.0501	0.7983	2.6	0.23
Na 11	0.1805	0.0705	0.4323	2.7	1.0
Na 12	0.2723	0.1111	0.3621	2.8	0.6
Na 13	0.2541	0.1110	0.3615	0.9	0.25
Na 14	0.2311	0.1084	0.3640	3.0	0.15
Si 1	0.2481	0.0633	0.6252	0.4	1.0
Si 2	0.3103	0.1213	0.7456	0.5	1.0
Si 3	0.1717	0.0154	0.9540	0.4	1.0
Si 4	0.2230	0.0852	0.2858	0.7	1.0
Al 1	0.3141	-0.0016	0.8749	0.5	1.0
Al 2	0.2484	0.1221	0.8066	0.5	1.0
Al 3	0.2965	0.0164	0.0794	0.4	1.0
Al 4	0.2850	0.0853	0.2273	0.7	1.0
O 1	0.2151	0.0365	0.6145	1.6	1.0
O 2	0.1613	0.0917	0.7357	1.0	1.0
O 3	0.3857	0.0308	0.0360	1.7	1.0
O 4	0.2580	0.0866	0.5894	1.3	1.0
O 5	0.1135	0.0417	0.4616	1.4	1.0
O 6	0.1982	0.0495	0.9583	1.6	1.0
O 7	0.3626	0.0346	0.7917	1.4	1.0
O 8	0.3261	0.0877	0.5060	1.8	1.0
O 9	0.2529	0.0944	0.8444	1.4	1.0
O 10	0.3209	0.0698	0.2537	1.9	1.0
O 11	0.2160	0.1228	0.9583	1.7	1.0
O 12	0.2652	0.0686	0.9861	1.8	1.0
O 13	0.2454	0.1656	0.8233	1.9	1.0
O 14	0.1723	0.0018	0.2433	2.0	1.0
O 15	0.2803	0.0436	0.3807	1.7	1.0
O 16	0.2839	0.0653	0.1852	1.8	1.0
H_2O 1	0.2685	0.2685	0.2685	7.3	0.89
H_2O 2	0.3699	0.0673	0.1659	2.6	0.17

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Atom	x	y	z	B_{iso}	occ
H_2O 3	0.3693	0.0758	0.1748	3.8	0.63
H_2O 4	0.3679	0.0911	0.1828	2.3	0.2
H_2O 5	0.0754	0.0754	0.0754	6.3	0.4
H_2O 6	0.3268	0.1250	0.6250	5.5	0.86
H_2O 7	0.1558	0.0849	0.8880	5.4	0.6
H_2O 8	0.1471	0.1066	0.8896	4.6	0.36
H_2O 9	0.3553	0.0276	0.3912	6.3	0.38
H_2O 10	0.3496	0.0471	0.3987	3.4	0.61
H_2O 11	0.2063	0.0449	0.1043	3.8	0.29

REFINED COMPOSITION: $|Na_{0.3}K_{2.52}Ca_{1.06}Mg_2(H_2O)_{31.48}|\ [Si_{26.28}Al_{9.72}O_{72}]$
Mont Semiol, Loire, France

CRYSTAL DATA: $P6_3/mmc$ (No. 194)
$a = 18.392$ Å $b = 18.392$ Å $c = 7.646$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.05$

REFERENCE: E. Galli,
Rend. Soc. Ital. Mineral. Petrol. **31** 599–612 (1975).

Atom	x	y	z	B_{iso}	occ
Na	0.5	0.0	0.0	4.61	0.05
K	0.5	0.0	0.0	4.61	0.42
Mg	0.3333	0.6667	-0.25	2.71	1.0
Ca 1	0.5	0.0	0.0	4.61	0.03
Ca 2	0.0	0.0	0.072	23.2	0.22
Si 1	0.1584	0.4902	0.25	1.05	0.73
Si 2	0.3536	0.0933	0.0444	1.05	0.73
Al 1	0.1584	0.4902	0.25	1.05	0.27
Al 2	0.3536	0.0933	0.0444	1.05	0.27
O 1	0.2589	0.5178	0.25	2.38	1.0
O 2	0.4249	0.8498	0.25	1.9	1.0
O 3	0.3822	0.1004	0.25	2.14	1.0
O 4	0.4352	0.1114	-0.0721	2.27	1.0
O 5	0.1614	0.3228	-0.0016	1.96	1.0
O 6	0.2741	0.0	0.0	2.37	1.0
H_2O 1	0.467	0.934	0.661	6.4	0.5
H_2O 2	0.3333	0.6667	0.016	4.3	1.0
H_2O 3	0.271	0.542	-0.25	5.4	0.44
H_2O 4	0.566	0.355	0.25	6.9	0.44
H_2O 5	0.028	0.148	0.030	7.7	0.23
H_2O 6	0.088	0.176	0.25	21.8	0.89
H_2O 7	0.076	0.152	-0.25	31.2	0.45

REFINED COMPOSITION: $[Si_{34}O_{68}]$

CRYSTAL DATA: $P6_3/m$ (No. 176)
$a = 13.175$ Å $b = 13.175$ Å $c = 15.848$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
DLS refinement

REFERENCE: S. L. Lawton and W. J. Rohrbaugh,
Science **247** 1319–1322 (1990).

Atom	x	y	z
Si 1	0.6667	0.3333	0.3495
Si 2	0.6713	0.1500	0.4700
Si 3	0.4522	0.1161	0.5682
Si 4	0.5266	0.2118	0.75
O 1	0.6667	0.3333	0.25
O 2	0.6623	0.2169	0.3878
O 3	0.5793	0.1388	0.5411
O 4	0.4217	0.1984	0.5101
O 5	0.4540	0.1495	0.6663
O 6	0.6506	0.2126	0.75
O 7	0.6443	0.0200	0.4453

REFINED COMPOSITION: $[Si_{96}O_{192}]$

CRYSTAL DATA: $I\bar{4}m2$ (No. 119)
$a = 20.067$ Å $b = 20.067$ Å $c = 13.411$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_p = 0.13$

REFERENCE: C. A. Fyfe, H. Gies, G. T. Kokotailo, C. Pasztor, H. Strobl and D. E. Cox, *J. Am. Chem. Soc.* **111** 2470–2474 (1989).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0777	0.0777	0.0000	0.34	1.0
Si 2	0.1212	0.1860	0.1451	1.64	1.0
Si 3	0.0775	0.2219	0.3569	1.29	1.0
Si 4	0.2801	0.1882	0.1403	0.39	1.0
Si 5	0.3053	0.0768	-0.0079	0.28	1.0
Si 6	0.1938	0.1938	0.5	1.1	1.0
Si 7	0.0761	0.3819	0.3589	-0.20	1.0
O 1	0.0873	0.0	0.0279	3.30	1.0
O 2	0.1067	0.1179	0.0975	2.83	1.0
O 3	0.0926	0.1856	0.2550	1.71	1.0
O 4	0.2018	0.1993	0.1506	1.79	1.0
O 5	0.3309	0.1186	0.0889	1.62	1.0
O 6	0.3003	0.0	0.0247	0.77	1.0
O 7	0.3095	0.1905	0.25	3.27	1.0
O 8	0.1204	0.1931	0.4478	0.24	1.0
O 9	0.2511	0.1927	0.4252	1.43	1.0
O 10	0.0905	0.3010	0.3497	1.16	1.0
O 11	0.0	0.2090	0.3875	3.49	1.0
O 12	0.0	0.3960	0.3871	-0.34	1.0
O 13	0.0926	0.2437	0.0900	1.59	1.0
O 14	0.1295	0.4078	0.4348	0.03	1.0
O 15	0.0875	0.4125	0.25	-1.59	1.0

REFINED COMPOSITION: $|C_8|$ $[Si_{46}O_{92}]$
Mt. Hamilton, California, U.S.A.

CRYSTAL DATA: $Pm\bar{3}n$ (No. 223)
$a = 13.436$ Å $b = 13.436$ Å $c = 13.436$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.04$

REFERENCE: H. Gies,
Z. Kristallogr. **164** 247–257 (1983).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0	0.3098	0.1142	1.71	1.0
Si 2	0.1826	0.1826	0.1826	1.72	1.0
Si 3	0.25	0.0	0.5	1.43	1.0
O 1	0.0963	0.2465	0.1360	4.88	1.0
O 2	0.0	0.4056	0.1813	4.78	1.0
O 3	0.3423	0.0	0.0	2.76	1.0
O 4	0.25	0.25	0.25	5.81	1.0
C 1	0.25	0.5	0.0	39.37	1.0
C 2	0.0	0.0	0.0	13.74	1.0

C1 represents guest molecules N_2 and CO_2 collapsed to a site.

REFINED COMPOSITION: $|Na_{0.68}K_{5.28}Ca_{1.844}Ba_{0.444}(H_2O)_{19.44}|\ [Si_{22.72}Al_{9.28}O_{64}]$
Cupaello, Italy

CRYSTAL DATA: *Immm* (No. 71)
$a = 14.116$ Å $b = 14.229$ Å $c = 9.946$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.09$

REFERENCE: E. Galli, G. Gottardi and D. Pongiluppi,
Neues Jahrb. Miner. Monatsh. **1** 1–9 (1979).

Atom	x	y	z	B_{iso}	occ
Na 3	0.5	0.5	0.275	12.0	0.054
Na 4	0.390	0.363	0.0	12.0	0.022
Na 5	0.333	0.380	0.0	12.0	0.036
K 1	0.156	0.5	0.0	3.8	0.419
K 2	0.5	0.192	0.0	3.8	0.419
K 3	0.5	0.5	0.275	12.0	0.09
K 4	0.390	0.363	0.0	12.0	0.136
K 5	0.333	0.380	0.0	12.0	0.06
Ca 3	0.5	0.5	0.275	12.0	0.147
Ca 4	0.390	0.363	0.0	12.0	0.059
Ca 5	0.333	0.380	0.0	12.0	0.098
Ba 1	0.156	0.5	0.0	3.8	0.041
Ba 2	0.5	0.192	0.0	3.8	0.041
Ba 3	0.5	0.5	0.275	12.0	0.009
Ba 4	0.390	0.363	0.0	12.0	0.004
Ba 5	0.333	0.380	0.0	12.0	0.006
Si 1	0.1097	0.2473	0.1563	1.0	0.71
Si 2	0.2816	0.1102	0.1596	1.0	0.71
Al 1	0.1097	0.2473	0.1563	1.0	0.29
Al 2	0.2816	0.1102	0.1596	1.0	0.29
O 1	0.1235	0.2830	0.0	1.8	1.0
O 2	0.3089	0.1177	0.0	1.5	1.0
O 3	0.0	0.2155	0.1839	1.8	1.0
O 4	0.2767	0.0	0.2096	1.9	1.0
O 5	0.1765	0.1568	0.1924	2.3	1.0
O 6	0.3661	0.1638	0.2454	2.6	1.0
H_2O 1	0.5	0.0	0.0	6.8	1.0
H_2O 2	0.0	0.5	0.158	4.9	1.0
H_2O 3	0.385	0.5	0.159	9.8	0.6
H_2O 4	0.5	0.5	0.0	3.7	0.2
H_2O 5	0.459	0.274	0.0	5.8	0.2
H_2O 6	0.251	0.464	0.0	3.6	0.21
H_2O 7	0.446	0.420	0.062	11.2	0.2
H_2O 8	0.443	0.5	0.5	12.0	0.44

MER Barium Chloroaluminosilicate

REFINED COMPOSITION: $|(Ba_3Cl_2O)_4|\ [Si_{21.34}Al_{10.66}O_{64}]$

CRYSTAL DATA: $I\,4/m\,mm$ (No. 139)
$a = 14.194$ Å $b = 14.194$ Å $c = 9.234$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.14$

REFERENCE: L. P. Solov'eva, S. V. Borisov and V. V. Bakakin, *Sov. Phys. – Crystallogr.* **16** 1035–1038 (1972).

Atom	x	y	z	B_{iso}	occ
Ba 1	0.1816	0.5	0.5	5.0	1.0
Ba 2	0.5	0.5	0.288	14.5	1.0
Cl	0.375	0.375	0.5	5.1	1.0
O^{2-}	0.0	0.5	0.25	4.8	1.0
Si	0.2386	0.3917	0.157	2.2	0.6667
Al	0.2386	0.3917	0.157	2.2	0.3333
O 1	0.193	0.390	0.0	3.6	1.0
O 2	0.350	0.350	0.156	4.6	1.0
O 3	0.158	0.342	0.25	7.0	1.0
O 4	0.257	0.5	0.213	3.3	1.0

REFINED COMPOSITION: $|(C_{12}N)_4|\ [Si_{96}O_{192}]$

CRYSTAL DATA: *Pnma* (No. 62)
$a = 20.022$ Å $b = 19.899$ Å $c = 13.383$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: H. van Koningsveld, H. van Bekkum and J. C. Jansen, *Acta Cryst.* **B43** 127–132 (1987).

Atom	x	y	z	B_{iso}	occ
Si 1	0.42238	0.05650	-0.33598	1.39	1.0
Si 2	0.30716	0.02772	-0.18930	1.63	1.0
Si 3	0.27911	0.06127	0.03120	1.52	1.0
Si 4	0.12215	0.06298	0.02670	1.43	1.0
Si 5	0.07128	0.02722	-0.18551	1.26	1.0
Si 6	0.18641	0.05896	-0.32818	1.41	1.0
Si 7	0.42265	-0.17250	-0.32718	1.46	1.0
Si 8	0.30778	-0.13016	-0.18548	1.57	1.0
Si 9	0.27554	-0.17279	0.03109	1.39	1.0
Si 10	0.12058	-0.17310	0.02979	1.52	1.0
Si 11	0.07044	-0.13037	-0.18200	1.52	1.0
Si 12	0.18706	-0.17327	-0.31933	1.58	1.0
O 1	0.3726	0.0534	-0.2442	3.87	1.0
O 2	0.3084	0.0587	-0.0789	3.16	1.0
O 3	0.2007	0.0592	0.0289	5.05	1.0
O 4	0.0969	0.0611	-0.0856	3.47	1.0
O 5	0.1149	0.0541	-0.2763	2.68	1.0
O 6	0.2435	0.0553	-0.2460	3.63	1.0
O 7	0.3742	-0.1561	-0.2372	3.71	1.0
O 8	0.3085	-0.1552	-0.0728	3.47	1.0
O 9	0.1980	-0.1554	0.0288	3.16	1.0
O 10	0.0910	-0.1614	-0.0777	4.58	1.0
O 11	0.1169	-0.1578	-0.2694	3.79	1.0
O 12	0.2448	-0.1594	-0.2422	4.34	1.0
O 13	0.3047	-0.0510	-0.1866	5.61	1.0
O 14	0.0768	-0.0519	-0.1769	3.71	1.0
O 15	0.4161	0.1276	-0.3896	3.47	1.0
O 16	0.4086	-0.0017	-0.4136	3.63	1.0
O 17	0.4020	-0.1314	-0.4239	3.16	1.0
O 18	0.1886	0.1298	-0.3836	2.84	1.0
O 19	0.1940	0.0007	-0.4082	3.55	1.0
O 20	0.1951	-0.1291	-0.4190	3.4	1.0
O 21	-0.0037	0.0502	-0.2080	2.61	1.0
O 22	-0.0040	-0.1528	-0.2078	3.16	1.0
O 23	0.4192	-0.2500	-0.3540	3.47	1.0
O 24	0.1884	-0.2500	-0.3538	2.68	1.0
O 25	0.2883	-0.2500	0.0579	2.61	1.0
O 26	0.1085	-0.2500	0.0611	2.37	1.0
N	0.4762	0.250	-0.1095	5.45	1.0
C 1	0.495	0.233	-0.221	4.58	0.3

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Atom	x	y	z	B_{iso}	occ
C 2	0.568	0.250	-0.241	7.66	0.6
C 3	0.578	0.250	-0.362	7.74	0.6
C 4	0.399	0.274	-0.100	5.05	0.3
C 5	0.355	0.228	-0.150	10.74	0.3
C 6	0.278	0.250	-0.147	8.21	0.6
C 7	0.505	0.319	-0.089	5.13	0.3
C 8	0.473	0.334	-0.019	6.55	0.3
C 9	0.496	0.412	0.045	6.95	0.5
C 10	0.508	0.199	-0.032	9.55	0.5
C 11	0.490	0.124	-0.045	8.61	0.5
C 12	0.529	0.088	0.033	5.68	0.5
C 21	0.413	0.229	-0.166	6.55	0.2
C 22	0.355	0.272	-0.150	10.74	0.2
C 23	0.285	0.250	-0.195	8.69	0.4
C 24	0.534	0.279	-0.185	5.29	0.2
C 25	0.546	0.225	-0.263	5.76	0.2
C 26	0.601	0.250	-0.332	10.19	0.4
C 27	0.468	0.315	-0.060	4.82	0.2
C 28	0.516	0.335	0.020	4.82	0.2

REFINED COMPOSITION: $[Si_{96}O_{192}]$

CRYSTAL DATA: $P1\,2_1/n\,1$ (No. 14) unique axis **b**, cell choice 2
$a = 19.879$ Å $b = 20.107$ Å $c = 13.369$ Å
$\alpha = 90°$ $\beta = 90.67°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.045$

REFERENCE: H. van Koningsveld, J. C. Jansen and H. van Bekkum, *Zeolites* **10** 235–242 (1990).

Atom	x	y	z	B_{iso}	occ
Si 1	0.05546	0.42056	-0.31990	0.26	1.0
Si 2	0.03090	0.31368	-0.16358	0.29	1.0
Si 3	0.06249	0.27960	0.05346	0.29	1.0
Si 4	0.06233	0.12395	0.03674	0.29	1.0
Si 5	0.02804	0.07678	-0.15797	0.26	1.0
Si 6	0.05585	0.19556	-0.31331	0.26	1.0
Si 7	-0.17148	0.42542	-0.31930	0.29	1.0
Si 8	-0.12653	0.31225	-0.17388	0.29	1.0
Si 9	-0.17590	0.27325	0.03597	0.26	1.0
Si 10	-0.17634	0.11895	0.03436	0.29	1.0
Si 11	-0.12939	0.07156	-0.17516	0.29	1.0
Si 12	-0.16528	0.19079	-0.31408	0.29	1.0
Si 13	0.44297	0.42837	-0.33456	0.26	1.0
Si 14	0.47305	0.31237	-0.18814	0.29	1.0
Si 15	0.43889	0.27704	0.02940	0.29	1.0
Si 16	0.43563	0.12155	0.03380	0.29	1.0
Si 17	0.47315	0.07096	-0.17844	0.26	1.0
Si 18	0.43778	0.18737	-0.31743	0.29	1.0
Si 19	0.67204	0.42389	-0.31417	0.26	1.0
Si 20	0.63130	0.31278	-0.16836	0.32	1.0
Si 21	0.66892	0.27312	0.04608	0.29	1.0
Si 22	0.67007	0.11867	0.03868	0.29	1.0
Si 23	0.63082	0.07268	-0.17757	0.32	1.0
Si 24	0.68070	0.19446	-0.29789	0.26	1.0
O 1	0.0588	0.3779	-0.2194	0.79	1.0
O 2	0.0662	0.3106	-0.0564	0.63	1.0
O 3	0.0472	0.2018	0.0465	0.92	1.0
O 4	0.0671	0.1032	-0.0784	0.63	1.0
O 5	0.0443	0.1230	-0.2693	0.66	1.0
O 6	0.0477	0.2483	-0.2248	0.89	1.0
O 7	-0.1533	0.3769	-0.2289	0.89	1.0
O 8	-0.1669	0.3050	-0.0725	0.79	1.0
O 9	-0.1558	0.1960	0.0316	0.76	1.0
O 10	-0.1689	0.0885	-0.0753	0.89	1.0
O 11	-0.1511	0.1208	-0.2630	0.87	1.0
O 12	-0.1376	0.2483	-0.2424	0.95	1.0
O 13	-0.0485	0.3189	-0.1490	1.03	1.0
O 14	-0.0509	0.0781	-0.1529	0.74	1.0
O 15	0.1253	0.4145	-0.3771	0.82	1.0
O 16	-0.0041	0.3923	-0.3892	0.87	1.0

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Atom	x	y	z	B_{iso}	occ
O 17	-0.1340	0.4022	-0.4186	0.71	1.0
O 18	0.1298	0.2003	-0.3583	0.63	1.0
O 19	0.0026	0.2099	-0.4008	0.82	1.0
O 20	-0.1275	0.1948	-0.4188	0.68	1.0
O 21	0.0515	0.0032	-0.2041	0.58	1.0
O 22	-0.1475	-0.0023	-0.2098	0.68	1.0
O 23	-0.2501	0.4239	-0.3413	0.82	1.0
O 24	-0.2435	0.1987	-0.3356	0.68	1.0
O 25	-0.2525	0.2822	0.0676	0.61	1.0
O 26	-0.2526	0.1101	0.0697	0.53	1.0
O 27	0.4503	0.3799	-0.2408	0.92	1.0
O 28	0.4480	0.3143	-0.0754	0.68	1.0
O 29	0.4318	0.1991	0.0094	0.82	1.0
O 30	0.4478	0.0812	-0.0669	0.84	1.0
O 31	0.4351	0.1206	-0.2527	0.63	1.0
O 32	0.4401	0.2505	-0.2451	0.79	1.0
O 33	0.6590	0.3797	-0.2169	0.74	1.0
O 34	0.6459	0.3148	-0.0508	0.58	1.0
O 35	0.6513	0.1961	0.0270	0.68	1.0
O 36	0.6559	0.0822	-0.0653	0.92	1.0
O 37	0.6678	0.1232	-0.2504	0.92	1.0
O 38	0.6694	0.2497	-0.2144	0.84	1.0
O 39	0.5530	0.3054	-0.1913	1.05	1.0
O 40	0.5519	0.0851	-0.1834	0.84	1.0
O 41	0.3714	0.4186	-0.3885	0.89	1.0
O 42	0.5015	0.4154	-0.4135	0.76	1.0
O 43	0.6320	0.3938	-0.4087	0.74	1.0
O 44	0.3711	0.1900	-0.3847	0.66	1.0
O 45	0.5032	0.1862	-0.3863	0.74	1.0
O 46	0.6326	0.2074	-0.3914	0.92	1.0
O 47	0.4576	-0.0039	-0.2104	0.66	1.0
O 48	0.6481	-0.0013	-0.2120	0.71	1.0

REFINED COMPOSITION: $[Si_{36}O_{72}]$

CRYSTAL DATA: $Imm2$ (No. 44)
$a = 7.4510$ Å $b = 14.1711$ Å $c = 18.767$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
DLS refinement.

REFERENCE: J. L. Schlenker, J. B. Higgins and E. W. Valyocsik, *Zeolites* **10** 293–296 (1990).

Atom	x	y	z
Si 1	0.0	0.0	0.0
Si 2	0.0	0.2043	0.9486
Si 3	0.0	0.6998	0.7986
Si 4	0.2941	0.0	0.1176
Si 5	0.2057	0.1963	0.1848
Si 6	0.2939	0.7017	0.0427
Si 7	0.0	0.5	0.8668
Si 8	0.2945	0.5	0.9848
O 1	0.0	0.0915	0.9503
O 2	0.1754	0.0	0.0473
O 3	0.0	0.2369	0.8678
O 4	0.1755	0.2405	0.9876
O 5	0.8255	0.7253	0.7524
O 6	0.0	0.5912	0.8173
O 7	0.5	0.0	0.0946
O 8	0.2531	0.0916	0.1632
O 9	0.0	0.2031	0.2079
O 10	0.2441	0.2688	0.1221
O 11	0.5	0.7234	0.0276
O 12	0.5	0.5	0.9611
O 13	0.1748	0.5	0.9149
O 14	0.2570	0.5917	0.0319

MON Montesommaite

REFINED COMPOSITION: $|K_{4.24}(H_2O)_4|\ [Si_{11.3}Al_{4.7}O_{32}]$
Pollena, Mt. Somma-Vesuvius, Italy

CRYSTAL DATA: $I\,4_1/a\,md$ (No. 141) origin at centre $(2/m)$
$a = 7.141$ Å $b = 7.141$ Å $c = 17.307$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray powder refinement of idealized substructure, $R = 0.10$

REFERENCE: R. C. Rouse, P. J. Dunn, J. D. Grice, J. L. Schlenker and J. B. Higgins, *American Mineralogist* **75** 1415–1420 (1990).

Atom	x	y	z	B_{iso}	occ
K	0.000	0.000	0.500	1.97	0.53
Si	0.000	0.463	0.090	0.39	0.706
Al	0.000	0.463	0.090	0.39	0.294
O 1	0.000	0.250	0.116	1.18	1.0
O 2	0.186	0.436	0.875	1.18	1.0
O 3	0.000	0.000	0.000	1.18	1.0
H_2O	0.000	0.250	0.342	1.18	0.5

REFINED COMPOSITION: $|Na_8(H_2O)_{25}|\ [Si_{40}Al_8O_{96}]$
Challis, Idaho, U.S.A.

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 18.11$ Å $b = 20.53$ Å $c = 7.528$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: V. Gramlich,
PhD dissertation, ETH, Zurich, (1971).
And V. Gramlich, Private communication.

Atom	x	y	z	B_{iso}	occ
Na 1	0.0	0.5	0.0	2.50	1.0
Na 2	0.0	0.4335	0.75	4.95	1.0
Si 1	0.19897	0.42771	0.5418	1.37	1.0
Si 2	0.19656	0.19092	0.5454	1.49	1.0
Si 3	0.0871	0.3840	0.25	1.21	0.5
Si 4	0.0866	0.2280	0.25	1.32	0.5
Al 3	0.0871	0.3840	0.25	1.21	0.5
Al 4	0.0866	0.2280	0.25	1.32	0.5
O 1	0.1232	0.4170	0.4292	3.09	1.0
O 2	0.1226	0.1946	0.4262	2.95	1.0
O 3	0.2632	0.3776	0.4887	3.63	1.0
O 4	0.0974	0.3057	0.25	3.61	1.0
O 5	0.1694	0.1946	0.75	3.62	1.0
O 6	0.1769	0.4212	0.75	2.66	1.0
O 7	0.2324	0.5	0.5	2.35	1.0
O 8	0.25	0.25	0.5	4.72	1.0
O 9	0.0	0.4071	0.25	2.17	1.0
O 10	0.0	0.2061	0.25	3.00	1.0
H_2O 1	0.040	0.303	0.75	16.32	0.5
H_2O 2	0.0	0.181	0.75	13.84	1.0
H_2O 3	0.0	0.094	0.502	21.32	1.0
H_2O 4	0.109	0.030	0.75	17.5	1.0
H_2O 5	0.0	-0.009	0.25	22.84	0.25

REFINED COMPOSITION: $|Pb_{10.68}(H_2O)_{26.5}O_4|\ [Si_{36.38}Al_{11.02}O_{100}]$
Moon Anchor Mine, Tonopah, AZ, U.S.A.

CRYSTAL DATA: $Cm2m$ (No. 38) **bca** setting
$a = 19.432$ Å $b = 19.702$ Å $c = 7.538$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.051$

REFERENCE: R. C. Rouse and D. R. Peacor,
American Mineralogist **79** 175–184 (1994).

Atom	x	y	z	B_{iso}	occ
Pb 1	0.0975	0.1044	0.500	2.25	0.83
Pb 2	0.0977	0.8988	0.0	1.83	0.245
Pb 3	0.0	0.9662	0.2377	2.29	0.622
Pb 4	0.0	0.0359	0.2516	3.4	0.175
Si 1	0.1790	0.2907	0.2956	1.17	0.736
Si 2	0.3211	0.2169	0.2043	1.38	0.735
Si 3	0.2546	0.9283	0.2076	1.18	0.736
Si 4	0.1395	0.9238	0.500	1.0	0.736
Si 5	0.1342	0.0843	0.0	1.1	1.0
Si 6	0.2554	0.0779	0.2885	1.26	0.736
Si 7	0.0794	0.2311	0.0	1.6	0.736
Si 8	0.0817	0.7763	0.500	1.1	0.736
Al 1	0.1790	0.2907	0.2956	1.17	0.264
Al 2	0.3211	0.2169	0.2043	1.38	0.264
Al 3	0.2546	0.9283	0.2076	1.18	0.264
Al 4	0.1395	0.9238	0.500	1.0	0.234
Al 6	0.2554	0.0779	0.2885	1.26	0.234
Al 7	0.0794	0.2311	0.0	1.6	0.234
Al 8	0.0817	0.7763	0.500	1.1	0.234
O 1	0.1861	0.9200	0.3250	2.9	1.0
O 2	0.0810	0.144	0.0	2.3	1.0
O 3	0.0932	0.9916	0.500	3.8	1.0
O 4	0.0862	0.8586	0.500	1.4	1.0
O 5	0.3443	0.2307	0.0	2.2	1.0
O 6	0.1820	0.0864	0.1811	1.7	1.0
O 7	0.3134	0.1342	0.2417	2.3	1.0
O 8	0.1607	0.2769	0.500	3.5	1.0
O 9	0.0863	0.0162	0.0	2.4	1.0
O 10	0.1865	0.3708	0.2641	2.0	1.0
O 11	0.2500	0.2536	0.2506	3.6	1.0
O 12	0.1164	0.2604	0.1761	3.0	1.0
O 13	0.3832	0.2424	0.3218	3.3	1.0
O 14	0.2897	0.0030	0.2460	2.5	1.0
O 15	0.2278	0.9219	0.0	2.5	1.0
O 16	0.2340	0.0838	0.500	2.0	1.0
O 17	0.0	0.2530	0.0	2.5	1.0
O 18	0.0	0.7557	0.500	2.6	1.0
H_2O 19	0.0	0.0828	0.3098	2.2	0.925
H_2O 20	0.0	0.231	0.500	2.6	0.95

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Atom	x	y	z	B_{iso}	occ
H_2O 21	0.085	0.561	0.0	2.6	0.6
H_2O 22	0.0	0.501	0.099	2.6	0.5
H_2O 23	0.061	0.594	0.500	2.6	0.275
H_2O 24	0.077	0.456	0.241	2.6	0.175
H_2O 25	0.074	0.457	0.385	2.6	0.2
H_2O 26	0.079	0.871	0.0	2.6	0.575
H_2O 27	0.070	0.151	0.500	2.6	0.175
H_2O 28	0.0	0.933	0.215	2.6	0.475

Interrupted mordenite framework. O3 and O9 are terminal oxygens, where the framework is not fully connected.

REFINED COMPOSITION: $|K_{9.38}C_{12}H_{48}|\ [Si_{36}O_{78}]$

CRYSTAL DATA: $R\bar{3}m$ (No. 166) rhombohedral setting
$a = 11.841$ Å $b = 11.841$ Å $c = 11.841$ Å
$\alpha = 93.29°$ $\beta = 93.29°$ $\gamma = 93.29°$
X-ray Rietveld refinement, $R_p = 0.0533$, $R_{wp} = 0.0704$

REFERENCE: D. F. Shantz, A. Burton and R. F. Lobo,
Microporous and Mesoporous Materials **31** 61–73 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	-0.0002	0.1797	0.2725	0.58	1.0
Si 2	0.0002	0.1795	0.1129	0.58	1.0
Si 3	0.0	0.3073	0.0	0.58	1.0
O 1	0.093	0.1861	0.295	1.43	1.0
O 2	0.9232	0.0768	0.2889	1.43	1.0
O 3	0.9845	0.2469	0.32	1.43	1.0
O 4	-0.0012	0.2058	0.1927	1.43	1.0
O 5	0.0755	0.151	0.1005	1.43	1.0
O 6	0.0205	0.2648	0.0667	1.43	1.0
O 7	0.9044	0.0955	0.09	1.43	1.0
K 1	-0.6667	-0.3333	0.2355	6.59	0.5
K 2	0.0	0.0	0.0057	6.9	0.344
K 3	-0.6667	-0.3333	0.2829	1.7	0.167
C	0.5504	-0.2694	0.1662	10.0	1.0
O 8	-0.5198	-0.3338	0.1231	9.86	0.5
H	-0.5346	-0.0692	0.1486	12.0	4.0

Typographic errors in the published coordinates for O2 and O6 have been corrected.

REFINED COMPOSITION: $[Si_{44}O_{88}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.5000$ Å $b = 30.7096$ Å $c = 7.3133$ Å
$\alpha = 90.0°$ $\beta = 91.7113°$ $\gamma = 90.0°$
X-ray synchrotron Rietveld refinement, $R_p = 0.0729$, $R_{wp} = 0.0916$, $R_b = 0.0302$

REFERENCE: P. A. Barrett, M.-J. Diaz-Cabanas and M. A. Camblor,
Chemistry of Materials **11** 2919–2927 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0	0.08356	0.0	0.41	1.0
Si 2	0.191	0.15359	-0.1667	1.25	1.0
Si 3	-0.0048	0.22858	-0.2913	0.29	1.0
Si 4	-0.1271	0.04862	-0.371	0.73	1.0
Si 5	-0.3049	0.19803	-0.1822	0.47	1.0
Si 6	-0.3391	0.12303	-0.4749	0.24	1.0
O 1	-0.0756	0.05227	-0.1609	1.62	1.0
O 2	-0.5	0.10684	-0.5	1.62	1.0
O 3	0.0	0.23506	-0.5	1.62	1.0
O 4	0.0	0.06345	-0.5	1.62	1.0
O 5	0.2923	0.17606	-0.0075	1.62	1.0
O 6	-0.2593	0.08102	-0.4062	1.62	1.0
O 7	0.0624	0.269	-0.1981	1.62	1.0
O 8	0.1281	0.11111	-0.0804	1.62	1.0
O 9	-0.2807	0.13899	-0.6705	1.62	1.0
O 10	0.0798	0.18695	-0.2331	1.62	1.0
O 11	-0.1766	0.0	-0.4029	1.62	1.0
O 12	-0.1646	0.22635	-0.223	1.62	1.0
O 13	-0.3268	0.16144	-0.3269	1.62	1.0

MTN Dodecasil 3C

REFINED COMPOSITION: $|N_{24}|\ [Si_{136}O_{272}]$

CRYSTAL DATA: $Fd\overline{3}$ (No. 203) origin at centre ($\overline{3}$)
$a = 19.402$ Å $b = 19.402$ Å $c = 19.402$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.06$

REFERENCE: H. Gies,
Z. Kristallogr. **167** 73–82 (1984).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0676	0.0676	0.3700	2.04	1.0
Si 2	0.2164	0.2164	0.2164	1.53	1.0
Si 3	0.125	0.125	0.125	1.42	1.0
O 1	0.0932	0.4065	-0.0001	4.97	1.0
O 2	0.0433	0.2995	0.4505	6.24	1.0
O 3	0.125	0.3734	0.125	4.29	1.0
O 4	0.1704	0.1704	0.1704	9.32	1.0
N 1	0.0	0.0	0.0	20.0	1.0
N 2	0.625	0.625	0.625	20.0	1.0

REFINED COMPOSITION: $|(NH_4F)_{1.72}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: $P12_11$ (No. 4) unique axis **b**
$a = 11.129$ Å $b = 5.025$ Å $c = 21.519$ Å
$\alpha = 90°$ $\beta = 89.85°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.033$, $R_{wp} = 0.085$, $R_F = 0.089$

REFERENCE: B. Marler, C. Deroche, H. Gies, C. A. Fyfe, H. Grondey, G. T. Kokotailo, Y. Feng, S. Ernst, J. Weitkamp and D. E. Cox, *J. Appl. Cryst.* **26** 636–644 (1993).

Atom	x	y	z	B_{iso}	occ
Si 1	-0.009	-0.02	0.4578	1.10	1.0
Si 2	0.726	-0.082	0.425	1.10	1.0
Si 3	0.228	-0.112	0.384	1.10	1.0
Si 4	0.312	0.00	0.251	1.10	1.0
Si 5	0.476	0.503	0.249	1.10	1.0
Si 6	0.346	0.390	0.434	1.10	1.0
Si 7	0.600	0.417	0.378	1.10	1.0
Si 8	-0.010	-0.10	0.0422	1.10	1.0
Si 9	0.726	-0.012	0.077	1.10	1.0
Si 10	0.232	-0.077	0.118	1.10	1.0
Si 11	0.355	0.424	0.063	1.10	1.0
Si 12	0.603	0.487	0.120	1.10	1.0
O 1	0.012	0.27	0.487	1.03	1.0
O 2	0.866	-0.02	0.422	1.03	1.0
O 3	0.093	-0.09	0.408	1.03	1.0
O 4	0.683	-0.04	0.495	1.03	1.0
O 5	0.655	0.122	0.381	1.03	1.0
O 6	0.231	-0.05	0.311	1.03	1.0
O 7	0.317	0.085	0.419	1.03	1.0
O 8	0.368	0.292	0.254	1.03	1.0
O 9	0.564	0.49	0.308	1.03	1.0
O 10	0.486	0.44	0.423	1.03	1.0
O 11	0.866	-0.07	0.079	1.03	1.0
O 12	0.100	-0.05	0.089	1.03	1.0
O 13	0.679	-0.03	0.008	1.03	1.0
O 14	0.226	-0.03	0.192	1.03	1.0
O 15	0.553	0.43	0.189	1.03	1.0
O 16	0.497	0.46	0.071	1.03	1.0
O 17	0.708	0.28	0.103	1.03	1.0
O 18	0.322	0.130	0.086	1.03	1.0
O 19	-0.001	0.11	-0.014	1.03	1.0
O 20	0.701	0.621	0.401	1.03	1.0
O 21	0.269	0.584	0.392	1.03	1.0
O 22	0.422	0.797	0.246	1.03	1.0
O 23	0.652	0.786	0.120	1.03	1.0
O 24	0.285	0.632	0.106	1.03	1.0
F	0.938	0.55	0.215	31.58	0.86
N	0.89	0.06	0.261	31.58	0.86

MTW ZSM-12, Calcined

REFINED COMPOSITION: $[Si_{56}O_{112}]$

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 24.8633$ Å $b = 5.01238$ Å $c = 24.3275$ Å
$\alpha = 90°$ $\beta = 107.7215°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.058$, $R_{wp} = 0.181$, $R_I = 0.069$

REFERENCE: C. A. Fyfe, H. Gies, G. T. Kokotailo, B. Marler and D. E. Cox, *J. Phys. Chem.* **94** 3718–3721 (1990).

Atom	x	y	z
Si 1	0.4402	0.5319	0.4129
Si 2	0.0678	-0.0708	0.4589
Si 3	0.3754	0.0320	0.3609
Si 4	0.1338	0.4218	0.4484
Si 5	0.2836	0.0822	0.4275
Si 6	0.2139	0.5853	0.3832
Si 7	0.2869	0.0100	0.2463
O 1	0.4280	0.5053	0.4730
O 2	0.5034	0.4725	0.4225
O 3	0.4245	0.8220	0.3872
O 4	0.3301	-0.0045	0.3956
O 5	0.0841	-0.3624	0.4513
O 6	0.3452	-0.0218	0.2972
O 7	0.2504	0.2441	0.2629
O 8	0.2602	0.3716	0.4078
O 9	0.1554	0.5101	0.3911
O 10	0.1853	0.4480	0.5026
O 11	0.2997	0.0905	0.1886
O 12	0.3995	0.3370	0.3702
O 13	0.1069	0.1372	0.4394
O 14	0.2343	0.8828	0.4093

Overall thermal parameter $B_{iso} = 0.01$ was used in the refinement.

ITQ-1, Calcined (Siliceous MCM-22) MWW

REFINED COMPOSITION: $[Si_{72}O_{144}]$

CRYSTAL DATA: $P6/mmm$ (No. 191)
$a = 14.2081$ Å $b = 14.2081$ Å $c = 24.945$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement. $R_{exp} = 0.103$, $R_{wp} = 0.159$, $R_F = 0.065$

REFERENCE: M. A. Camblor, A. Corma, M.-J. Diaz-Cabanas and Ch. Baerlocher, *J. Phys. Chem. B* **102** 44–51 (1998).

Atom	x	y	z	B_{iso}	occ
Si 1	0.6667	0.3333	0.0633	1.10	1.0
Si 2	0.4685	0.2342	0.1356	1.10	1.0
Si 3	0.3904	0.0000	0.1607	1.10	1.0
Si 4	0.6667	0.3333	0.2108	1.10	1.0
Si 5	0.6667	0.3333	0.3404	1.10	1.0
Si 6	0.3895	0.0000	0.2872	1.10	1.0
Si 7	0.4215	0.2108	0.3470	1.10	1.0
Si 8	0.2544	0.1272	0.4407	1.10	1.0
O 1	0.6667	0.3333	0.0000	1.50	1.0
O 2	0.5411	0.2705	0.0822	1.50	1.0
O 3	0.3942	0.1048	0.1348	1.50	1.0
O 4	0.5453	0.2726	0.1882	1.50	1.0
O 5	0.6667	0.3333	0.2755	1.50	1.0
O 6	0.3763	0.0000	0.2239	1.50	1.0
O 7	0.5000	0.0000	0.1449	1.50	1.0
O 8	0.5000	0.0000	0.3021	1.50	1.0
O 9	0.3945	0.1063	0.3116	1.50	1.0
O 10	0.5469	0.2735	0.3638	1.50	1.0
O 11	0.3536	0.1768	0.4014	1.50	1.0
O 12	0.1835	0.0000	0.4300	1.50	1.0
O 13	0.3017	0.1508	0.5000	1.50	1.0

NAT Natrolite

REFINED COMPOSITION: $|Na_{16}(H_2O)_{16}|\ [Si_{24}Al_{16}O_{80}]$
Aussig, Bohemia

CRYSTAL DATA: *Fdd*2 (No. 43)
$a = 18.30$ Å $b = 18.63$ Å $c = 6.60$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{wp} = 0.08$

REFERENCE: W. M. Meier,
Z. Kristallogr. **113** 430–444 (1960).

Atom	x	y	z	B_{iso}	occ
Na	0.2208	0.0305	0.6120	2.00	1.0
Si 1	0.0	0.0	0.0	1.07	1.0
Si 2	0.1532	0.2112	0.6181	1.0	1.0
Al	0.0376	0.0936	0.6119	1.12	1.0
O 1	0.0227	0.0683	0.8594	1.81	1.0
O 2	0.0704	0.1824	0.6011	1.10	1.0
O 3	0.0986	0.0346	0.4997	1.55	1.0
O 4	0.2063	0.1526	0.7166	1.24	1.0
O 5	0.1799	0.2272	0.3860	1.83	1.0
H_2O	0.0564	0.1893	0.1085	2.50	1.0

REFINED COMPOSITION: $|Na_{6.528}Ca_{1.472}(H_2O)_{12}H_8|\ [Si_{10.25}Al_{9.75}O_{40}]$
Tvedalen, Langesund District, Norway

CRYSTAL DATA: $I\bar{4}2d$ (No. 122)
$a = 13.21$ Å $b = 13.21$ Å $c = 6.622$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.03$

REFERENCE: F. Mazzi, A. O. Larsen, G. Gottardi and E. Galli, *Neues Jarhb. Mineral. Monatsh.* 219–228 (1986).

Atom	x	y	z	B_{iso}	occ
Na^+	0.3084	0.2500	0.1250	2.35	0.816
Ca^{2+}	0.3084	0.2500	0.1250	2.35	0.184
Si	0.0	0.0	0.0	0.84	0.284
Si^{4+}	0.0	0.0	0.0	0.84	0.29
Si	0.1332	0.0536	0.3789	0.78	0.292
Si^{4+}	0.1332	0.0536	0.3789	0.78	0.205
Al	0.0	0.0	0.0	0.84	0.189
Al^{3+}	0.0	0.0	0.0	0.84	0.237
Al	0.1332	0.0536	0.3789	0.78	0.238
Al^{3+}	0.1332	0.0536	0.3789	0.78	0.265
O	0.25	0.1037	0.375	1.16	0.271
O^{2-}	0.25	0.1037	0.375	1.16	0.729
O	0.0917	0.4497	0.1094	1.71	0.271
O^{2-}	0.0917	0.4497	0.1094	1.71	0.729
O	0.4369	0.3674	0.0210	1.64	0.271
O^{2-}	0.4369	0.3674	0.0210	1.64	0.729
H_2O	0.2500	0.3652	0.3750	3.36	1.0
H_2O	0.1280	0.2434	0.0545	6.02	0.25
H	0.2500	0.4272	0.3750	0.11	1.0

Occupancy of second Si^{4+} site has been corrected from 0.265 to 0.205.

NAT Mesolite

REFINED COMPOSITION: $|Na_{16}Ca_{16}(H_2O)_{64}|\ [Si_{72}Al_{48}O_{240}]$
Poona, India

CRYSTAL DATA: $Fdd2$ (No. 43)
$a = 18.4049$ Å $b = 56.655$ Å $c = 6.5443$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.052$

REFERENCE: G. Artioli, J. V. Smith and J. J. Pluth,
Acta Cryst. **C42** 937–942 (1986).

Atom	x	y	z	B_{iso}	occ
Na	0.96736	0.76089	0.63172	1.48	1.0
Ca	0.22807	0.82737	0.88068	0.91	1.0
Si 1	0.75000	0.75000	0.00000	0.55	1.0
Si 2	0.15499	0.76432	0.87210	0.48	1.0
Si 3	0.90188	0.81979	0.65040	0.50	1.0
Si 4	0.08794	0.84688	0.65213	0.52	1.0
Si 5	0.00435	0.83180	0.27740	0.53	1.0
Al 1	0.78689	0.78025	0.61310	0.50	1.0
Al 2	0.03630	0.80211	0.89287	0.52	1.0
Al 3	0.95155	0.86233	0.89294	0.51	1.0
O 1	0.76818	0.77289	0.86482	1.03	1.0
O 2	0.02298	0.80800	0.15228	0.98	1.0
O 3	0.98498	0.85319	0.12809	1.18	1.0
O 4	0.82365	0.80837	0.59682	0.70	1.0
O 5	0.07262	0.77385	0.86425	0.72	1.0
O 6	0.16644	0.85935	0.67096	0.83	1.0
O 7	0.84335	0.75866	0.51529	1.00	1.0
O 8	0.09631	0.82339	0.79447	0.93	1.0
O 9	0.88933	0.84183	0.80185	0.98	1.0
O 10	0.95568	0.80062	0.75319	1.06	1.0
O 11	0.20947	0.78462	0.95950	0.86	1.0
O 12	0.02193	0.86358	0.71805	1.00	1.0
O 13	0.93735	0.82799	0.43383	1.09	1.0
O 14	0.18020	0.75695	0.64166	1.06	1.0
O 15	0.07638	0.83892	0.41273	0.99	1.0
H 11	0.0450	0.7813	0.322	0.7	1.0
H 12	0.0881	0.7679	0.420	0.9	1.0
H 21	0.7773	0.8037	0.018	1.0	1.0
H 22	0.8085	0.8232	0.004	2.7	1.0
H 31	0.2274	0.8560	0.247	2.1	1.0
H 32	0.1685	0.8438	0.260	1.2	1.0
H 41	0.8072	0.8702	0.387	0.6	1.0
H 42	0.8615	0.8525	0.359	2.0	1.0
O 21	0.05347	0.76839	0.37684	1.67	1.0
O 22	0.78167	0.81598	0.07685	2.83	1.0
O 23	0.20069	0.84820	0.18338	2.46	1.0
O 24	0.81793	0.85687	0.36556	2.05	1.0

REFINED COMPOSITION: $|Ca_4(H_2O)_{12}|\ [Si_{12}Al_8O_{40}]$
Bombay, India

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 6.5222$ Å $b = 18.9678$ Å $c = 9.8398$ Å
$\alpha = 90°$ $\beta = 109.972°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.031$

REFERENCE: J. V. Smith, J. J. Pluth, G. Artioli and F. K. Ross,
in *Proceedings of the 6th International Zeolite Conference, Reno 1983*,
Ed. by D. H. Olson and A. Bisio (Butterworth: Guildford) 842–850 (1984).

Atom	x	y	z	B_{iso}	occ
Ca	0.16217	0.14321	0.05204	0.76	1.0
Si 1	0.5	0.37057	0.0	0.44	1.0
Si 2	0.22996	0.33185	0.20022	0.43	1.0
Si 3	0.54002	0.08259	0.33102	0.42	1.0
Al 1	0.93441	0.46209	0.09971	0.45	1.0
Al 2	0.35577	0.21663	0.43387	0.43	1.0
O 1	0.5425	0.03146	0.4608	0.85	1.0
O 2	0.4471	0.04597	0.1174	0.66	1.0
O 3	0.3834	0.15127	0.3157	0.77	1.0
O 4	0.1153	0.19942	0.4684	0.79	1.0
O 5	0.3536	0.29954	0.3584	0.63	1.0
O 6	0.0863	0.27133	0.0907	0.80	1.0
O 7	0.4143	0.35860	0.1343	0.91	1.0
O 8	0.0764	0.39545	0.2150	0.89	1.0
O 9	0.7889	0.11007	0.3566	0.82	1.0
O 10	0.6603	0.43692	0.0339	0.92	1.0
H_2O 1	0.8906	0.0803	0.1082	2.22	1.0
H_2O 2	0.9080	0.3263	0.4407	2.33	1.0
H_2O 3	0.5787	0.4454	0.3742	1.81	1.0

REFINED COMPOSITION: $|(H_2O)_{20}|\ [Si_{68}O_{136}]$

CRYSTAL DATA: $P1\,2_1/c\,1$ (No. 14) unique axis **b**, cell choice 1
$a = 14.324$ Å $b = 22.376$ Å $c = 25.092$ Å
$\alpha = 90°$ $\beta = 151.515°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.075$, $R_{wp} = 0.14$, $R_I = 0.065$

REFERENCE: M. D. Shannon, J. L. Casci, P. A. Cox and S. J. Andrews, *Nature* **353** 417–420 (1991).

Atom	x	y	z
Si 1	0.640	0.1717	0.324
Si 2	0.473	0.1970	0.738
Si 3	0.028	0.2218	0.500
Si 4	0.228	0.0010	0.178
Si 5	0.226	0.0039	0.048
Si 6	0.412	0.1280	0.108
Si 7	0.421	0.1200	0.308
Si 8	0.666	0.1299	0.737
Si 9	0.654	0.1237	0.924
Si 10	0.606	0.1816	0.496
Si 11	0.604	0.1838	0.109
Si 12	0.456	0.1822	0.536
Si 13	0.451	0.1837	0.917
Si 14	0.035	0.1941	0.100
Si 15	0.038	0.2969	0.406
Si 16	0.033	0.2154	0.307
Si 17	0.031	0.2175	0.697
O 1	0.242	0.009	0.121
O 2	0.550	0.2367	0.284
O 3	0.870	0.1734	0.434
O 4	0.242	0.194	0.614
O 5	0.588	0.133	0.349
O 6	0.553	0.141	0.228
O 7	0.579	0.168	0.741
O 8	0.533	0.159	0.818
O 9	0.002	0.2773	0.526
O 10	-0.006	0.2429	0.423
O 11	0.001	0.003	0.083
O 12	0.350	0.0523	0.269
O 13	0.318	0.0626	0.066
O 14	0.675	0.0611	0.757
O 15	0.651	0.0530	0.911
O 16	0.240	0.163	0.206
O 17	0.244	0.1761	0.023
O 18	0.880	0.152	0.833
O 19	0.873	0.146	1.031
O 20	0.508	0.133	0.409
O 21	0.535	0.134	0.116
O 22	0.533	0.137	0.619
O 23	0.563	0.138	0.935

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Atom	x	y	z
O 24	0.521	0.2479	0.440
O 25	0.526	0.2499	0.587
O 26	0.555	0.163	0.531
O 27	0.509	0.167	0.006
O 28	0.838	0.178	0.605
O 29	0.837	0.180	0.221
O 30	0.223	0.176	0.414
O 31	0.219	0.176	0.793
O 32	0.026	0.2544	0.640
O 33	0.037	0.2734	0.345
O 34	0.036	0.2360	0.2480
H_2O 1	0.233	0.037	0.568
H_2O 2	0.39	0.016	0.917
H_2O 3	0.08	0.044	0.268
H_2O 4	-0.03	0.037	0.313
H_2O 5	0.01	0.065	0.61

No temperature factors or occupancies were reported.

REFINED COMPOSITION: $|Na_{66.8}|^{\dagger}$ $[Si_{115.6}Al_{20.4}O_{272}]$
Mt. Adamson, Northern Victoria Land, Antarctica

CRYSTAL DATA: *Cmce* (No. 64)
$a = 13.698$ Å $b = 25.213$ Å $c = 22.660$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_F = 0.1195$, $R_w = 0.0968$

REFERENCE: A. Alberti, G. Vezzalini, E. Galli and S. Quartieri, *Eur. J. Mineral.* **8** 69–75 (1996).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0	0.0804	0.1973	1.18	0.85
Si 2	0.0	0.1784	0.2828	1.47	0.85
Si 3	0.0	0.2884	0.2204	1.39	0.85
Si 4	0.0	0.3841	0.3023	1.34	0.85
Si 5	0.0	0.4818	0.2235	1.68	0.85
Si 6	0.2102	0.0023	0.316	1.95	0.85
Si 7	0.1934	0.0978	0.1253	1.34	0.85
Si 8	0.2122	0.1948	0.3174	1.11	0.85
Si 9	0.2143	0.3111	0.1846	1.32	0.85
Si 10	0.1873	0.4049	0.3752	1.18	0.85
Si 11	0.1151	0.0634	0.0009	1.53	0.85
Al 1	0.0	0.0804	0.1973	1.18	0.15
Al 2	0.0	0.1784	0.2828	1.47	0.15
Al 3	0.0	0.2884	0.2204	1.39	0.15
Al 4	0.0	0.3841	0.3023	1.34	0.15
Al 5	0.0	0.4818	0.2235	1.68	0.15
Al 6	0.2102	0.0023	0.316	1.95	0.15
Al 7	0.1934	0.0978	0.1253	1.34	0.15
Al 8	0.2122	0.1948	0.3174	1.11	0.15
Al 9	0.2143	0.3111	0.1846	1.32	0.15
Al 10	0.1873	0.4049	0.3752	1.18	0.15
Al 11	0.1151	0.0634	0.0009	1.53	0.15
O 1	0.0	0.0208	0.2214	3.92	1.0
O 2	0.0969	0.0897	0.1594	5.84	1.0
O 3	0.0	0.1213	0.2499	3.76	1.0
O 4	0.0955	0.1833	0.3238	2.63	1.0
O 5	0.0	0.2249	0.2361	3.11	1.0
O 6	0.0928	0.304	0.181	2.87	1.0
O 7	0.0	0.3225	0.2802	2.53	1.0
O 8	0.084	0.395	0.3443	6.37	1.0
O 9	0.0	0.4225	0.2462	6.55	1.0
O 10	0.0928	0.492	0.1818	3.74	1.0
O 11	0.228	0.1576	0.135	2.66	1.0
O 12	0.2242	0.0598	0.3504	3.61	1.0
O 13	0.2381	0.4586	0.3559	5.9	1.0
O 14	0.1754	0.0893	0.0555	3.0	1.0
O 15	0.2329	0.2564	0.3357	3.16	1.0
O 16	0.25	0.1829	0.25	2.03	1.0
O 17	0.2381	0.3553	0.1332	2.79	1.0

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Atom	x	y	z	B_{iso}	occ
O 18	0.25	0.329	0.25	1.89	1.0
O 19	0.25	0.005	0.25	5.66	1.0
O 20	0.0	0.0807	0.0048	2.82	1.0
O 21	0.1276	0.0	0.0	3.26	1.0
O 22	0.1627	0.4084	0.4406	5.34	1.0
Na 1	0.0	0.386	0.999	1.7	0.48
Na 2	0.0	0.183	0.43	4.6	0.77
Na 3	0.0	0.263	0.996	3.9	0.45
Na 4	0.0	0.081	0.404	6.5	0.64
Na 5	0.067	0.281	0.421	9.1	0.59
Na 6	0.121	0.458	0.019	3.9	0.24
Na 7	0.0	0.192	0.071	11.0	0.57
Na 8	0.151	0.349	0.994	6.6	0.4
Na 9	0.0	0.39	0.103	8.9	0.63
Na 10	0.12	0.268	0.558	9.4	0.56
Na 11	0.193	0.271	0.473	12.3	0.36
Na 12	0.0	0.301	0.064	8.9	0.51

In editions of the *International Tables For Crystallography* published after 1995, space group symbol *Cmce* replaces *Cmca*.

[†]Na atoms have been used to represent the average scattering curve for the unresolved cations and water in the channels which, from chemical analysis, amount to $Na_{2.5}K_{0.2}Mg_{3.1}Ca_{4.9}(H_2O)_{93}$ per unit cell. The refinement accounts for only 59% of these extraframework electrons.

NON 2-aminopentane Nonasil

REFINED COMPOSITION: $|C_{36}|\ [Si_{88}O_{176}]$

CRYSTAL DATA: *Fmmm* (No. 69)
$a = 22.232$ Å $b = 15.058$ Å $c = 13.627$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.125$

REFERENCE: B. Marler, N. Dehnbostel, H. H. Eulert, H. Gies and F. Liebau, *J. Inclusion Phenomena* **4** 339–349 (1986).

Atom	x	y	z	B_{iso}	occ
Si 1	0.3745	0.1635	0.3103	1.66	1.0
Si 2	0.2798	0.5000	0.5000	2.05	1.0
Si 3	0.2950	0.3270	0.0000	2.84	1.0
Si 4	0.5000	0.1051	0.6156	0.32	1.0
Si 5	0.3173	0.5000	0.2831	2.29	1.0
O 1	0.3356	0.3282	0.9056	5.13	1.0
O 2	0.4427	0.1462	0.3374	1.97	1.0
O 3	0.3520	0.4050	0.2525	10.11	1.0
O 4	0.2702	0.4329	0.0000	12.79	1.0
O 5	0.3197	0.5000	0.5937	3.4	1.0
O 6	0.3667	0.2500	0.2500	17.13	1.0
O 7	0.0000	0.0000	0.1392	2.05	1.0
O 8	0.5000	0.1155	0.5000	0.39	1.0
O 9	0.2500	0.0000	0.2500	1.82	1.0
O 10	0.2500	0.2500	0.0000	9.95	1.0
C 1	0.5000	0.4489	0.5700	19.11	1.0
C 2	0.4659	0.3547	0.5000	10.11	1.0
C 3	0.0000	0.0000	0.5000	32.37	1.0

REFINED COMPOSITION: $|KMgCa_{1.32}O_{16.04}|\ [Si_{12.6}Al_{5.4}O_{36}]$
Poia Creek, Adamello, Italy

CRYSTAL DATA: $P\overline{6}m2$ (No. 187)
$a = 13.331$ Å $b = 13.291$ Å $c = 7.593$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.058$, $R_w = 0.038$

REFERENCE: A. Alberti, G. Cruciani, E. Galli and G. Vezzalini, *Zeolites* **17** 457–461 (1996).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0007	0.2334	0.2089	0.92	0.7
Si 2	0.0923	0.4236	0.5	0.71	0.7
Al 1	0.0007	0.2334	0.2089	0.92	0.3
Al 2	0.0923	0.4236	0.5	0.71	0.3
O 1	0.0243	0.3486	0.3213	2.21	1.0
O 2	0.0961	0.9039	0.2558	1.72	1.0
O 3	0.8738	0.1262	0.2603	2.5	1.0
O 4	0.0103	0.2718	0.0	2.46	1.0
O 5	0.2286	0.7714	0.5	2.38	1.0
O 6	0.4570	0.5430	0.5	2.01	1.0
K	0.0	0.0	0.5	2.37	1.0
Mg	0.3333	0.6667	0.0	1.62	1.0
Ca 1	0.6667	0.3333	0.3947	2.25	0.32
Ca 2	0.6667	0.3333	0.2812	6.61	0.34
O 7	0.3333	0.6667	0.2676	2.10	1.0
O 8	0.2446	0.7554	0.0	3.86	0.38
O 9	0.1670	0.5266	0.0	5.97	0.48
O 10	0.7635	0.2365	0.5	6.43	1.0
O 11	-0.4369	0.4369	0.1881	10.2	1.0
O 12	0.2310	0.2310	0.0	2.6	0.17

REFINED COMPOSITION: $[Al_{16}P_{16}O_{64}]$

CRYSTAL DATA: $Imm2$ (No. 44)
$a = 18.3549$ Å $b = 18.3206$ Å $c = 5.0530$ Å
$\alpha = 90.0°$ $\beta = 90.0°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.044$, $R_{wp} = 0.059$

REFERENCE: D. E. Akporiaye, H. Fjellvåg, E. N. Halvorsen, T. Haug, A. Karlsson, and K. P Lillerud, *J. Chem. Soc., Chem. Commun.* 1553–1554 (1996).

Atom	x	y	z
Al 1	0.5	0.2867	0.0
Al 2	0.6179	0.5	0.604
Al 3	0.7205	0.1659	0.528
P 1	0.5	0.3795	0.527
P 2	0.7221	0.5	0.081
P 3	0.3554	0.7691	0.068
O 1	0.5	0.3073	-0.3398
O 2	0.5	0.3556	0.2413
O 3	0.4353	0.2154	0.0247
O 4	0.6491	0.5	0.9332
O 5	0.6738	0.5	0.3272
O 6	0.5724	0.4185	0.5300
O 7	0.6709	0.1950	0.8099
O 8	0.6977	0.1764	0.1912
O 9	0.8081	0.2030	0.5110
O 10	0.7376	0.0718	0.5281

Refined from simulated annealing and low-resolution powder X-ray diffraction. Temperature factors and occupancies were not provided.

REFINED COMPOSITION: $|K_{5.37}(H_2O)_9|\ [Be_{3.51}Si_{5.52}O_{18}]$

CRYSTAL DATA: $P3_2$ (No. 145)
$a = 10.0928$ Å $b = 10.0928$ Å $c = 7.6264$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.0596$

REFERENCE: K. O. Kongshaug, H. Fjellvåg, K. P. Lillerud, T. E. Gier, G. D. Stucky and A. K. Cheetham, Private communication (2000).

Atom	x	y	z	B_{iso}	occ
Si 1	0.5818	0.2893	0.7241	1.03	0.58
Be 1	0.5818	0.2893	0.7241	1.03	0.42
Si 2	0.2899	0.5811	0.0599	0.71	0.53
Be 2	0.2899	0.5811	0.0599	0.71	0.47
Si 3	0.0007	0.4976	0.2277	1.03	0.73
Be 3	0.0007	0.4976	0.2277	1.03	0.28
O 1	0.68	0.3710	0.5540	1.58	1.0
O 2	0.312	0.6910	0.8820	2.45	1.0
O 3	0.465	0.1070	0.6810	1.66	1.0
O 4	0.349	0.4560	0.0180	2.21	1.0
O 5	0.107	0.4640	0.1020	1.97	1.0
O 6	0.469	0.3560	0.7720	1.74	1.0
K 11	0.005	0.4620	0.7200	3.95	0.44
K 12	-0.006	0.5270	0.7180	4.50	0.56
K 2	0.185	0.0750	0.7140	20.53	0.79
H_2O 1	0.115	0.1710	0.0510	9.24	1.0
H_2O 2	0.136	0.3270	0.5840	15.00	1.0
H_2O 3	-0.138	0.1890	-0.0790	14.21	1.0

REFINED COMPOSITION: $|Ca_8(H_2O)_{16}|\ [Si_{16}Al_{16}O_{60}(OH)_8]$
Taurus Mountains, Turkey

CRYSTAL DATA: $C1\,2/c\,1$ (No. 15) unique axis **b**, cell choice 1
$a = 21.555$ Å $b = 8.761$ Å $c = 9.304$ Å
$\alpha = 90°$ $\beta = 91.55°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.07$

REFERENCE: N. Engel and K. Yvon,
Z. Kristallogr. **169** 165–175 (1984).

Atom	x	y	z	B_{iso}	occ
Ca	0.35586	0.1991	0.0444	0.93	1.0
Si 1	0.06729	0.1832	0.2896	0.53	1.0
Si 2	0.23983	0.0077	0.4621	0.46	1.0
Al 1	0.1161	0.0844	0.6006	0.56	1.0
Al 2	0.1999	0.3162	0.2858	0.51	1.0
O 1	0.0695	0.0181	0.2162	0.73	1.0
O 2	0.0725	0.1719	0.4626	0.84	1.0
O 3	0.1222	0.2883	0.2295	0.89	1.0
O 4	0.1722	0.0363	0.0250	0.86	1.0
O 5	0.2081	0.4669	0.4096	0.71	1.0
O 6	0.2345	0.1550	0.3605	0.84	1.0
O 7	0.2340	0.3599	0.1221	0.76	1.0
O 8	0.0	0.2632	0.2500	0.63	1.0
OH	0.3523	0.2673	0.2918	1.11	1.0
H_2O 1	0.0712	0.5050	0.0159	2.62	1.0
H_2O 2	0.4541	0.3070	0.0800	1.72	1.0

REFINED COMPOSITION: $|Na_{9.68}K_{50.51}Ca_{26.75}Ba_{1.06}(H_2O)_{452}|\ [Si_{520.12}Al_{151.88}O_{1344}]$
Rock Island Dam, Washington, U.S.A.

CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 35.093$ Å $b = 35.093$ Å $c = 35.093$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.14$

REFERENCE: E. K. Gordon, S. Samson and W. B. Kamb, *Science* **154** 1004–1007 (1966).

Atom	x	y	z	B_{iso}	occ
Na 1	0.1788	0.1788	0.1788	2.4	0.11
Na 2	0.2543	0.2543	0.0	3.0	0.11
Na 3	0.3975	0.3975	0.1445	5.5	0.11
K 1	0.1788	0.1788	0.1788	2.4	0.574
K 2	0.2543	0.2543	0.0	3.0	0.574
K 3	0.3975	0.3975	0.1445	5.5	0.574
Ca 1	0.1788	0.1788	0.1788	2.4	0.304
Ca 2	0.2543	0.2543	0.0	3.0	0.304
Ca 3	0.3975	0.3975	0.1445	5.5	0.304
Ba 1	0.1788	0.1788	0.1788	2.4	0.012
Ba 2	0.2543	0.2543	0.0	3.0	0.012
Ba 3	0.3975	0.3975	0.1445	5.5	0.012
Si 1	0.3137	0.25	0.1863	0.47	0.774
Si 2	0.4021	0.25	0.0979	0.46	0.774
Si 3	0.3132	0.2498	0.0979	0.48	0.774
Si 4	0.4558	0.1072	0.0443	0.54	0.774
Si 5	0.4019	0.1782	0.0448	0.45	0.774
Si 6	0.3126	0.1785	0.0446	0.40	0.774
Si 7	0.2592	0.1073	0.0445	0.36	0.774
Si 8	0.1708	0.1076	0.0441	0.44	0.774
Al 1	0.3137	0.25	0.1863	0.47	0.226
Al 2	0.4021	0.25	0.0979	0.46	0.226
Al 3	0.3132	0.2498	0.0979	0.48	0.226
Al 4	0.4558	0.1072	0.0443	0.54	0.226
Al 5	0.4019	0.1782	0.0448	0.45	0.226
Al 6	0.3126	0.1785	0.0446	0.40	0.226
Al 7	0.2592	0.1073	0.0445	0.36	0.226
Al 8	0.1708	0.1076	0.0441	0.44	0.226
O 1	0.1635	0.0933	0.0	1.4	1.0
O 2	0.2679	0.0968	0.0	1.3	1.0
O 3	0.3041	0.1886	0.0	1.4	1.0
O 4	0.4092	0.1900	0.0	1.8	1.0
O 5	0.4484	0.0952	0.0	1.6	1.0
O 6	0.4489	0.3794	0.0	1.8	1.0
O 7	0.0713	0.0713	0.1610	1.4	1.0
O 8	0.4308	0.4308	0.2322	1.9	1.0
O 9	0.1437	0.1437	0.0545	1.5	1.0
O 10	0.2860	0.2860	0.1965	1.6	1.0
O 11	0.2868	0.2868	0.0890	1.7	1.0

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Atom	x	y	z	B_{iso}	occ
O 12	0.4299	0.4299	0.0548	2.0	1.0
O 13	0.2152	0.1211	0.0496	1.2	1.0
O 14	0.2870	0.1414	0.0582	1.8	1.0
O 15	0.3573	0.1672	0.0525	1.5	1.0
O 16	0.4278	0.1417	0.0573	2.3	1.0
O 17	0.3002	0.2163	0.0693	1.9	1.0
O 18	0.4148	0.2142	0.0710	1.9	1.0
O 19	0.3576	0.2623	0.0909	1.6	1.0
O 20	0.3080	0.2351	0.1419	1.5	1.0
H_2O 1	0.140	0.140	0.140	5.7	1.0
H_2O 2	0.217	0.217	0.217	4.2	1.0
H_2O 3	0.209	0.209	0.053	6.2	1.0
H_2O 4	0.348	0.348	0.200	5.5	1.0
H_2O 5	0.350	0.350	0.082	11.5	1.0
H_2O 6	0.220	0.220	0.140	15.0	1.0
H_2O 7	0.139	0.139	0.217	15.0	1.0
H_2O 8	0.334	0.275	0.0	15.0	1.0
H_2O 9	0.422	0.285	0.0	15.0	1.0
H_2O 10	0.292	0.5	0.0	15.0	1.0
H_2O 11	0.367	0.367	0.0	15.0	1.0
H_2O 12	0.178	0.0	0.0	15.0	1.0
H_2O 13	0.270	0.0	0.0	15.0	1.0
H_2O 14	0.458	0.0	0.0	15.0	1.0

REFINED COMPOSITION: $|K_2Ca_{1.648}(H_2O)_{12}|\ [Si_{10.7}Al_{5.3}O_{32}]$
Casal Brunori, Rome, Italy

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 9.865$ Å $b = 14.300$ Å $c = 8.668$ Å
$\alpha = 90°$ $\beta = 124.20°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.057$

REFERENCE: R. Rinaldi, J. J. Pluth and J. V. Smith,
Acta Cryst. **B30** 2426–2433 (1974).

Atom	x	y	z	B_{iso}	occ
K	0.8480	0.2500	0.2076	2.4	1.0
Ca	0.6080	0.6262	0.4401	2.14	0.412
Si 1	0.7362	0.0248	0.2805	1.08	0.669
Si 2	0.4206	0.1409	0.0019	1.06	0.669
Si 3	0.0604	0.0078	0.2844	1.11	0.669
Si 4	0.1204	0.1396	0.0421	1.14	0.669
Al 1	0.7362	0.0248	0.2805	1.08	0.331
Al 2	0.4206	0.1409	0.0019	1.06	0.331
Al 3	0.0604	0.0078	0.2844	1.11	0.331
Al 4	0.1204	0.1396	0.0421	1.14	0.331
O 1	0.1335	0.0976	0.2289	2.04	1.0
O 2	0.6445	0.5766	0.1878	1.94	1.0
O 3	0.6100	0.1130	0.1728	1.89	1.0
O 4	0.0254	0.9154	0.1494	1.85	1.0
O 5	0.8957	0.0440	0.2713	2.06	1.0
O 6	0.3022	0.3738	0.0783	2.32	1.0
O 7	0.7872	0.4795	0.4982	1.9	1.0
O 8	0.5814	0.7500	0.0616	1.94	1.0
O 9	0.0665	0.2500	0.0196	2.12	1.0
H_2O 1	0.7551	0.7500	0.4733	7.8	1.0
H_2O 2	0.1552	0.7500	0.4382	7.3	1.0
H_2O 3	0.3208	0.8525	0.1740	8.8	1.0
H_2O 4	0.5085	0.2500	0.4384	18.7	1.0
H_2O 5	0.5	0.5	0.5	16.6	1.0

REFINED COMPOSITION: $|Ba_2Ca_{0.6}(H_2O)_{12}|\ [Si_{12}Al_4O_{32}]$
Andreasberg, Hartz, Germany

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 9.879$ Å $b = 14.139$ Å $c = 8.693$ Å
$\alpha = 90°$ $\beta = 124.81°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.039$

REFERENCE: R. Rinaldi, J. J. Pluth and J. V. Smith,
Acta Cryst. **B30** 2426–2433 (1974).

Atom	x	y	z	B_{iso}	occ
Ba	0.86290	0.25	0.19441	1.79	1.0
Ca	0.5869	0.6286	0.4799	0.0	0.15
Si 1	0.7367	0.0248	0.2840	0.82	0.75
Si 2	0.4214	0.1410	0.0136	0.77	0.75
Si 3	0.0577	0.0075	0.2898	0.78	0.75
Si 4	0.1216	0.1390	0.0375	0.85	0.75
Al 1	0.7367	0.0248	0.2840	0.82	0.25
Al 2	0.4214	0.1410	0.0136	0.77	0.25
Al 3	0.0577	0.0075	0.2898	0.78	0.25
Al 4	0.1216	0.1390	0.0375	0.85	0.25
O 1	0.1042	0.0896	0.1958	2.45	1.0
O 2	0.6470	0.5726	0.1679	1.80	1.0
O 3	0.6163	0.1186	0.1792	1.58	1.0
O 4	0.0050	0.9083	0.1711	2.05	1.0
O 5	0.9057	0.0515	0.2955	1.47	1.0
O 6	0.3137	0.3709	0.1017	1.84	1.0
O 7	0.7808	0.4856	0.4976	1.68	1.0
O 8	0.5885	0.75	0.0573	1.76	1.0
O 9	0.0661	0.25	0.0256	1.99	1.0
H_2O 1	0.8004	0.75	0.4889	5.5	1.0
H_2O 2	0.1148	0.75	0.4593	4.8	1.0
H_2O 3	0.3027	0.8628	0.1324	5.8	1.0
H_2O 4	0.4611	0.75	0.5134	47.0	1.0
H_2O 5	0.5	0.5	0.5	35.0	1.0

REFINED COMPOSITION: $|Na_{2.88}Cs_{3.12}(H_2O)_{73.27}|\ [Si_{35.95}Al_{12.05}O_{96}]$

CRYSTAL DATA: $Im\overline{3}m$ (No. 229)
$a = 15.031$ Å $b = 15.031$ Å $c = 15.031$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.18$, $R_F = 0.134$

REFERENCE: L. B. McCusker and Ch. Baerlocher,
in *Proceedings of the 6th International Zeolite Conference, Reno 1983*,
Ed. by D. H. Olson and A. Bisio (Butterworth: Guildford) 812–822 (1984).

Atom	x	y	z	B_{iso}	occ
Na	0.2768	0.2768	0.2768	6.3	0.180
Cs	0.0	0.0	0.3554	0.3	0.260
Si	0.25	0.1042	0.3958	3.2	0.749
Al	0.25	0.1042	0.3958	3.2	0.251
O 1	0.2107	0.0	0.3834	5.6	1.0
O 2	0.1652	0.1652	0.3654	5.6	1.0
H_2O 1	0.0749	0.2096	0.2096	5.5	0.204
H_2O 2	0.0542	0.0542	0.2756	15.0	0.504
H_2O 3	0.0636	0.1180	0.1735	15.0	0.305
H_2O 4	0.0	0.0	0.4295	15.0	0.717
H_2O 5	0.0	0.0	0.0	15.0	0.70

RHO Pahasapaite

REFINED COMPOSITION: $|Li_{11.6}Na_{0.192}K_{1.2}Ca_{5.5}(H_2O)_{38}|\ [Be_{24}P_{24}O_{96}]$
Custer, S. Dakota, U.S.A.

CRYSTAL DATA: $I23$ (No. 197)
$a = 13.781$ Å $b = 13.781$ Å $c = 13.781$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.035$

REFERENCE: R. C. Rouse, D. R. Peacor and S. Merlino, *American Mineralogist* **74** 1195–1202 (1989).

Atom	x	y	z	B_{iso}	occ
Li 1	0.3615	0.0357	0.0301	3.66	0.15
Li 2	0.3013	0.3013	0.3013	1.89	1.0
Na	0.3615	0.0357	0.0301	3.66	0.008
K	0.3615	0.0357	0.0301	3.66	0.05
Ca	0.3615	0.0357	0.0301	3.66	0.229
Be	0.4207	0.1210	0.2675	0.76	1.0
P	0.2771	0.1240	0.4224	0.71	1.0
O 1	0.2246	0.2178	0.3914	0.95	1.0
O 2	0.3781	0.1245	0.3766	1.16	1.0
O 3	0.3791	0.0329	0.2041	1.18	1.0
O 4	0.2160	0.0383	0.3889	1.16	1.0
H_2O 1	0.3851	0.3851	0.3851	3.08	1.0
H_2O 2	0.4768	0.0	0.0	1.68	0.5
H_2O 3	0.2171	0.1095	0.0714	4.0	0.5
H_2O 4	0.2459	0.0765	0.0504	6.58	0.5

REFINED COMPOSITION: $|Rb_{24}(D_2O)_{3.6}|\ [Be_{24}As_{24}O_{96}]$

CRYSTAL DATA: $I23$ (No. 197)
$a = 14.001$ Å $b = 14.001$ Å $c = 14.001$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
neutron $R_{wp} = 0.041$, X-ray $R_{wp} = 0.145$

REFERENCE: J. B. Parise, D. R. Corbin, T. E. Gier, R. L. Harlow, L. Abrams and R. B. Von Dreele, *Zeolites* **12** 360–368 (1992).
And J. B. Parise, Private communication (1994).

Atom	x	y	z	B_{iso}	occ
Rb 1	0.5	0.0	0.0	4.89	1.0
Rb 2	0.1903	0.1903	0.1903	7.74	1.0
Rb 3	0.3716	0.3716	0.3716	7.74	0.87
Rb 4	0.244	0.0	0.0	7.74	0.25
Be	0.2173	0.9311	0.3717	4.34	1.0
As	0.27446	0.12749	0.42737	0.79	1.0
O 1	0.2296	0.2349	0.3988	1.5	1.0
O 2	0.3882	0.1265	0.3899	0.95	1.0
O 3	0.2852	0.1055	0.5429	4.42	1.0
O 4	0.2094	0.0467	0.3679	1.34	1.0
D_2O 1	0.244	0.0	0.0	4.74	0.10
D_2O 2	0.066	0.066	0.066	4.74	0.23
D_2O 3	0.441	0.441	0.441	4.74	0.07

REFINED COMPOSITION: $|Ca_{16}(H_2O)_{18.72}|\ [(Be(OH)_2)_8Si_{32}Al_{16}O_{104}]$
Pizzo Marcio, Val Vigezzo, Italy

CRYSTAL DATA: $I\,4/m\,cm$ (No. 140)
$a = 18.33$ Å $b = 18.33$ Å $c = 9.16$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{obs} = 0.034$

REFERENCE: G. Giuseppetti, F. Mazzi, C. Tadini and E. Galli, *Neues Jahrb. Mineral. Monatsh.* **7** 307–314 (1991).

Atom	x	y	z	B_{iso}	occ
Ca	0.1769	0.1769	0.25	1.34	1.0
Si 1	0.1044	0.2810	0.0	0.95	1.0
Si 2	0.1159	0.0408	0.0	0.79	1.0
Be	0.2619	0.2381	0.0000	1.42	1.0
Al	0.2177	0.0000	0.25	0.87	1.0
O 1	0.1353	0.3647	0.0000	1.26	1.0
O 2	0.1641	0.0579	0.1457	1.26	1.0
O 3	0.0579	0.2673	0.1461	1.74	1.0
O 4	0.0451	0.0936	0.0000	1.66	1.0
O 5	0.1725	0.2246	0.0	1.18	1.0
O 6	0.2935	0.2065	0.1512	1.34	1.0
H	0.324	0.176	0.145	2.37	1.0
H_2O 1	0.409	0.091	0.154	11.05	0.49
H_2O 2	0.375	0.079	0.0	10.26	0.27
H_2O 1	0.445	0.055	0.264	17.37	0.41

O6 is a terminal oxygen, where the framework is not fully connected.

REFINED COMPOSITION: $|K_4Na_{12}(H_2O)_{20.7}|\ [Si_{28}Zn_8O_{72}]$

CRYSTAL DATA: $C1m1$ (No. 8) unique axis **b**, cell choice 1
$a = 7.238$ Å $b = 40.56$ Å $c = 7.308$ Å
$\alpha = 90°$ $\beta = 91.8°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.238$, $R_{wp} = 0.164$, $R_I = 0.090$

REFERENCE: C. Röhrig and H. Gies,
Angew. Chem., Int. ed. **34** 63–65 (1995).

Atom	x	y	z	B_{iso}	occ
Na 1	-0.141	0.0	0.224	1.97	1.0
Na 2	-0.164	0.0	0.795	1.97	1.0
Na 3	-0.002	0.2469	0.84	1.97	1.0
Na 4	0.05	0.1309	0.574	1.97	1.0
K	0.063	0.3865	0.442	1.97	1.0
Si 1	0.317	0.0382	0.308	0.79	1.0
Si 2	0.299	0.0379	0.72	0.79	1.0
Si 3	0.572	0.0671	0.017	0.79	1.0
Si 4	-0.195	0.1277	-0.024	0.79	1.0
Si 5	0.755	0.1991	0.096	0.79	1.0
Si 6	0.038	0.2185	0.397	0.79	1.0
Si 7	0.467	0.2105	0.388	0.79	1.0
Zn 1	0.0	0.0605	0.0	0.79	1.0
Zn 2	0.7484	0.1832	0.6786	0.79	1.0
O 1	0.377	0.0	0.298	1.18	1.0
O 2	0.317	0.052	0.515	1.18	1.0
O 3	0.111	0.0427	0.224	1.18	1.0
O 4	0.467	0.0603	0.205	1.18	1.0
O 5	0.365	0.0	0.735	1.18	1.0
O 6	0.086	0.042	0.773	1.18	1.0
O 7	0.433	0.0609	0.844	1.18	1.0
O 8	0.7478	0.043	0.004	1.18	1.0
O 9	-0.002	0.1084	0.01	1.18	1.0
O 10	0.626	0.1058	0.022	1.18	1.0
O 11	-0.203	0.1599	0.106	1.18	1.0
O 12	0.784	0.1378	0.762	1.18	1.0
O 13	0.737	0.2124	0.888	1.18	1.0
O 14	-0.079	0.2182	0.204	1.18	1.0
O 15	0.561	0.2066	0.192	1.18	1.0
O 16	-0.029	0.1919	0.544	1.18	1.0
O 17	0.521	0.1815	0.53	1.18	1.0
O 18	0.247	0.2091	0.346	1.18	1.0
O 19	0.023	0.2549	0.485	1.18	1.0
H_2O 1	-0.1	0.0753	0.501	4.74	1.15
H_2O 2	0.257	0.2093	0.898	4.74	1.15
H_2O 3	0.299	0.1398	0.775	4.74	1.15
H_2O 4	0.21	0.1324	0.293	4.74	1.15
H_2O 5	0.746	0.0	0.487	4.74	1.15

REFINED COMPOSITION: $|C_{17.6}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 14.018$ Å $b = 13.612$ Å $c = 7.418$ Å
$\alpha = 90°$ $\beta = 102.12°$ $\gamma = 90°$
X-ray single crystal refinement, $R_1 = 0.099$

REFERENCE: B. Marler, A. Grünewald-Lüke and H. Gies,
Microporous and Mesoporous Materials **26** 49–59 (1998).

Atom	x	y	z	B_{iso}	occ
Si 1	0.6021	0.1135	0.4515	2.13	1.0
Si 2	0.7308	0.1133	0.8427	1.89	1.0
Si 3	0.6111	0.2237	0.0859	1.89	1.0
O 1	0.5	0.1473	0.5	3.08	1.0
O 2	0.5966	0.0	0.3917	2.61	1.0
O 3	0.6869	0.1288	0.6265	2.76	1.0
O 4	0.6239	0.1784	0.2882	26.06	1.0
O 5	0.7551	0.0	0.8826	24.48	1.0
O 6	0.8826	0.1749	0.9047	2.37	1.0
O 7	0.6414	0.1465	0.9575	2.84	1.0
O 8	0.5	0.2477	0.0	2.53	1.0
C 1	0.422	0.477	0.432	22.9	0.63
C 2	0.489	0.414	0.428	18.16	0.63
C 3	0.943	0.0	0.277	18.95	0.31
C 4	0.967	0.0	0.63	16.58	0.31
C 5	0.858	0.097	0.358	30.79	0.63

REFINED COMPOSITION: $[Si_{31}O_{64}]$

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 9.659$ Å $b = 20.461$ Å $c = 9.831$ Å
$\alpha = 90°$ $\beta = 96.58°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.06$

REFERENCE: S. Vortmann, B. Marler, H. Gies and P. Daniels, *Microporous Materials* **4** 111–121 (1995).

Atom	x	y	z	B_{iso}	occ
Si 1	-0.00071	0.32074	0.34243	0.96	0.969
Si 2	0.40984	0.07574	0.12008	1.21	0.969
Si 3	0.25048	0.26603	0.21513	1.37	0.969
Si 4	0.15487	0.15272	0.01508	1.69	0.969
O 1	0.0	0.34053	0.5	1.76	1.0
O 2	0.0	0.12655	0.0	1.94	1.0
O 3	0.151	0.29265	0.3211	2.07	1.0
O 4	0.16628	0.21447	0.11538	2.59	1.0
O 5	0.25098	0.09473	0.07707	2.22	1.0
O 6	0.31018	0.32663	0.12877	2.43	1.0
O 7	-0.11737	0.26658	0.30066	2.6	1.0
O 8	0.42048	0.0	0.15383	2.3	1.0
O 9	-0.03047	0.38601	0.25539	2.53	1.0
O 10	0.5	0.09471	0.0	2.68	1.0

RUT RUB-10, SiO_2 Framework

REFINED COMPOSITION: $[Si_{36}O_{72}]$

CRYSTAL DATA: $P1\,2_1/a\,1$ (No. 14) unique axis **b**, cell choice 3
$a = 13.112$ Å $b = 12.903$ Å $c = 12.407$ Å
$\alpha = 90°$ $\beta = 113.50°$ $\gamma = 90°$
DLS refinement.

REFERENCE: H. Gies and J. Rius,
Z. Kristallogr. **210** 475–480 (1995).

Atom	x	y	z
Si 1	0.3003	0.1257	0.1207
Si 2	0.2975	0.1210	0.3594
Si 3	0.0627	0.1268	0.3183
Si 4	0.9222	0.1899	0.0622
Si 5	0.0007	0.2581	0.4892
Si 6	0.2992	0.8890	0.1088
Si 7	0.2864	0.8847	0.3504
Si 8	0.0468	0.8885	0.3340
Si 9	0.9254	0.8006	0.0773
O 1	0.1789	0.1393	0.0177
O 2	0.3410	0.0078	0.1248
O 3	0.3869	0.1999	0.0963
O 4	0.2960	0.1544	0.2447
O 5	0.1930	0.1528	0.3686
O 6	0.3934	0.1688	0.4555
O 7	0.3082	0.0070	0.3699
O 8	0.0446	0.0110	0.3542
O 9	0.0011	0.2062	0.3720
O 10	0.0111	0.1359	0.1779
O 11	0.9756	0.2048	0.9673
O 12	0.8142	0.1180	0.0063
O 13	0.1123	0.3247	0.5507
O 14	0.9967	0.1694	0.5780
O 15	0.2787	0.8539	0.2222
O 16	0.3906	0.8156	0.0936
O 17	0.1721	0.8541	0.3608
O 18	0.9673	0.8607	0.2007

REFINED COMPOSITION: $[P_{28}Al_{28}O_{112}]$

CRYSTAL DATA: $P\bar{4}n2$ (No. 118)
$a = 13.620$ Å $b = 13.620$ Å $c = 21.649$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.059$, $R_w = 0.076$; At $T = 200$K.

REFERENCE: G. W. Noble, P. A. Wright, P. Lightfoot, R. E. Morris, K. J. Hudson, Å. Kvick and H. Graafsma, *Angew. Chem., Int. ed.* **36** 81–83 (1997).

Atom	x	y	z	B_{iso}	occ
P 1	0.3905	0.1197	0.1332	1.60	1.0
P 2	0.1100	0.1207	0.1892	1.69	1.0
P 3	0.2094	-0.1143	0.0563	1.70	1.0
P 4	0.2953	-0.2047	0.2500	1.73	1.0
Al 1	0.2022	0.1119	0.0597	1.76	1.0
Al 2	0.1156	-0.1114	0.1885	1.85	1.0
Al 3	0.3900	-0.1082	0.1346	1.96	1.0
Al 4	0.2950	0.2050	0.2500	1.57	1.0
O 1	0.3220	0.1410	0.0821	3.0	1.0
O 2	0.3706	0.1832	0.1872	3.3	1.0
O 3	0.3763	0.0132	0.1538	2.4	1.0
O 4	0.4928	0.1360	0.1110	2.5	1.0
O 5	0.1959	-0.0099	0.0369	3.7	1.0
O 6	0.1260	0.1403	0.1220	2.6	1.0
O 7	0.1812	0.1848	-0.0039	3.1	1.0
O 8	0.1737	0.1878	0.2267	2.5	1.0
O 9	0.1332	0.0152	0.2036	2.5	1.0
O 10	0.3141	-0.1304	0.0715	3.8	1.0
O 11	0.1439	-0.1372	0.1105	2.9	1.0
O 12	0.0057	0.1434	0.2061	2.5	1.0
O 13	0.1906	-0.1879	0.2353	2.8	1.0
O 14	0.3577	-0.1789	0.1965	4.0	1.0

REFINED COMPOSITION: $|C_{19.44}N_{5.04}|\ [Mg_{2.4}Al_{13.6}P_{16}O_{64}]$

CRYSTAL DATA: $P\,4/m\,nc$ (No. 128)
$a = 14.322$ Å $b = 14.322$ Å $c = 10.424$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray synchrotron single crystal refinement, $R_F = 0.094$, $wR_2 = 0.313$

REFERENCE: V. Patinec, P. A. Wright, P. Lightfoot, R. A. Aitken and P. A. Cox, *J. Chem. Soc., Dalton Trans.* **22** 3909–3911 (1999).

Atom	x	y	z	B_{iso}	occ
Al 1	0.2689	0.1091	0.0	1.66	0.85
Al 2	0.3907	0.8907	0.75	2.45	0.85
Mg 1	0.2689	0.1091	0.0	1.66	0.15
Mg 2	0.3907	0.8907	0.75	2.45	0.15
P 1	0.6101	0.8899	0.75	2.45	1.0
P 2	0.2666	0.8863	0.0	1.89	1.0
O 1	0.2414	0.9886	0.0	3.0	1.0
O 2	0.3209	0.8603	0.8826	3.87	1.0
O 3	0.5093	0.8722	0.7865	3.87	1.0
O 4	0.175	0.8339	0.0	3.4	1.0
O 5	0.6683	0.8619	0.8614	5.05	1.0
N 1	0.5595	0.6718	0.0547	23.7	0.09
N 2	0.5368	0.3621	0.0	23.7	0.09
N 3	0.4221	0.5146	0.2956	23.7	0.09
N 4	0.4938	0.5105	0.7902	23.7	0.09
C 1	0.4937	0.7371	1.0	23.7	0.09
C 2	0.6187	0.3376	0.0918	23.7	0.09
C 3	0.4966	0.4748	0.3812	23.7	0.09
C 4	0.4092	0.5505	0.7258	23.7	0.09
C 5	0.4451	0.32	0.0477	23.7	0.09
C 6	0.4066	0.348	0.1815	23.7	0.09
C 7	0.3685	0.4473	0.2101	23.7	0.09
C 8	0.4508	0.605	0.2332	23.7	0.09
C 9	0.5145	0.5906	0.1159	23.7	0.09
C 10	0.646	0.6501	0.9782	23.7	0.09
C 11	0.648	0.5692	0.8802	23.7	0.09
C 12	0.581	0.5662	0.7643	23.7	0.09
C 13	0.5025	0.4061	0.7672	23.7	0.09
C 14	0.5593	0.3481	0.8665	23.7	0.09

REFINED COMPOSITION: $|(C_{22}H_{50}N_2)_3|\ [Al_{36}P_{36}O_{144}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 12.726$ Å $b = 12.726$ Å $c = 30.939$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement at 200 K. $R_F = 0.0757$

REFERENCE: G. W. Noble, P. A. Wright and Å. Kvick,
J. Chem. Soc., Dalton Trans. 4485–4490 (1997).

Atom	x	y	z	B_{iso}	occ
Al 1	0.7533	0.7572	0.2954	1.30	1.0
Al 2	0.5762	0.9023	0.2165	1.71	1.0
P 1	0.5778	0.9043	0.1144	1.53	1.0
P 2	0.7568	1.0013	0.2914	1.08	1.0
O 1	0.6138	0.9393	0.1617	2.75	1.0
O 2	0.5341	0.7532	0.2251	2.76	1.0
O 3	0.7928	0.9072	0.2939	3.05	1.0
O 4	0.4612	0.9280	0.2310	2.81	1.0
O 5	0.7014	0.9959	0.2472	2.66	1.0
O 6	0.8644	1.1224	0.2968	2.75	1.0
O 7	0.6689	0.9831	0.3267	3.64	1.0
O 8	0.6563	0.0092	0.0856	2.70	1.0
N	0.0000	0.0000	0.1025	5.43	1.0
C 1	0.0000	0.0000	0.1842	7.76	1.0
C 2	-0.0415	0.0827	0.1662	10.66	1.0
C 3	-0.0415	0.0787	0.1177	11.13	1.0
C 4	-0.0312	0.0351	0.0556	17.02	1.0
C 5	0.0000	0.0000	0.0241	14.90	1.0
H 1	0.0000	0.0000	0.2147	0.0	1.0
H 2	0.0103	0.1631	0.1757	0.0	1.0
H 3	-0.1222	0.0567	0.1762	0.0	1.0
H 4	0.0090	0.1580	0.1069	0.0	1.0
H 5	-0.1226	0.0498	0.0498	0.0	1.0
H 6	0.0075	0.1208	0.0540	0.0	1.0
H 7	-0.1164	0.0017	0.0540	0.0	1.0
H 8	0.0851	0.0322	0.0249	0.0	1.0
H 9	-0.0211	0.0263	-0.0015	0.0	1.0

REFINED COMPOSITION: $[Mg_{4.8}Al_{19.2}P_{24}O_{96}]$

CRYSTAL DATA: $P\,4/n$ (No. 85) origin at centre $\overline{1}$
$a = 18.7732$ Å $b = 18.7732$ Å $c = 9.4537$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray synchrotron single crystal refinement, $R_p = 0.0539$, $wR_{wp} = 0.1422$

REFERENCE: P. A. Wright, M. J. Maple, A. M. Z. Slawin, V. Patinec, R. A. Aitken, S. Welsh and P. A. Cox, *J. Chem. Soc., Dalton Trans.* 1243–1248 (2000).

Atom	x	y	z	B_{iso}	occ
Al 1	0.06412	0.66568	0.08090	2.04	0.8
Al 2	0.95577	0.83599	0.84220	2.13	0.8
Al 3	0.94930	0.43481	0.33580	1.99	0.8
Mg 1	0.06412	0.66568	0.08090	2.04	0.2
Mg 2	0.95577	0.83599	0.84220	2.13	0.2
Mg 3	0.94930	0.43481	0.33580	1.99	0.2
P 1	0.06413	0.55768	0.33630	2.12	1.0
P 2	0.94979	0.66685	0.83780	2.12	1.0
P 3	0.06624	0.83420	0.09420	2.15	1.0
O 1	0.05740	0.62430	0.24630	3.78	1.0
O 2	0.07540	0.58070	0.48780	3.73	1.0
O 3	0.12730	0.51280	0.29030	3.67	1.0
O 4	0.99500	0.51620	0.32390	3.8	1.0
O 5	0.98490	0.65670	0.98110	3.6	1.0
O 6	0.99740	0.63590	0.72250	3.6	1.0
O 7	0.87790	0.62920	0.84020	3.9	1.0
O 8	0.93760	0.74420	0.80680	4.1	1.0
O 9	0.99790	0.84490	0.01270	3.88	1.0
O 10	0.12970	0.86300	0.01460	3.62	1.0
O 11	0.05990	0.87030	0.23630	4.14	1.0
O 12	0.07950	0.75560	0.12070	3.97	1.0

REFINED COMPOSITION: $|C_{32}N_{16}|$ $[Al_{32}Co_{32}P_{64}O_{256}]$

CRYSTAL DATA: $P\,4/n\,nc$ (No. 126) origin at centre $\overline{1}$
$a = 19.0654$ Å $b = 19.0654$ Å $c = 27.594$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_F = 0.098$, $R_w = 0.26$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

Atom	x	y	z	B_{iso}	occ
Al 1	0.4567	0.1672	0.5127	2.30	0.50
Co 1	0.4567	0.1672	0.5127	2.30	0.50
Al 2	0.3317	0.0477	0.8051	2.40	0.50
Co 2	0.3317	0.0477	0.8051	2.40	0.50
Al 3	0.3269	-0.0423	0.5995	2.30	0.50
Co 3	0.3269	-0.0423	0.5995	2.30	0.50
Al 4	0.4015	-0.1712	0.9551	2.40	0.50
Co 4	0.4015	-0.1712	0.9551	2.40	0.50
P 1	0.3358	0.0490	0.5055	2.60	1.0
P 2	0.3335	0.0501	0.6916	2.10	1.0
P 3	0.3381	-0.0486	0.8941	2.40	1.0
P 4	0.3991	-0.1636	0.5484	2.40	1.0
O 1	0.3443	0.0224	0.7421	3.00	1.0
O 2	0.3817	0.1116	0.4947	4.80	1.0
O 3	0.3797	-0.1151	0.9041	4.50	1.0
O 4	0.3798	-0.1174	0.5918	3.90	1.0
O 5	0.3495	-0.0085	0.6576	4.30	1.0
O 6	0.3491	-0.0278	0.8419	3.80	1.0
O 7	0.3475	-0.1555	0.0081	3.90	1.0
O 8	0.3524	0.0209	0.5559	3.90	1.0
O 9	0.3808	0.1121	0.6815	4.90	1.0
O 10	0.5292	0.1415	0.4681	4.30	1.0
O 11	0.3969	-0.2397	0.5644	4.50	1.0
O 12	0.2391	-0.0627	0.5963	4.80	1.0
O 13	0.2585	0.0743	0.6842	3.20	1.0
O 14	0.4306	0.2596	0.5031	4.30	1.0
O 15	0.3519	-0.0073	0.4685	4.30	1.0
O 16	0.4888	0.1397	0.5740	4.50	1.0
N	0.4831	0.0187	0.4150	6.10	1.0
C 1	0.4727	0.0323	0.3615	7.70	1.0
C 2	0.4080	0.1047	0.3607	2.20	1.0

REFINED COMPOSITION: $|C_{16}N_{16}O_{12}|$ $[Ga_{24}Co_{24}P_{48}O_{192}]$

CRYSTAL DATA: $P\bar{3}1c$ (No. 163)
$a = 17.8356$ Å $b = 17.8356$ Å $c = 27.1816$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_F = 0.070$, $R_w = 0.201$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

Atom	x	y	z	B_{iso}	occ
Ga 1	-0.1059	0.2593	0.5978	3.10	1.0
Ga 2	-0.3132	-0.0696	0.5392	2.80	1.0
Co 3	-0.3324	0.1607	0.6925	1.80	1.0
Co 4	0.1597	0.4754	0.4858	2.30	1.0
P 1	0.0636	0.3015	0.5490	2.00	1.0
P 2	-0.2758	0.0833	0.6104	2.40	1.0
P 3	0.3445	0.4963	0.4890	2.40	1.0
P 4	-0.1572	0.3339	0.6866	2.20	1.0
O 1	-0.1815	0.1465	0.6031	8.50	1.0
O 2	-0.0993	0.3059	0.6604	3.70	1.0
O 3	-0.3021	0.0832	0.6645	5.40	1.0
O 4	-0.4440	0.1312	0.6708	3.90	1.0
O 5	0.1005	0.3966	0.5389	3.50	1.0
O 6	0.0043	0.2744	0.5940	2.90	1.0
O 7	-0.2905	-0.0069	0.5983	3.80	1.0
O 8	0.2840	0.5324	0.4864	4.20	1.0
O 9	0.3446	0.4533	0.4400	3.40	1.0
O 10	-0.2789	-0.1458	0.5616	3.90	1.0
O 11	-0.3289	0.1432	0.7592	4.60	1.0
O 12	0.1071	0.4363	0.4219	4.00	1.0
O 13	-0.2515	0.2760	0.6719	4.00	1.0
O 14	0.1302	0.5642	0.5001	3.50	1.0
O 15	0.3173	0.4293	0.5305	4.30	1.0
O 16	-0.2357	0.0127	0.4954	4.00	1.0
N 1	-0.3333	0.3333	0.5967	4.30	1.0
N 2	0.0266	0.5103	0.5912	4.40	1.0
C 3	0.0863	0.5395	0.6361	10.90	1.0
C 4	0.3333	0.6667	0.5770	17.50	1.0
O 17	-0.1496	0.1913	0.5275	10.30	1.0

REFINED COMPOSITION: $|C_{30}N_{24}|$ $[Ga_{36}Zn_{36}P_{72}O_{288}]$

CRYSTAL DATA: $R\overline{3}$ (No. 148) hexagonal setting
$a = 18.0804$ Å $b = 18.0804$ Å $c = 41.9511$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_F = 0.045$, $R_w = 0.140$

REFERENCE: X. Bu, P. Feng and G. D. Stucky,
Science **278** 2080–2085 (1997).

Atom	x	y	z	B_{iso}	occ
Zn 1	0.8424	0.3247	-0.0100	1.90	1.0
Zn 2	0.5111	0.8371	0.1286	1.70	1.0
Ga 3	0.7579	0.0668	0.0283	1.70	1.0
Ga 4	0.0998	0.3663	0.0679	2.20	1.0
P 5	0.1544	0.4958	0.1257	1.70	1.0
P 6	0.8467	0.5083	-0.0071	1.80	1.0
P 7	0.9384	0.2394	0.0315	1.60	1.0
P 8	0.6378	0.9116	0.0709	1.80	1.0
O 1	0.9897	0.2715	0.0634	2.70	1.0
O 2	0.8712	0.1447	0.0378	2.80	1.0
O 3	0.7166	0.0023	0.0655	2.90	1.0
O 4	0.8693	0.4399	0.0021	2.80	1.0
O 5	0.8991	0.2943	0.0229	3.00	1.0
O 6	0.0990	0.4105	0.1077	3.30	1.0
O 7	0.6173	0.9034	0.1071	2.80	1.0
O 8	0.1818	0.3362	0.0595	3.60	1.0
O 9	0.4685	0.7195	0.1183	3.70	1.0
O 10	0.5324	0.8575	0.1724	3.90	1.0
O 11	0.6965	0.1221	0.0207	3.10	1.0
O 12	0.4312	0.8690	0.1134	3.20	1.0
O 13	0.7589	0.9997	-0.0051	2.80	1.0
O 14	0.7192	0.2499	-0.0127	3.50	1.0
O 15	0.1045	0.4472	0.0383	3.30	1.0
O 16	0.9003	0.3389	-0.0512	3.50	1.0
N 1	0.3333	0.6667	0.0655	5.20	1.0
N 2	0.5103	0.0289	0.0608	4.70	1.0
C 1	0.3333	0.6667	0.1050	4.20	1.0
C 2	0.5501	0.0936	0.0891	13.20	1.0
C 3	0.6667	0.3333	0.0461	9.90	1.0

REFINED COMPOSITION: $[Si_{14}O_{28}]$

CRYSTAL DATA: $P2_1$ (No. 4) unique axis **b**
$a = 11.1527$ Å $b = 5.002$ Å $c = 13.667$ Å
$\alpha = 90°$ $\beta = 100.633°$ $\gamma = 90°$
Electron diffraction, and X-ray powder, $R_w = 0.0971$, $R_p = 0.0887$

REFERENCE: P. Wagner, O. Terasaki, S. Ritsch, J. G. Nery, S. I. Zones, M. E. Davis and K. Hiraga, *J. Phys. Chem. B* **103** 8245–8250 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.2558	0.3385	0.1869	1.50	1.0
Si 2	0.3963	0.3355	0.3874	5.05	1.0
Si 3	0.4323	0.3363	0.6058	7.50	1.0
Si 4	0.6337	0.338	0.8955	0.32	1.0
Si 5	0.3516	0.4094	0.7996	0.32	1.0
Si 6	0.7451	0.4067	0.1181	0.24	1.0
Si 7	0.9952	0.3947	0.0657	1.11	1.0
O 1	0.282	0.3816	0.3036	3.55	1.0
O 2	0.3294	0.5403	0.1315	0.16	1.0
O 3	0.1138	0.3692	0.1504	0.08	1.0
O 4	0.2936	0.0386	0.162	1.89	1.0
O 5	0.3565	0.3572	0.4942	0.95	1.0
O 6	0.4574	1.0463	0.3752	9.95	1.0
O 7	0.502	0.5462	0.3807	3.47	1.0
O 8	0.343	0.3596	0.6825	5.76	1.0
O 9	0.4891	0.3747	0.8557	0.16	1.0
O 10	0.6629	0.3845	0.0099	0.16	1.0
O 11	0.2652	0.2098	0.8435	5.76	1.0
O 12	0.3071	0.7112	0.8097	4.26	1.0
O 13	0.8812	0.341	0.1139	0.16	1.0
O 14	0.0061	0.1947	0.9774	6.47	1.0

REFINED COMPOSITION: $[Si_{32}O_{64}]$

CRYSTAL DATA: $P1\,2_1/m\,1$ (No. 11) unique axis **b**
$a = 11.4853$ Å $b = 21.9458$ Å $c = 7.3881$ Å
$\alpha = 90.0°$ $\beta = 94.702°$ $\gamma = 90.0°$
X-ray Rietveld refinement, $R_p = 0.0892$, $R_{wp} = 0.1058$

REFERENCE: P. Wagner, S. I. Zones, M. E. Davis and R. C. Medrud, *Angew. Chem., Int. ed.* **38** 1269–1272 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.27227	0.97791	0.93601	-0.35	1.0
Si 2	0.13548	0.62930	0.10193	-0.18	1.0
Si 3	0.23886	0.67904	0.47825	1.12	1.0
Si 4	0.39323	0.56890	0.59794	0.15	1.0
Si 5	0.03652	0.68184	0.74254	1.27	1.0
Si 6	0.05149	0.04087	0.76211	0.91	1.0
Si 7	0.11053	0.06798	0.36508	-0.47	1.0
Si 8	0.35948	0.02838	0.29204	0.31	1.0
O 1	0.22578	0.91806	0.02742	0.87	1.0
O 2	0.32885	0.96241	0.75474	2.61	1.0
O 3	0.36382	0.01059	0.08089	2.88	1.0
O 4	0.16115	0.02349	0.89856	1.28	1.0
O 5	0.02146	0.59436	0.15514	-0.33	1.0
O 6	0.19913	0.66360	0.27348	0.77	1.0
O 7	0.09682	0.67737	0.94529	3.58	1.0
O 8	0.27877	0.75000	0.49498	1.01	1.0
O 9	0.34544	0.63729	0.55819	2.04	1.0
O 10	0.13244	0.66902	0.60239	1.72	1.0
O 11	0.36967	0.53179	0.41218	0.69	1.0
O 12	0.53084	0.57271	0.65389	1.53	1.0
O 13	0.93509	0.63319	0.70903	2.04	1.0
O 14	0.98407	0.75000	0.71105	2.39	1.0
O 15	0.96479	0.98471	0.73380	1.16	1.0
O 16	0.09791	0.06329	0.57827	0.69	1.0
O 17	0.24371	0.06267	0.32726	2.88	1.0

SGT 1-aminoadamantane Sigma-2

REFINED COMPOSITION: $|C_{43.84}|\ [Si_{64}O_{128}]$

CRYSTAL DATA: $I\,4_1/a\,md$ (No. 141) origin at centre $(\,2/m\,)$
$a = 10.2387$ Å $\quad b = 10.2387$ Å $\quad c = 34.3829$ Å
$\alpha = 90°$ $\quad \beta = 90°$ $\quad \gamma = 90°$
X-ray Rietveld refinement, $R_{\rm wp} = 0.225$, $R_{\rm F} = 0.100$

REFERENCE: L. B. McCusker,
J. Appl. Cryst. **21** 305–310 (1988).

Atom	x	y	z	$B_{\rm iso}$	occ
Si 1	0.2843	0.2500	0.1182	0.08	1.0
Si 2	0.2811	0.0000	0.0000	0.16	1.0
Si 3	0.1539	0.2500	0.0349	0.08	1.0
Si 4	0.1510	0.2500	0.1954	0.24	1.0
O 1	0.0000	0.2500	0.2072	1.03	1.0
O 2	0.2165	0.1201	0.2131	1.03	1.0
O 3	0.2297	0.2500	0.0754	0.32	1.0
O 4	0.1689	0.2500	0.1493	0.55	1.0
O 5	0.0000	0.2500	0.043	1.5	1.0
O 6	0.1913	0.1219	0.010	0.63	1.0
O 7	0.3729	0.1229	0.125	1.66	1.0
C 1	0.124	-0.126	0.125	7.9	0.3
C 2	0.000	-0.250	0.073	7.9	0.3
C 3	0.000	-0.126	0.099	7.9	0.3
C 4	0.000	-0.003	0.103	7.9	0.46
C 5	0.115	-0.151	0.086	7.9	0.53
C 6	0.000	-0.077	0.145	7.9	0.47

REFINED COMPOSITION: $|Na_6(H_2O)_8|\ [Si_6Al_6O_{24}]$

CRYSTAL DATA: $P\bar{4}3n$ (No. 218)
$a = 8.848$ Å $b = 8.848$ Å $c = 8.848$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.091$, $R_F = 0.047$

REFERENCE: J. Felsche, S. Luger and Ch. Baerlocher, *Zeolites* **6** 367–372 (1986).

Atom	x	y	z	B_{iso}	occ
Na	0.1504	0.1504	0.1504	3.71	0.75
Si	0.25	0.0	0.5	0.79	1.0
Al	0.25	0.5	0.0	1.18	1.0
O	0.1366	0.4338	0.1490	1.5	1.0
H_2O	0.3753	0.3753	0.3753	3.08	1.0

REFINED COMPOSITION: $|Ca_8(H_2O)_8|\ [Si_4Al_8O_{24}]$
Synthetic material

CRYSTAL DATA: $I\bar{4}3m$ (No. 217)
$a = 8.825$ Å $b = 8.825$ Å $c = 8.825$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.012$

REFERENCE: K. Sahl,
Z. Kristallogr. **152** 13–21 (1980).

Atom	x	y	z	B_{iso}	occ
Ca	0.1434	0.1434	0.1434	0.75	1.0
Si	0.25	0.5	0.0	0.49	0.3333
Al	0.25	0.5	0.0	0.49	0.6667
O	0.1407	0.1407	0.4220	0.94	1.0
OH	0.3845	0.3845	0.3845	0.93	1.0
H	0.328	0.328	0.328	0.0	1.0

REFINED COMPOSITION: $|Na_8Cl_2|\ [Si_8Al_2Be_2O_{24}]$
Ilimaussaq, South Greenland

CRYSTAL DATA: $I\overline{4}$ (No. 82)
$a = 8.640$ Å $b = 8.640$ Å $c = 8.873$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.030$

REFERENCE: I. Hassan and H. D. Grundy,
Canadian Mineralogist **29** 385–390 (1991).

Atom	x	y	z	B_{iso}	occ
Na	0.1563	0.1972	0.1818	1.48	1.0
Cl	0.0	0.0	0.0	1.85	1.0
Si	0.0127	0.2533	0.4958	0.58	1.0
Al	0.0	0.5	0.75	0.6	1.0
Be	0.0	0.5	0.25	0.77	1.0
O 1	0.1504	0.1343	0.4417	0.97	1.0
O 2	0.3472	0.0385	0.6488	0.94	1.0
O 3	0.4256	0.1486	0.1377	0.95	1.0

REFINED COMPOSITION: $[Si_{16}O_{32}]$

CRYSTAL DATA: $P\overline{1}$ (No. 2)
$a = 11.4114$ Å $b = 11.5268$ Å $c = 7.3770$ Å
$\alpha = 94.661°$ $\beta = 96.206°$ $\gamma = 104.892°$
X-ray Rietveld refinement, $R_p = 0.0995$, $R_{wp} = 0.1188$

REFERENCE: P. Wagner, S. I. Zones, M. E. Davis and R. C. Medrud, *Angew. Chem., Int. ed.* **38** 1269–1272 (1999).

Atom	x	y	z	B_{iso}	occ
Si 1	0.36019	0.35630	0.61106	1.04	1.0
Si 2	0.41221	0.42852	0.21918	1.49	1.0
Si 3	0.14209	0.64205	0.40966	1.72	1.0
Si 4	0.36181	0.85678	0.57148	2.06	1.0
Si 5	0.13396	0.44151	0.67151	1.52	1.0
Si 6	0.23859	0.56731	0.04636	1.77	1.0
Si 7	0.46001	0.75796	0.92351	2.31	1.0
Si 8	0.55968	0.87468	0.30376	1.76	1.0
O 1	0.36502	0.37709	0.40067	1.87	1.0
O 2	0.23168	0.36461	0.67114	0.89	1.0
O 3	0.47018	0.45770	0.73017	3.15	1.0
O 4	0.37472	0.22510	0.64375	2.07	1.0
O 5	0.30673	0.47043	0.10734	2.60	1.0
O 6	0.44890	0.32523	0.09908	2.49	1.0
O 7	0.22725	0.77005	0.50790	1.84	1.0
O 8	0.16588	0.54074	0.53230	2.01	1.0
O 9	0.17639	0.61558	0.20899	2.46	1.0
O 10	0.00178	0.64477	0.39598	1.13	1.0
O 11	0.43707	0.85788	0.39827	3.01	1.0
O 12	0.35217	0.99191	0.62479	1.61	1.0
O 13	0.43055	0.81119	0.73707	2.31	1.0
O 14	0.13629	0.50548	0.87315	1.20	1.0
O 15	0.33382	0.67945	0.98040	2.47	1.0
O 16	0.52218	0.86584	0.08546	1.83	1.0

REFINED COMPOSITION: $|Na_{1.76}Ca_4(H_2O)_{29.4}|\ [Si_{25.68}Al_{10.32}O_{72}]$
Iceland

CRYSTAL DATA: $C1\,2/m\,1$ (No. 12) unique axis **b**, cell choice 1
$a = 13.64$ Å $b = 18.24$ Å $c = 11.27$ Å
$\alpha = 90°$ $\beta = 128.0°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.123$

REFERENCE: E. Galli,
Acta Cryst. **B27** 833–841 (1971).

Atom	x	y	z	B_{iso}	occ
Na	0.5055	0.0659	0.0392	4.28	0.22
Ca	0.2805	0.0	0.0949	2.15	1.0
Si 1	0.4830	0.3042	0.2420	0.46	0.5
Si 2	0.2653	0.3097	0.2619	0.33	0.73
Si 3	0.1892	0.0893	0.4846	0.40	0.73
Si 4	0.1124	0.3166	0.5013	0.43	1.0
Si 5	0.0	0.2610	0.0	0.42	0.5
Al 1	0.4830	0.3042	0.2420	0.46	0.5
Al 2	0.2653	0.3097	0.2619	0.33	0.27
Al 3	0.1892	0.0893	0.4846	0.40	0.27
Al 5	0.0	0.2610	0.0	0.42	0.5
O 1	0.4645	0.2911	0.0842	1.40	1.0
O 2	0.1164	0.3162	0.1189	1.38	1.0
O 3	0.0512	0.2661	0.3516	2.03	1.0
O 4	0.0638	0.1199	0.3226	1.41	1.0
O 5	0.2935	0.2308	0.3453	2.01	1.0
O 6	0.3001	0.3796	0.3714	1.76	1.0
O 7	0.3406	0.3162	0.1914	1.40	1.0
O 8	0.3157	0.1119	0.5024	1.78	1.0
O 9	0.1863	0.0	0.4876	1.75	1.0
O 10	0.0	0.3509	0.5	1.15	1.0
H_2O 1	0.1347	0.0776	0.1067	7.45	0.84
H_2O 2	0.3306	0.1258	0.1013	4.71	0.91
H_2O 3	0.3691	0.0	0.3549	3.58	0.85
H_2O 4	0.5124	0.0	0.2416	9.98	1.0
H_2O 5	0.4028	0.5	0.1632	4.72	1.0
H_2O 6	0.1712	0.5	0.1040	10.16	1.0

REFINED COMPOSITION: $|Ca_8(H_2O)_{55.52}|\ [Si_{56}Al_{16}O_{144}]$
Villanova-Monteleone, Sardinia, Italy

CRYSTAL DATA: *Fmmm* (No. 69)
$a = 13.599$ Å $b = 18.222$ Å $c = 17.863$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.082$

REFERENCE: E. Galli and A. Alberti,
Bull. Soc. Fr. Minéral. Crystallogr. **98** 11–18 (1975).

Atom	x	y	z	B_{iso}	occ
Ca	0.5	0.0	0.2910	3.23	1.0
Si 1	0.3857	0.3072	0.3769	0.78	0.778
Si 3	0.3013	0.4112	0.5	0.85	0.778
Si 4	0.3883	0.1833	0.5	0.83	0.778
Si 5	0.25	0.25	0.25	1.04	0.778
Al 1	0.3857	0.3072	0.3769	0.78	0.222
Al 3	0.3013	0.4112	0.5	0.85	0.222
Al 4	0.3883	0.1833	0.5	0.83	0.222
Al 5	0.25	0.25	0.25	1.04	0.222
O 1	0.3175	0.3046	0.3018	2.46	1.0
O 3	0.3721	0.2321	0.4251	3.07	1.0
O 4	0.3577	0.3802	0.4239	2.87	1.0
O 7	0.5	0.3141	0.3493	2.1	1.0
O 8	0.3135	0.1129	0.5	2.37	1.0
O 9	0.3100	0.5	0.5	2.44	1.0
O 10	0.5	0.1495	0.5	2.13	1.0
H_2O 1	0.395	0.098	0.313	4.9	0.2
H_2O 2	0.5	0.128	0.303	7.8	0.8
H_2O 3	0.459	0.0	0.423	3.3	0.37
H_2O 4	0.376	0.0	0.390	13.0	0.45
H_2O 5	0.459	0.5	0.339	4.5	0.43
H_2O 6	0.368	0.5	0.312	10.8	0.62
H_2O 7	0.321	0.056	0.288	9.1	0.2

REFINED COMPOSITION: $|Na_{9.812}K_{1.912}Mg_{0.032}Ca_{1.52}(H_2O)_{58.56}|\ [Si_{55.58}Al_{16.42}O_{144}]$
Capo Pula, Sardinia, Italy

CRYSTAL DATA: *Amma* (No. 63) **cab** setting
$a = 13.643$ Å $b = 18.200$ Å $c = 17.842$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.067$

REFERENCE: E. Galli and A. Alberti,
Bull. Soc. Fr. Minéral. Crystallogr. **98** 331–340 (1975).

Atom	x	y	z	B_{iso}	occ
Na 1	0.25	0.0	0.0417	10.05	0.521
Na 11	0.25	0.0	0.4558	3.82	0.442
Na 2	0.0482	0.0624	0.0446	12.98	0.101
Na 21	0.0369	0.0634	0.4792	18.26	0.181
Na 3	0.1611	0.0	0.2386	15.68	0.181
K 1	0.25	0.0	0.0417	10.05	0.102
K 11	0.25	0.0	0.4558	3.82	0.086
K 2	0.0482	0.0624	0.0446	12.98	0.02
K 21	0.0369	0.0634	0.4792	18.26	0.035
K 3	0.1611	0.0	0.2386	15.68	0.035
Mg 1	0.25	0.0	0.0417	10.05	0.001
Mg 11	0.25	0.0	0.4558	3.82	0.001
Mg 21	0.0369	0.0634	0.4792	18.26	0.001
Mg 3	0.1611	0.0	0.2386	15.68	0.001
Ca 1	0.25	0.0	0.0417	10.05	0.08
Ca 11	0.25	0.0	0.4558	3.82	0.068
Ca 2	0.0482	0.0624	0.0446	12.98	0.016
Ca 21	0.0369	0.0634	0.4792	18.26	0.028
Ca 3	0.1611	0.0	0.2386	15.68	0.028
Si 1	0.1356	0.3037	0.1245	1.19	0.772
Si 2	0.1363	0.3122	0.3724	1.21	0.772
Si 3	0.0512	0.4110	0.2433	1.21	0.772
Si 4	0.1386	0.1846	0.2541	1.05	0.772
Si 5	0.0	0.2399	0.0	1.40	0.772
Al 1	0.1356	0.3037	0.1245	1.19	0.228
Al 2	0.1363	0.3122	0.3724	1.21	0.228
Al 3	0.0512	0.4110	0.2433	1.21	0.228
Al 4	0.1386	0.1846	0.2541	1.05	0.228
Al 5	0.0	0.2399	0.0	1.40	0.228
O 1	0.0699	0.2937	0.0495	2.86	1.0
O 11	0.0664	0.3136	0.4475	2.73	1.0
O 3	0.1195	0.2338	0.1806	2.95	1.0
O 31	0.1247	0.2331	0.3299	2.32	1.0
O 4	0.1062	0.3806	0.1677	3.13	1.0
O 41	0.1060	0.3810	0.3188	3.01	1.0
O 7	0.25	0.3104	0.0971	2.76	1.0
O 71	0.25	0.3219	0.4007	2.21	1.0
O 8	0.0656	0.1142	0.2550	2.54	1.0
O 9	0.0546	0.5	0.2435	2.79	1.0

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Atom	x	y	z	B_{iso}	occ
O 10	0.25	0.1508	0.2540	2.13	1.0
H_2O 1	0.1911	0.1160	0.0519	10.3	0.49
H_2O 11	0.0894	0.0824	0.4356	8.1	0.41
H_2O 2	0.25	0.1259	0.0557	2.3	0.32
H_2O 21	0.25	0.1313	0.4421	9.3	0.91
H_2O 3	0.1750	0.0	0.1764	7.4	0.38
H_2O 31	0.2177	0.0	0.3221	6.0	0.46
H_2O 4	0.0915	0.0	0.1217	13.7	0.50
H_2O 41	0.1479	0.0	0.3869	14.2	0.50
H_2O 5	0.2174	0.5	0.0917	2.9	0.20
H_2O 51	0.1966	0.5	0.4154	8.0	0.42
H_2O 6	0.1251	0.5	0.0607	8.1	0.83
H_2O 61	0.0814	0.5	0.4349	11.4	0.50
H_2O 8	0.25	0.5	0.1615	19.9	0.50
H_2O 81	0.25	0.5	0.3615	1.2	0.50

REFINED COMPOSITION: $|C_{52}N_4F_{2.84}|$ $[Si_{64}O_{128}]$

CRYSTAL DATA: $P1\,2_1/n\,1$ (No. 14) unique axis **b**, cell choice 2
$a = 12.9594$ Å $b = 21.7919$ Å $c = 13.5980$ Å
$\alpha = 90.0°$ $\beta = 101.855°$ $\gamma = 90.0°$
X-ray single crystal refinement, $R_{F_{obs}} = 0.0811$, $wR_{F^2} = 0.1657$

REFERENCE: M. A. Camblor, M.-J. Diaz-Cabanas, J. Perez-Pariente, S. J. Teat, W. Clegg, I. J. Shannon, P. Lightfoot, P. A. Wright and R. E. Morris, *Angew. Chem., Int. Ed.* **37** 2122–2126 (1998).

Atom	x	y	z	B_{iso}	occ
Si 1	0.59105	0.16686	0.20389	0.77	1.0
Si 2	0.6351	0.16809	0.44152	1.0	1.0
Si 3	0.69632	0.57232	-0.0374	0.84	1.0
Si 4	0.66614	0.49124	0.13311	0.74	1.0
Si 5	0.6625	0.29875	0.21813	0.88	1.0
Si 6	0.6889	0.30373	0.44861	0.88	1.0
Si 7	0.5039	0.4046	0.1951	1.17	1.0
Si 8	0.4663	0.09638	0.52554	0.93	1.0
Si 9	0.7777	0.55142	0.33339	0.92	1.0
Si 10	0.36884	0.00001	0.37794	0.65	1.0
Si 11	0.1541	0.50214	0.35464	0.94	1.0
Si 12	0.8221	0.38557	0.1683	1.05	1.0
Si 13	0.5381	0.41447	0.424	1.6	1.0
Si 14	0.8892	0.37328	0.55406	0.85	1.0
Si 15	0.3487	0.46238	0.503	1.26	1.0
Si 16	0.9363	0.44089	0.3693	1.29	1.0
O 1	0.638	0.5326	0.0329	1.07	1.0
O 2	0.5926	0.166	0.3221	1.91	1.0
O 3	0.9008	0.4015	0.2708	2.76	1.0
O 4	0.6618	0.236	0.4841	1.5	1.0
O 5	0.5436	0.145	0.493	1.74	1.0
O 6	0.7546	0.3237	0.1668	1.41	1.0
O 7	0.7534	0.4429	0.1182	1.72	1.0
O 8	0.6365	0.2305	0.1751	1.24	1.0
O 9	0.4366	0.4154	0.4794	1.84	1.0
O 10	0.9431	0.3958	0.4641	1.61	1.0
O 11	0.3965	0.1321	0.5894	1.04	1.0
O 12	0.5605	0.4591	0.1489	1.64	1.0
O 13	0.6119	0.6022	-0.1252	1.48	1.0
O 14	0.7357	0.1251	0.4725	2.05	1.0
O 15	0.4869	0.4187	0.3065	2.12	1.0
O 16	0.3942	0.0661	0.4285	1.48	1.0
O 17	0.7114	0.5353	0.2244	1.73	1.0
O 18	0.6618	0.1137	0.1752	2.38	1.0
O 19	0.4741	0.1588	0.1421	1.82	1.0
O 20	0.5929	0.3488	0.4575	1.65	1.0
O 21	0.5313	0.0435	0.5938	1.82	1.0
O 22	0.255	0.4651	0.4069	2.14	1.0
O 23	0.7727	0.5288	-0.0852	2.43	1.0
O 24	0.6977	0.5644	0.4059	2.37	1.0

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Atom	x	y	z	B_{iso}	occ
O 25	0.1585	0.5697	0.4003	2.08	1.0
O 26	0.7033	0.2962	0.3361	1.78	1.0
O 27	0.558	0.3389	0.1887	1.64	1.0
O 28	0.8602	0.498	0.3767	1.93	1.0
O 29	0.0522	0.466	0.3707	2.84	1.0
O 30	0.3415	0.0086	0.2609	2.31	1.0
O 31	0.7965	0.3253	0.5173	1.73	1.0
O 32	0.6054	0.4709	0.4705	2.92	1.0
N	0.2428	0.7703	0.155	6.4	1.0
C 1	0.3457	0.7267	0.1737	2.68	1.0
C 2	0.5292	0.7219	0.1601	13.5	1.0
C 3	0.3687	0.7103	0.2776	9.16	1.0
C 4	0.4504	0.6122	0.2391	6.16	1.0
C 5	0.4773	0.6709	0.2948	7.66	1.0
C 6	0.2674	0.8296	0.2124	8.29	1.0
C 7	0.5595	0.7035	0.2696	10.82	1.0
C 8	0.3194	0.6723	0.1102	10.26	1.0
C 9	0.4313	0.2629	0.1453	7.9	1.0
C 10	0.425	0.63	0.1223	11.76	1.0
C 11	0.1602	0.7437	0.1979	16.19	1.0
C 12	0.5153	0.6654	0.1113	12.48	1.0
C 13	0.2111	0.7845	0.0455	14.84	1.0
F 1	0.7395	0.404	0.2683	1.97	0.317
F 2	0.6632	0.4191	0.3659	1.97	0.262
F 3	0.6473	0.414	0.2743	1.97	0.131

REFINED COMPOSITION: $|Na_{4.23}K_{0.167}Mg_{0.167}Ca_{3.74}|$ $[Al_{12.32}Si_{67.68}O_{160}]$
Mt. Adamson, N. Victoria Land, Antarctica

CRYSTAL DATA: *Cmcm* (No. 63)
$a = 9.747$ Å $b = 23.880$ Å $c = 20.068$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R = 0.071$, $R_w = 0.068$

REFERENCE: E. Galli, S. Quartieri, G. Vezzalini, A. Alberti and M. Franzini, *American Mineralogist* **82** 423–429 (1997).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0	0.4524	0.3281	1.01	0.846
Al 1	0.0	0.4524	0.3281	1.01	0.154
Si 2	0.0	0.5440	0.4396	1.18	0.846
Al 2	0.0	0.5440	0.4396	1.18	0.154
Si 3	0.7919	0.3604	0.3728	1.28	0.846
Al 3	0.7919	0.3604	0.3728	1.28	0.154
Si 4	0.7917	0.6392	0.4694	1.13	0.846
Al 4	0.7917	0.6392	0.4694	1.13	0.154
Si 5	0.0	0.1806	0.4414	1.07	0.846
Al 5	0.0	0.1806	0.4414	1.07	0.154
Si 6	0.0	0.7321	0.4365	1.01	0.846
Al 6	0.0	0.7321	0.4365	1.01	0.154
Si 7	0.0	0.2697	0.3272	1.15	0.846
Al 7	0.0	0.2697	0.3272	1.15	0.154
Si 8	0.0	0.8252	0.3289	1.02	0.846
Al 8	0.0	0.8252	0.3289	1.02	0.154
O 1	0.0	0.4692	0.25	3.41	1.0
O 2	0.0	0.5113	0.3679	3.97	1.0
O 3	0.1367	0.4160	0.3453	3.74	1.0
O 4	0.0	0.5	0.5	5.66	1.0
O 5	0.8630	0.5836	0.4415	3.97	1.0
O 6	0.1958	0.3583	0.4512	5.04	1.0
O 7	0.6325	0.3623	0.3488	3.16	1.0
O 8	0.8661	0.3057	0.3415	3.47	1.0
O 9	0.3663	0.6374	0.4453	2.34	1.0
O 10	0.8655	0.6932	0.4377	3.03	1.0
O 11	0.0	0.2124	0.3685	2.93	1.0
O 12	0.0	0.7751	0.4970	3.09	1.0
O 13	0.0	0.7648	0.3656	2.39	1.0
O 14	0.0	0.2515	0.25	3.28	1.0
O 15	0.0	0.8123	0.25	4.01	1.0
Na 1	0.0	0.0458	0.4442	0.7	0.03632
Na 2	0.0	0.0403	0.25	1.6	0.05564
Na 3	0.3578	0.4603	0.25	9.2	0.07573
Na 4	0.1457	0.0399	0.3495	9.5	0.05718
Na 5	0.0	0.6982	0.25	9.5	0.04327
Na 6	0.0	0.9509	0.4405	9.5	0.04327
Na 7	0.9089	0.1288	0.25	9.5	0.04327
Na 8	0.3519	0.4804	0.4598	8.2	0.02859

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Atom	x	y	z	B_{iso}	occ
Na 9	0.0	0.9651	0.3547	4.1	0.02009
Na 10	0.0	0.5972	0.25	11.8	0.04327
Na 11	0.3056	0.1983	0.25	9.5	0.03709
Na 12	0.1901	0.0815	0.1907	8.7	0.01545
K 1	0.0	0.0458	0.4442	0.7	0.00142
K 2	0.0	0.0403	0.25	1.6	0.00218
K 3	0.3578	0.4603	0.25	9.2	0.00297
K 4	0.1457	0.0399	0.3495	9.5	0.00224
K 5	0.0	0.6982	0.25	9.5	0.00170
K 6	0.0	0.9509	0.4405	9.5	0.00170
K 7	0.9089	0.1288	0.25	9.5	0.00170
K 8	0.3519	0.4804	0.4598	8.2	0.00112
K 9	0.0	0.9651	0.3547	4.1	0.00079
K 10	0.0	0.5972	0.25	11.8	0.00170
K 11	0.3056	0.1983	0.25	9.5	0.00145
K 12	0.1901	0.0815	0.1907	8.7	0.00061
Mg 1	0.0	0.0458	0.4442	0.7	0.00142
Mg 2	0.0	0.0403	0.25	1.6	0.00218
Mg 3	0.3578	0.4603	0.25	9.2	0.00297
Mg 4	0.1457	0.0399	0.3495	9.5	0.00224
Mg 5	0.0	0.6982	0.25	9.5	0.00170
Mg 6	0.0	0.9509	0.4405	9.5	0.00170
Mg 7	0.9089	0.1288	0.25	9.5	0.00170
Mg 8	0.3519	0.4804	0.4598	8.2	0.00112
Mg 9	0.0	0.9651	0.3547	4.1	0.00079
Mg 10	0.0	0.5972	0.25	11.8	0.00170
Mg 11	0.3056	0.1983	0.25	9.5	0.00145
Mg 12	0.1901	0.0815	0.1907	8.7	0.00061
Ca 1	0.0	0.0458	0.4442	0.7	0.03205
Ca 2	0.0	0.0403	0.25	1.6	0.04909
Ca 3	0.3578	0.4603	0.25	9.2	0.06682
Ca 4	0.1457	0.0399	0.3495	9.5	0.05045
Ca 5	0.0	0.6982	0.25	9.5	0.03818
Ca 6	0.0	0.9509	0.4405	9.5	0.03818
Ca 7	0.9089	0.1288	0.25	9.5	0.03818
Ca 8	0.3519	0.4804	0.4598	8.2	0.02523
Ca 9	0.0	0.9651	0.3547	4.1	0.01773
Ca 10	0.0	0.5972	0.25	11.8	0.03818
Ca 11	0.3056	0.1983	0.25	9.5	0.03273
Ca 12	0.1901	0.0815	0.1907	8.7	0.01364

Real symmetry is probably $C\ 2/c\ m$.
The Na, K, Mg and Ca cations share the same sites in the ratio ($Na_{0.51}K_{0.02}Mg_{0.02}Ca_{0.45}$).

REFINED COMPOSITION: $|Na_4Ca_{11.2}Sr_{0.8}(H_2O)_{24}|\ [Si_{20}Al_{20}O_{80}]$
Death Valley, California, U.S.A.

CRYSTAL DATA: *Pncn* (No. 52) **bca** setting
$a = 13.088$ Å $b = 13.052$ Å $c = 13.229$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Neutron single crystal refinement, $R_{F^2} = 0.048$

REFERENCE: J. J. Pluth, J. V. Smith and Å. Kvick, *Zeolites* **5** 74–80 (1985).

Atom	x	y	z	B_{iso}	occ
Na	0.0582	0.50360	0.36141	1.22	0.5
Ca 1	0.0582	0.50360	0.36141	1.22	0.5
Ca 2	0.49939	0.47837	0.49952	1.34	0.9
Sr	0.49939	0.47837	0.49952	1.34	0.1
Si 1	0.25	0.25	0.6885	0.51	1.0
Si 2	0.11291	0.69558	0.50065	0.51	1.0
Si 3	0.3082	0.38501	0.37805	0.49	1.0
Al 1	0.25	0.75	0.69049	0.48	1.0
Al 2	0.11939	0.30543	0.49655	0.5	1.0
Al 3	0.30947	0.62405	0.38045	0.51	1.0
O 1	0.16863	0.31051	0.61839	0.97	1.0
O 2	0.15818	0.69179	0.61444	0.95	1.0
O 3	0.31248	0.33136	0.75655	0.97	1.0
O 4	0.31152	0.65725	0.76318	0.98	1.0
O 5	0.00216	0.63793	0.50143	0.74	1.0
O 6	0.1838	0.6298	0.42414	1.02	1.0
O 7	0.19038	0.38476	0.41668	1.0	1.0
O 8	0.10438	0.81313	0.46106	0.94	1.0
O 9	0.11829	0.18031	0.45256	1.03	1.0
O 10	0.35586	0.49928	0.38346	0.72	1.0
O 20	0.12597	0.50192	0.18859	2.09	1.0
O 21	0.39173	0.49760	0.63937	2.19	1.0
O 22	0.0	0.64972	0.75	2.37	1.0
O 23	0.0	0.34436	0.75	2.19	1.0
H 1	0.15914	0.43727	0.66171	2.71	1.0
H 2	0.15747	0.55922	0.66161	2.95	1.0
H 3	0.37012	0.43800	0.67748	3.1	1.0
H 4	0.37158	0.55535	0.68126	3.1	1.0
H 5	0.04695	0.69037	0.71194	3.65	1.0
H 6	0.05008	0.30291	0.71828	4.19	1.0

TON Diethylamine Theta-1 (Silica ZSM-22)

REFINED COMPOSITION: $|C_{5.1}|\ [Si_{24}O_{48}]$

CRYSTAL DATA: $Cmc2_1$ (No. 36)
$a = 13.859$ Å $b = 17.420$ Å $c = 5.038$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.056$

REFERENCE: B. Marler,
Zeolites **7** 393–397 (1987).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0000	0.2737	0.25	0.67	1.0
Si 2	0.0000	0.3768	0.7465	0.58	1.0
Si 3	0.2951	0.0482	0.2265	0.80	1.0
Si 4	0.2055	0.2112	0.1445	0.58	1.0
O 1	0.0923	0.4268	0.6977	1.47	1.0
O 2	0.0942	0.2224	0.2068	1.90	1.0
O 3	0.2712	0.3789	0.6639	1.88	1.0
O 4	0.2288	0.4800	0.0234	1.05	1.0
O 5	0.2705	0.2584	0.3535	1.48	1.0
O 6	0.0	0.3062	0.5441	1.60	1.0
O 7	0.0	0.3450	0.0493	1.45	1.0
C 1	0.5	0.5195	0.1363	22.11	0.575
C 2	0.5	0.5124	0.3458	22.11	0.7

REFINED COMPOSITION: $|K_{12}Ca_{76}Sr_{12}Ba_{12}Cu_{48}Cl_{0.896}O_{327.448}(OH)_{128}|\ [Si_{192}Al_{192}O_{768}]$
Bellberg volcano, near Mayen, Eifel, Germany

CRYSTAL DATA: $Fm\bar{3}m$ (No. 225)
$a = 31.62$ Å $b = 31.62$ Å $c = 31.62$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
Single Crystal X-ray Refinement. $R_p = 0.065$, $R_{wp} = 0.156$

REFERENCE: H. Effenberger, G. Giester, W. Krause and H.-J. Bernhardt, *American Mineralogist* **83** 607–617 (1998).

Atom	x	y	z	B_{iso}	occ
Si 1	0.10993	0.18083	0.24967	0.92	0.5
Al 1	0.10993	0.18083	0.24967	0.92	0.5
Si 2	0.05044	0.12239	0.19243	0.95	0.5
Al 2	0.05044	0.12239	0.19243	0.95	0.5
O 1	0.0674	0.15559	0.23003	1.51	1.0
O 2	0.21169	0.21169	0.13239	1.37	1.0
O 3	0.21022	0.21022	0.40798	1.32	1.0
O 4	0.1464	0.1464	0.26611	1.72	1.0
O 5	0.14402	0.14402	0.05687	2.08	1.0
O 6	0.0772	0.0772	0.19159	2.01	1.0
O 7	0.11259	0.20286	0.0	2.05	1.0
Ca 1	0.09965	0.09965	0.09965	2.04	1.0
Ca 2	0.20984	0.20984	0.20984	1.23	1.0
K	0.17945	0.27909	0.0	2.68	0.125
Ca 3	0.17945	0.27909	0.0	2.68	0.125
Sr	0.17945	0.27909	0.0	2.68	0.125
Ba	0.17945	0.27909	0.0	2.68	0.125
Cu	0.07339	0.07339	0.0	2.31	1.0
OH 1	0.04506	0.04506	0.10539	2.16	1.0
OH 2	0.28335	0.28335	0.28335	1.29	1.0
Cl	0.0	0.0	0.0	0.87	0.224
O 8	0.041	0.0	0.0	5.37	0.181
O 9	0.0262	0.0262	0.0262	3.95	0.243
O 10	0.1467	0.1467	0.1467	9.71	1.0
O 11	0.0159	0.1842	0.0	8.76	0.305
O 12	0.2087	0.2339	0.0	3.71	0.5
O 13	0.0085	0.1316	0.3048	10.42	0.22
O 14	0.13599	0.13559	0.13559	5.68	1.0
O 15	0.0336	0.0336	0.2642	7.9	0.195
O 16	0.0714	0.0888	0.3105	7.9	0.189
O 17	0.0514	0.1204	0.3298	16.82	0.4

REFINED COMPOSITION: $[Si_{17}O_{34}]$

CRYSTAL DATA: $P\overline{4}$ (No. 81)
$a = 13.045$ Å $b = 13.045$ Å $c = 5.034$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{wp} = 0.125$, $R_p = 0.102$

REFERENCE: C. C. Freyhardt, R. F. Lobo, S. Khodabandeh, J. E. Lewis, Jr., M. Tsapatsis, M. Yoshikawa, M. A. Camblor, M. Pan, M. M. Helmkamp, S. I. Zones and M. E. Davis, *J. Am. Chem. Soc.* **118** 7299–7310 (1996).

Atom	x	y	z	B_{iso}	occ
Si 1	0.0000	0.0000	0.5000	1.03	1.0
Si 2	0.1991	0.0485	0.7568	1.03	1.0
Si 3	0.8341	0.2830	0.7444	1.03	1.0
Si 4	0.6512	0.1468	0.7630	1.03	1.0
Si 5	0.5182	0.12278	0.2656	1.03	1.0
O 34	0.7159	0.2492	0.7089	1.97	1.0
O 32	0.8867	0.2442	0.0133	1.97	1.0
O 35	0.8253	0.4062	0.748	1.97	1.0
O 24	0.7243	0.0464	0.7842	1.97	1.0
O 55	0.5000	0.0000	0.243	1.97	1.0
O 12	0.0746	0.0195	0.7489	1.97	1.0
O 54	0.5575	0.1441	0.5614	1.97	1.0
O 45	0.5998	0.1581	0.0521	1.97	1.0
O 23	0.9048	0.2340	0.5175	1.97	1.0

REFINED COMPOSITION: $|(H_2O)_{42}|\ [Al_{18}P_{18}O_{72}]$

CRYSTAL DATA: $P6_3$ (No. 173)
$a = 18.9752$ Å $b = 18.9752$ Å $c = 8.1044$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray Rietveld refinement, $R_{exp} = 0.108$, $R_{wp} = 0.141$, $R_F = 0.086$

REFERENCE: L. B. McCusker, Ch. Baerlocher, E. Jahn and M. Bülow, *Zeolites* **11** 308–313 (1991).

Atom	x	y	z	B_{iso}	occ
Al 1	0.385	-0.001	0.239	0.24	1.0
Al 2	0.474	-0.173	0.204	0.24	1.0
Al 3	0.654	0.169	0.198	0.24	1.0
P 1	0.550	-0.001	0.358	0.79	1.0
P 2	0.311	-0.185	0.320	0.79	1.0
P 3	0.507	0.185	0.309	0.79	1.0
O 1	0.470	0.001	0.339	1.5	1.0
O 2	0.431	0.009	0.037	1.5	1.0
O 3	0.322	-0.112	0.223	1.5	1.0
O 4	0.430	0.111	0.255	1.5	1.0
O 5	0.540	-0.074	0.264	1.5	1.0
O 6	0.619	0.072	0.278	1.5	1.0
O 7	0.512	-0.231	0.280	1.5	1.0
O 8	0.378	-0.206	0.280	1.5	1.0
O 9	0.474	-0.175	-0.015	1.5	1.0
O 10	0.311	-0.168	0.500	1.5	1.0
O 11	0.575	0.195	0.198	1.5	1.0
O 12	0.739	0.236	0.315	1.5	1.0
H_2O 1	0.339	0.005	0.465	2.13	1.0
H_2O 2	0.290	0.002	0.160	2.13	1.0
H_2O 3	0.314	0.130	-0.028	7.11	1.0
H_2O 4	0.248	0.055	-0.288	10.03	1.0
H_2O 5	0.193	0.045	-0.566	10.03	1.0
H_2O 6	0.319	0.189	-0.539	7.11	1.0
H_2O 7	0.100	0.053	-0.534	10.03	1.0

REFINED COMPOSITION: $|Rb_{44}K_4(H_2O)_{14}|\ [Si_{96}Zn_{24}O_{240}]$

CRYSTAL DATA: $P4_12_12$ (No. 92)
$a = 9.8837$ Å $b = 9.8837$ Å $c = 73.6505$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.099$, $R_{wp} = 0.147$, $R_F = 0.069$

REFERENCE: L. B. McCusker, R. W. Grosse-Kunstleve, Ch. Baerlocher, M. Yoshikawa, and M. E. Davis, *Microporous Materials* **6** 295–309 (1996).

Atom	x	y	z	B_{iso}	occ
Si 1	-0.05560	0.14097	0.04647	0.32	1.0
Si 2	0.12355	0.36647	0.03339	0.32	1.0
Si 3	0.34788	0.54161	0.04577	0.32	1.0
Si 4	0.64551	0.45059	0.04531	0.32	1.0
Si 5	0.70956	0.22908	0.01951	0.32	1.0
Si 6	0.91831	0.59382	0.03688	0.32	1.0
Zn 7	0.76905	0.26960	0.07855	0.79	1.0
Si 8	0.85239	0.37616	0.11695	0.32	1.0
Si 9	0.63992	0.15641	0.11374	0.32	1.0
Si 10	0.35908	0.14462	0.13017	0.32	1.0
Si 11	0.13640	0.35246	0.13429	0.32	1.0
Zn 12	0.27595	0.23519	0.16979	0.79	1.0
Si 13	0.43977	0.36294	0.20263	0.32	1.0
Si 14	0.21756	0.29059	0.22953	0.32	1.0
Zn 15	-0.00008	0.50334	0.24691	0.79	1.0
O 1	0.08204	0.21588	0.03997	1.97	1.0
O 2	-0.08423	0.17140	0.06759	1.97	1.0
O 3	-0.04109	-0.01758	0.04349	1.97	1.0
O 4	-0.17747	0.18145	0.03360	1.97	1.0
O 5	0.27867	0.39943	0.04014	1.97	1.0
O 6	0.02165	0.47477	0.04195	1.97	1.0
O 7	0.11120	0.37695	0.01106	1.97	1.0
O 8	0.50734	0.53146	0.04608	1.97	1.0
O 9	0.65363	0.37488	0.02615	1.97	1.0
O 10	0.77309	0.55290	0.04576	1.97	1.0
O 11	0.76847	0.24075	-0.00018	1.97	1.0
O 12	0.59335	0.11791	0.01974	1.97	1.0
O 13	0.91157	0.61905	0.01426	1.97	1.0
O 14	0.96658	0.72981	0.04654	1.97	1.0
O 15	0.64151	0.34871	0.06225	1.97	1.0
O 16	0.85799	0.39098	0.09506	1.97	1.0
O 17	0.66199	0.14092	0.09257	1.97	1.0
O 18	0.73381	0.27261	0.12267	1.97	1.0
O 19	0.68028	0.02001	0.12391	1.97	1.0
O 20	0.48533	0.19440	0.11787	1.97	1.0
O 21	0.23709	0.24422	0.12539	1.97	1.0
O 22	0.38915	0.14632	0.15157	1.97	1.0
O 23	0.31402	-0.00248	0.12264	1.97	1.0
O 24	0.13419	0.33967	0.15616	1.97	1.0
O 25	-0.00850	0.32063	0.12528	1.97	1.0

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Atom	x	y	z	B_{iso}	occ
O 26	0.36760	0.38136	0.18320	1.97	1.0
O 27	0.20338	0.09310	0.18492	1.97	1.0
O 28	0.33256	0.36743	0.21848	1.97	1.0
O 29	0.18986	0.14876	0.21931	1.97	1.0
O 30	0.08186	0.37815	0.23040	1.97	1.0
Rb 1	0.00301	0.00830	0.11980	2.92	0.875
Rb 2	0.16907	0.36207	0.08261	2.92	0.875
Rb 3	0.41652	0.41652	0.00000	2.92	0.75
O 31	0.41652	0.41652	0.00000	2.92	0.25
Rb 4	0.07877	0.07877	0.00000	2.92	1.0
Rb 5	0.64934	0.84320	0.03976	2.92	0.875
Rb 6	0.40656	0.13336	0.04950	2.92	0.75
K 6	0.32838	0.13511	0.03545	2.92	0.25
Rb 7	0.83939	0.69102	0.08693	2.92	0.75
K 7	0.86257	0.61323	0.07771	2.92	0.25
Rb 8	0.62218	0.62218	0.00000	2.92	0.25
O 32	0.62218	0.62218	0.00000	2.92	0.75
Rb 9	0.53776	0.56878	0.08892	2.92	0.375
O 33	0.56914	0.90441	0.07753	2.92	1.25

REFINED COMPOSITION: $|Na_{28.48}(H_2O)_{49.76}|\ [Si_{56}Zn_{16}O_{144}]$

CRYSTAL DATA: *Fdd*2 (No. 43)
$a = 39.88$ Å $b = 10.326$ Å $c = 10.219$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray Rietveld refinement, $R_{exp} = 0.248$, $R_{wp} = 0.162$, $R_I = 0.100$

REFERENCE: C. Röhrig, H. Gies and B. Marler,
Zeolites **14** 498–503 (1994).

Atom	x	y	z	B_{iso}	occ
Na 1	0.1269	0.201	0.059	1.58	0.89
Na 2	0.2549	0.069	0.762	1.58	0.89
Si 1	0.0	0.0	0.0	1.86	1.0
Si 2	0.0718	0.4537	0.565	1.86	1.0
Si 3	0.0868	0.1622	0.571	1.86	1.0
Si 4	0.0904	0.4481	0.855	1.86	1.0
Zn	0.05488	0.1640	0.856	1.86	1.0
O 1	0.0087	0.1255	0.910	0.87	1.0
O 2	0.0319	0.464	0.589	0.87	1.0
O 3	0.0850	0.054	0.955	0.87	1.0
O 4	0.0809	0.3082	0.519	0.87	1.0
O 5	0.0572	0.120	0.670	0.87	1.0
O 6	0.0610	0.3481	0.887	0.87	1.0
O 7	0.0902	0.488	0.702	0.87	1.0
O 8	0.1228	0.142	0.641	0.87	1.0
O 9	0.0836	0.081	0.435	0.87	1.0
H_2O 1	0.0889	0.299	0.213	5.53	1.23
H_2O 2	0.25	0.75	0.124	5.53	1.3
H_2O 3	0.2237	0.627	0.436	5.53	1.23

REFINED COMPOSITION: $|Ca_4(H_2O)_{16}|\ [Be_{12}P_8O_{32}(OH)_8]$
Weinebene Pass, Koralpe, Austria

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 11.897$ Å $b = 9.707$ Å $c = 9.633$ Å
$\alpha = 90°$ $\beta = 95.76°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: F. Walter,
Eur. J. Mineral. **4** 1275–1283 (1992).

Atom	x	y	z	B_{iso}	occ
Ca	0.1124	0.0853	0.3718	1.32	1.0
Be 1	-0.3006	0.8817	0.1613	0.65	1.0
Be 2	-0.1925	0.3821	0.3460	0.78	1.0
Be 3	0.0014	0.5184	0.2517	0.66	1.0
P 1	0.2785	0.0985	0.1409	0.54	1.0
P 2	-0.2780	0.0992	0.3606	0.71	1.0
O 1	-0.0939	0.6163	0.1650	0.87	1.0
O 2	0.2150	0.7795	0.6971	0.97	1.0
O 3	0.2388	0.9725	0.2213	0.71	1.0
O 4	0.2431	0.9230	0.4847	0.89	1.0
O 5	0.2853	0.7213	0.3029	1.02	1.0
O 6	0.2573	0.5836	0.5177	0.91	1.0
O 7	0.0943	0.6210	0.3323	1.25	1.0
O 8	0.2597	0.4676	0.2905	0.99	1.0
OH 9	0.0638	0.4212	0.1442	1.08	1.0
OH 10	-0.0622	0.4263	0.3603	1.04	1.0
H_2O 1	-0.5254	0.6453	0.1881	1.85	1.0
H_2O 2	0.4918	0.3807	0.3780	2.20	1.0
H_2O 3	0.4905	0.3629	0.0437	2.09	1.0
H_2O 41	0.2250	0.7474	0.0035	2.19	0.55
H_2O 42	0.1950	0.7323	0.0061	1.74	0.45

REFINED COMPOSITION: $|Na_{0.5}K_{0.5}Ca_{5.5}Ba_{3.5}S_3(OH)_{12}|\ [Si_{11}Al_9O_{41}(OH)_2]$
Candoglia, Italy

CRYSTAL DATA: $P\overline{6}2m$ (No. 189)
$a = 13.511$ Å $b = 13.511$ Å $c = 7.462$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R = 0.10$

REFERENCE: S. Merlino,
Acta Cryst. **B30** 1262–1266 (1974).

Atom	x	y	z	B_{iso}	occ
Na	0.4988	0.2743	0.0	2.42	0.083
K 1	0.0	0.0	0.5	2.04	0.125
K 2	0.3932	0.0	0.5	1.78	0.125
Ca	0.4988	0.2743	0.0	2.42	0.917
Ba 1	0.0	0.0	0.5	2.04	0.875
Ba 2	0.3932	0.0	0.5	1.78	0.875
S	0.5200	0.5200	0.0	1.3	1.0
Si 1	0.2666	0.1336	0.2178	0.8	0.60
Si 2	0.4380	0.3008	0.5	0.4	0.56
Si 3	0.66667	0.33333	0.3970	0.4	0.11
Al 1	0.2666	0.1336	0.2178	0.8	0.40
Al 2	0.4380	0.3008	0.5	0.4	0.44
Al 3	0.66667	0.33333	0.3970	0.4	0.39
O 1	0.296	0.145	0.0	0.2	1.0
O 2	0.392	0.215	0.317	1.4	1.0
O 3	0.216	0.0	0.294	0.8	1.0
O 4	0.170	0.170	0.275	1.0	1.0
O 5	0.399	0.399	0.5	2.2	1.0
O 6	0.580	0.378	0.5	1.3	1.0
O 7	0.66667	0.33333	0.170	3.0	0.5
OH 7	0.66667	0.33333	0.170	3.0	0.5
OH 8	0.421	0.402	-0.049	0.9	0.25
OH 9	0.492	0.606	0.074	2.6	0.25
OH 10	0.599	0.553	-0.158	1.6	0.25
OH 11	0.591	0.499	0.154	2.9	0.25

Si3, Al3, and the attached O7, are disordered over two positions, with the individual site occupancies being only 0.5. O7 is an OH^- when the T3 site is vacant, and an oxygen when T3 is occupied.

REFINED COMPOSITION: $|Ca_2H_{15.82}O_{8.136}|\ [Si_{12}Al_4O_{32}]$
Hvalfjördur, Iceland

CRYSTAL DATA: $P1c1$ (No. 7) unique axis **b**, cell choice 1
$a = 6.700$ Å $b = 13.972$ Å $c = 10.039$ Å
$\alpha = 90°$ $\beta = 111.07°$ $\gamma = 90°$
Neutron single crystal refinement at $T = 13$K, $R_w = 0.045$

REFERENCE: Å. Kvick, G. Artioli and J. V. Smith,
Z. Kristallogr. **174** 265–281 (1986).

Atom	x	y	z	B_{iso}	occ
Ca	0.05134	0.21654	0.42364	0.44	1.0
Si 1	0.34121	0.14798	0.98083	0.25	1.0
Si 2	0.71051	0.03650	0.19124	0.26	1.0
Si 3	0.40911	0.12450	0.69431	0.22	1.0
Si 4	0.02736	0.47598	0.43748	0.22	1.0
Si 5	0.36039	0.37327	0.96046	0.24	1.0
Si 6	0.74211	0.49757	0.62097	0.24	1.0
Al 1	0.0	0.00710	0.0	0.21	1.0
Al 2	0.39614	0.35598	0.65361	0.21	1.0
O 1	0.10689	0.10638	0.94844	0.54	1.0
O 2	0.85591	0.04834	0.09817	0.58	1.0
O 3	0.19153	0.07642	0.59056	0.48	1.0
O 4	0.50365	0.10778	0.13425	0.41	1.0
O 5	0.43489	0.11736	0.86004	0.65	1.0
O 6	0.61915	0.07317	0.67971	0.46	1.0
O 7	0.84451	0.06416	0.35574	0.44	1.0
O 8	0.33904	0.26252	-0.00394	0.64	1.0
O 9	0.39913	0.23277	0.63939	0.47	1.0
O 10	0.16380	0.42664	0.98834	0.47	1.0
O 11	0.83032	0.48293	0.49303	0.49	1.0
O 12	0.17154	0.38236	0.49904	0.42	1.0
O 13	0.57911	0.41154	0.08345	0.48	1.0
O 14	0.36053	0.39320	0.80583	0.54	1.0
O 15	0.62998	0.40026	0.64000	0.48	1.0
O 16	0.93634	0.47014	0.26478	0.40	1.0
O 100	0.98759	0.24929	0.17041	0.97	0.774
O 101	0.04165	0.27602	0.20621	3.79	0.182
H 11	0.95821	0.19582	0.10667	3.0	0.825
H 12	0.03505	0.30007	0.12817	3.55	0.883
H 13	0.05913	0.34986	0.21315	4.47	0.157
O 20	0.90310	0.23331	0.61844	0.89	1.0
H 21	0.87936	0.18305	0.67456	3.25	1.0
H 22	0.81676	0.28638	0.62799	2.36	1.0
O 30	0.70811	0.29016	0.32835	0.94	0.978
H 31	0.59175	0.27280	0.34773	3.00	0.482
H 32	0.65286	0.33338	0.39098	3.38	0.417
H 33	0.66062	0.32229	0.23748	2.31	1.001
O 40	0.36920	0.15938	0.36919	1.23	0.887
O 41	0.33283	0.12668	0.35814	1.35	0.128

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Atom	x	y	z	B_{iso}	occ
H 41	0.39007	0.14373	0.28329	2.50	0.910
H 42	0.49359	0.13517	0.44553	2.88	0.704
H 43	0.45146	0.15376	0.40785	15.99	0.314
H 51	0.90889	0.20607	0.91977	1.42	0.098
H 52	0.87863	0.31721	0.90312	4.90	0.119
O 50	0.81646	0.25961	0.92491	1.42	0.119

REFINED COMPOSITION: $|N_8C_{42.656}|$ $[Al_{25}Zn_7P_{32}O_{128}]$

CRYSTAL DATA: *Pbca* (No. 61)
$a = 14.226$ Å $b = 15.117$ Å $c = 17.557$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.069$

REFERENCE: B. Marler, J. Patarin and L. Sierra, *Microporous Materials* **5** 151–159 (1995).

Atom	x	y	z	B_{iso}	occ
Al 1	0.0532	0.7242	0.3410	1.56	0.639
Al 2	0.5553	0.9022	0.4377	1.56	0.794
Al 3	0.4234	0.6045	0.4306	1.56	0.814
Al 4	0.2111	0.8403	0.5378	1.56	0.877
Zn 1	0.0532	0.7242	0.3410	1.69	0.361
Zn 2	0.5553	0.9022	0.4377	1.69	0.206
Zn 3	0.4234	0.6045	0.4306	1.69	0.186
Zn 4	0.2111	0.8403	0.5378	1.69	0.123
P 1	0.4499	0.4048	0.4262	2.25	1.0
P 2	0.5849	0.1002	0.4250	2.25	1.0
P 3	0.5607	0.7292	0.3412	2.25	1.0
P 4	0.2147	0.6608	0.4506	2.25	1.0
O 1	0.0432	0.0001	0.3975	3.46	1.0
O 2	-0.5552	-0.0084	0.6006	3.46	1.0
O 3	0.0523	-0.1605	0.3570	3.46	1.0
O 4	-0.0558	0.3285	0.3629	3.46	1.0
O 5	-0.0494	-0.3296	0.3703	3.46	1.0
O 6	0.0279	0.1831	0.3709	3.46	1.0
O 7	0.1970	0.1063	0.4270	3.46	1.0
O 8	-0.3063	0.1053	0.4351	3.46	1.0
O 9	-0.4573	0.1168	0.5049	3.46	1.0
O 10	0.0359	0.1174	0.5247	3.46	1.0
O 11	0.3383	0.1058	0.5102	3.46	1.0
O 12	-0.0722	0.2158	0.2574	3.46	1.0
O 13	0.3486	0.1715	0.3817	3.46	1.0
O 14	0.2528	0.2463	0.4864	3.46	1.0
O 15	0.1399	-0.1002	0.4770	3.46	1.0
O 16	-0.1496	0.1936	0.3819	3.46	1.0
N	0.3047	0.9264	0.2574	4.41	1.0
C 1	0.2179	0.9808	0.2397	12.44	1.333
C 2	0.3954	0.9835	0.2517	12.44	1.333
C 3	0.3024	0.8446	0.2023	12.44	1.333
C 4	0.3006	0.8984	0.3392	12.44	1.333

Alpha Cristobalite

REFINED COMPOSITION: $[Si_4O_8]$
Ellora, Hyderabad, India

CRYSTAL DATA: $P4_12_12$ (No. 92)
$a = 4.97$ Å $b = 4.97$ Å $c = 6.94$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.044$

REFERENCE: W. A. Dollase,
Z. Kristallogr. **121** 369–377 (1965).

Atom	x	y	z	B_{iso}	occ
Si	0.30004	0.30004	0.0000	0.83	1.0
O	0.23976	0.10324	0.17844	1.55	1.0

Keatite

REFINED COMPOSITION: $[Si_{12}O_{24}]$
Synthetic material

CRYSTAL DATA: $P4_32_12$ (No. 96)
$a = 7.46$ Å $b = 7.46$ Å $c = 8.61$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$
X-ray single crystal refinement, $R_{hk0} = 0.129$, $R_{hhl} = 0.098$

REFERENCE: J. Shropshire, P. P. Keat and P. A. Vaughan,
Z. Kristallogr. **112** 409–413 (1959).

Atom	x	y	z	B_{iso}	occ
Si 1	0.326	0.120	0.248	2.34	1.0
Si 2	0.410	0.410	0.000	2.34	1.0
O 1	0.445	0.132	0.400	2.34	1.0
O 2	0.117	0.123	0.296	2.34	1.0
O 3	0.344	0.297	0.143	2.34	1.0

B_{iso} is the average of $B_{hk0} = 1.47$ Å^2 and $B_{hhl} = 3.22$ Å^2.

Moganite

REFINED COMPOSITION: $[Si_{12}O_{24}]$
Mogan formation, Gran Canaria, Canary Islands

CRYSTAL DATA: $I1\,2/a\,1$ (No. 15) unique axis **b**, cell choice 3
$a = 8.758$ Å $b = 4.876$ Å $c = 10.715$ Å
$\alpha = 90°$ $\beta = 90.08°$ $\gamma = 90°$

REFERENCE: G. Miehe and H. Graetsch,
Eur. J. Mineral. **4** 693–706 (1992).

Atom	x	y	z	B_{iso}	occ
Si 1	0.2500	0.9908	0.0000	3.2	1.0
Si 2	0.0115	0.2533	0.1678	0.5	1.0
O 1	0.9686	0.0680	0.2860	1.9	1.0
O 2	0.1711	0.1770	0.1050	5.0	1.0
O 3	0.8657	0.2148	0.0739	0.4	1.0

Alpha Quartz

REFINED COMPOSITION: $[Si_3O_6]$
Dextro-rotatory synthetic material

CRYSTAL DATA: $P3_221$ (No. 154)
$a = 4.916$ Å $b = 4.916$ Å $c = 5.4054$ Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 120°$
X-ray single crystal refinement, $R_w = 0.016$

REFERENCE: L. Levien, C. T. Prewitt and D. J. Weidner,
American Mineralogist **65** 920–930 (1980).

Atom	x	y	z	B_{iso}	occ
Si	0.5303	0.0000	0.6667	0.62	1.0
O	0.5865	0.7331	0.7142	1.05	1.0

Coordinates were transformed from the old setting of space group $P3_221$ to the new setting, using the transformation $(1 - x, 1 - y, 5/6 - z)$.

Tridymite

REFINED COMPOSITION: $[Si_{48}O_{96}]$
From the Steinbach meteorite, Harvard Museum, U.S.A.

CRYSTAL DATA: $C1c1$ (No. 9) unique axis **b**, cell choice 1
$a = 18.524$ Å $b = 5.0032$ Å $c = 23.810$ Å
$\alpha = 90°$ $\beta = 105.82°$ $\gamma = 90°$
X-ray single crystal refinement, $R_w = 0.069$

REFERENCE: W. A. Dollase and W. H. Baur,
American Mineralogist **61** 971–978 (1976).

Atom	x	y	z	B_{iso}	occ
Si 1	0.5507	0.541	0.5642	0.9	1.0
Si 2	0.7036	0.947	0.7374	1.2	1.0
Si 3	0.4198	0.549	0.6225	0.7	1.0
Si 4	0.5751	0.043	0.7955	1.1	1.0
Si 5	0.9247	0.548	0.6971	0.8	1.0
Si 6	0.7643	0.944	0.5386	0.9	1.0
Si 7	0.8023	0.449	0.7661	0.8	1.0
Si 8	0.6453	0.041	0.6027	0.7	1.0
Si 9	0.8531	0.463	0.9016	1.0	1.0
Si 10	0.9493	0.966	0.9358	1.0	1.0
Si 11	0.7244	0.559	0.9605	0.9	1.0
Si 12	0.5697	0.549	0.8702	1.1	1.0
O 1	0.5749	0.351	0.8182	1.2	1.0
O 2	0.5707	0.840	0.8476	1.5	1.0
O 3	0.7315	0.138	0.4851	1.8	1.0
O 4	0.7509	0.644	0.5152	1.7	1.0
O 5	0.4155	0.352	0.6741	2.9	1.0
O 6	0.4127	0.852	0.6434	1.9	1.0
O 7	0.8773	0.164	0.9213	1.8	1.0
O 8	0.9160	0.668	0.9361	2.4	1.0
O 9	0.7741	0.145	0.7538	1.8	1.0
O 10	0.7336	0.643	0.7402	2.2	1.0
O 11	0.6195	0.341	0.5847	1.2	1.0
O 12	0.5811	0.843	0.5661	1.9	1.0
O 13	0.4966	0.511	0.6062	2.7	1.0
O 14	0.3533	0.489	0.5665	1.0	1.0
O 15	0.6498	0.005	0.6711	1.8	1.0
O 16	0.6524	0.996	0.7805	2.0	1.0
O 17	0.8636	0.499	0.7328	1.8	1.0
O 18	0.8361	0.503	0.8333	2.6	1.0
O 19	0.5052	0.993	0.7398	1.8	1.0
O 20	0.6369	0.511	0.9268	2.9	1.0
O 21	0.9927	0.992	0.8868	1.4	1.0
O 22	0.5	0.468	0.5	2.2	1.0
O 23	0.7252	0.991	0.5898	2.3	1.0
O 24	0.7744	0.521	0.9155	1.5	1.0