Schemes for Building Zeolite Framework Models.

Systematics in the structures of zeolite frameworks.

INTRODUCTION

The "Atlas of Zeolite Framework Types" [1] contains 160 topological distinct tetrahedral TO_4 frameworks, where T may be Si, Al, P, Ga, B, Be etc.. The compiled framework types, characterized by Framework Type Codes consisting of three capital letters, do not depend on composition, distribution of the various T atoms, cell dimensions or symmetry. Their frameworks exhibit such a diversity of four-connected three-dimensional nets, that finite and infinite component units were introduced to describe their topologies.
Finite units were introduced by Meier [1.2] and Smith [3]. The secondary building units (SBUs) of Meier, e.g., 4-, 5- or 6-rings, are invariably non-chiral. This means that only one kind of SBU rather than enantiomeric pairs is needed to assemble the three-dimensional framework. The assemblage of the structure does not necessarily involve crystallographic symmetry operations.
The finite structural subunits (SSUs) developed by Smith are often of greater complexity (e.g., polyhedral cages). The SSUs represent a structural feature. They are not, however, SBUs in the sense just mentioned because very often the framework cannot be constructed from SSUs alone. Frequently, SSUs need to share corners, edges or faces to complete the framework.
The SBUs, as such, are not meant to describe precursors from which the zeolite grows. On the other hand, inspection of the systematics in existing framework types may give clues to choose targets for synthesis because equal segments in different frameworks, like (some of) the polyhedral cages, may play a role during crystal growth.
Infinite units, e.g. chains and layers, were extensively discussed by several authors [4-8]. The 5-ring zeolites were described in terms of component chains [9] as well as in terms of component layers [10].

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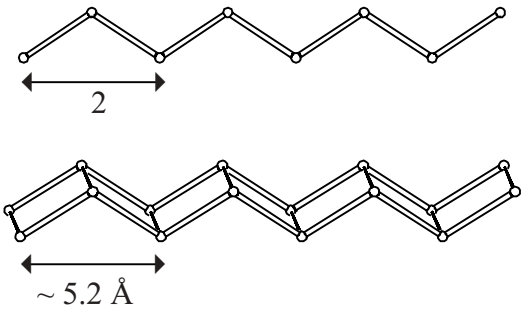
BUILDING UNITS USED IN THE PRESENT DESCRIPTION

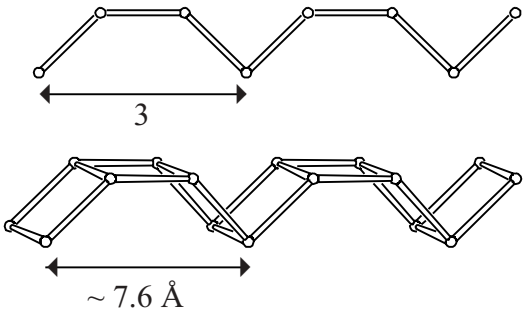
Crystal structures, which are periodically ordered in 3 dimensions, are ordered structures (regular crystalline solids). In this sense chemical disorder, e.g. different cations on a particular site, and dynamic disorder, e.g. rotational disorder of template molecules, is exluded. Structural disorder within cavities of zeolite frameworks is also excluded. In this "Schemes of Building Zeolite Framework Models" (hereafter called "Schemes") the frameworks are built from periodic 0-, 1-, or 2-dimensional structurally invariant **Periodic Building Units (PerBUs)**. The PerBUs are built from smaller units composed of a limited number of T-atoms by applying simple operation(s) to the smaller unit, e.g. translation, rotation. The zeolite framework types are analyzed in terms of these

component PerBUs. The infinite PerBUs, like (multiple) chains, tubes and layers, and finite PerBUs, like (double) 4-rings, (double) 6-rings and cages, are far from unique. However, they are common to several zeolite framework types and allow an easy description of the frameworks. Infinite PerBUs and finite PerBUs can be used to build the zeolite frameworks. 6-Ring layers are frequently curled up to form tubes of 6-rings.

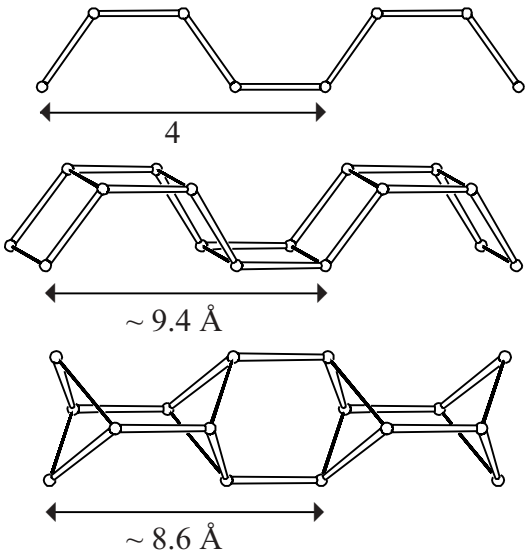
Many PerBUs can readily bee constructed from (infinite) chains shown in Scheme 1. Three of these chains, with identity periods of ~ m*2.5 Å, are referred to as zigzag (ZZ) chain, saw (SAW) chain and crankshaft (CRSHFT) chain with m = 2, 3 and 4, respectively. The number of T atoms in the independent repeat unit along the chain axis equals m. The fibrous zeolites can be built using the natrolite (NAT) chain. The unit cell dimension in a certain direction very often reflects the presence of ZZ, SAW or CRSHFT chains in that direction.



Single zigzag chain(top) and double zigzag chain (bottom).



Single saw chain(top) and double saw chain (bottom).



Single crankshaft chain(top), double crankshaft chain of the feldspar type(middle) and double crankshaft chain of the narsarsukite type (bottom).

Scheme 1. Some examples of frequently occurring chains in zeolite frameworks: open circles are tetrahedral coordinated T atoms (such as Si or Al); bridging oxygen atoms are left out for clarity. The number of T atoms in the repeat unit (of the single chain) and the length of the identity period are indicated.

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PORE DESCRIPTOR

According to the IUPAC Recommendations 2001 [11] the pore system is described with the general pore descriptor

$$\{ \boldsymbol{D}\ [n^m]_i\ (\boldsymbol{W}_{(\mathrm{eff})})\}$$

where

D is the dimensionality of the pore system. For cages ***D*** = 0, and for channels, ***D*** = 1. For systems of interconnected channels, ***D*** = 2 or 3;

$[n^m]_i$ is the shape of the pore, where *m* is the number of *n*-rings (or windows) defining the faces of the polyhedral pore and Óm_i is the total number of faces;

[*uvw*] the direction of the channel. The term [*uvw*] can be replaced by <*uvw*> to indicate that all crystallographic equivalent directions are involved;

and ($\boldsymbol{W}_{(\mathrm{eff})}$) is the effective channel width. In topological description this is the smallest *n*-ring that determines the accessibility of the pore system to guest species along the dimension of infinite extension.

If more than one pore system is present, the descriptions are separated by a slash(/). **TOP**

ZIGZAG CHAINS

In the following framework types at least one of the unit cell dimensions is about (n∗)5.2 Å indicating the presence of zigzag (ZZ) chains: **ABW, ATN, ATO, ATS, BCT, BIK, CAN, CAS, CFI, -CHI, DAC, EPI, EUO, GON, ITW, JBW, MTT, MTW, NES, NON, NPO, NSI, OSI, SFE, SFH, SFN, SSY, TON,** and **VET**. A detailed description of the framework type is given in the building scheme concerned.

All PerBUs consist of ZZ chains connected to 4-rings, of (double) layers of (corrugated) fused 6-rings with additional zigzag chains or 4-rings, or of tubular pores of rolled-up honeycomb-like sheets of (fused) 6-rings. These pores are different from the 6-ring pores in which crankshaft chains determine the cell repeat along the pore axis.

For a summary of the PerBUs: click **ZZ**. **TOP**

SAW CHAINS

In the following framework types at least one of the unit cell dimensions is about n*7.6 Å indicating the presence of (twisted) saw (SAW) chains. Saw chains can be connected into several PerBUs. A detailed description of the framework types obtained is given in de building schemes of **ATT**, **ATV**, **AWO**, **CDO**, **DAC**, **EON**, **EPI**, **FER**, **JBW**, **LTL**, **MAZ**, **MFS**, **MOR**, **OFF**, **RWR** and **UEI**.

For a summary of the PerBUs: click **SAW**. **TOP**

CRANKSHAFT CHAINS

In the following framework types at least one of the unit cell dimensions is between 8.3 and 9.9 Å indicating the presence of crankshaft (CRSHFT) chains. Crankshaft chains can be connected into several PerBUs. A detailed description of the framework types obtained is given in the building schemes of **ACO**, **AEL**, **AET**, **AFI**, **AFO**, **AHT**, **APC**, **APD**, **ATT**, **ATV**, **AWO**, **DFT**, **DON**, **GIS**, **-LIT**, **MER**, **PHI**, **GME**, **UEI** and **VFI**.

Several PerBUs consist of pores of rolled-up honeycomb-like sheets of (fused) 6-rings. These pores are different from the 6-ring pores in which ZZ chains determine the cell repeat along the pore axis.

For a summary of the PerBUs: click **CRSHFT**. **TOP**

SINGLE 3- AND/OR 4-RINGS

Single 3- and/or 4-rings (S3/4R) can be connected into several PerBUs. In some cases additional T atoms are needed to build the PerBU. A detailed description of the framework types obtained is given in the building schemes of (in alphabetic order) **EDI**, **ITE**, **LOV**, **MEI**, **MON**, **NAB**, **NAT**, **NPO**, **OBW**, **OSO**, **PAR**, **PON**, **-RON**, **RSN**, **RTH**, **RWY**, **THO**, **VNI**, **VSV** and **WEI**.
For a summary of the PerBUs: click **S3/4R** **TOP**

DOUBLE 4-RINGS

Double 4-rings (D4Rs) can be connected in several ways. In some cases the 4-rings of the D4Rs are not 4-fold connected and/or additional T atoms are needed to build the framework. A detailed description of the framework types obtained is given in the building schemes of (in alphabetic order) **ACO**, **AFI**, **AFN**, **AFR**, **AFS**, **AFY**, **APC**, **APD**, **AST**, **ASV**, **BOG**, **BPH**, **BRE**, **CGF**, **CGS**, **-CLO**, **DFO**, **DFT**, **ETR**, **GIS**, **GOO**, **HEU**, **ITW**, **LAU**, **LTA**, **MEI**, **MER**, **OWE**, **PHI**, **RRO**, **SAS**, **SFO**, **STI**, **TER**, **UOZ**, **USI**, **YUG** and **ZON**.
For a summary of the PerBUs: click **D4R**. **TOP**

5-RINGS

5-Rings (5RINGS) can be connected into several PerBUs. In all cases additional T atoms, connected to the 5-rings, are needed to build the PerBU. A detailed description of the framework types obtained is given in the building schemes of (in alphabetic order) **BIK**, **CAS**, **CDO**, **CFI**, **-CHI**, **CON**, **DAC**, **DON**, **EPI**, **ESV**, **FER**, **GON**, **IWR**, **MAZ**, **MEL**, **MFI**, **MFS**, **MOR**, **MTF**, **MTT**, **MTW**, **NSI**, **RTE**, **SFE**, **SFF**, **SFH**, **SFN**, **SGT**, **SSY**, **STF**, **STT** and **TON**.
For a summary of the PerBUs: click **5RINGS** **TOP**

DOUBLE 6-RINGS

Double 6-rings (D6Rs) can be connected into several PerBUs. In some cases the 6-rings of the D6Rs are not 6-fold connected and/or additional T atoms are needed to build the PerBU. A detailed description of the framework types obtained is given in de building schemes of **AEI**, **AEN**, **AFI**, **AFO**, **AFT**, **AFX**, **ATT**, **ATV**, **AWO**, **AWW**, **BOG**, **CGS**, **CHA**, **EMT**, **ETR**, **FAU**, **GME**, **IFR**, **KFI**, **LAU**, **-LIT**, **MSO**, **RTE**, **RUT**, **SAO**, **SAS**, **SAV**, **SOS**, **TSC** and **UEI**.
For a summary of the PerBUs: click **D6R**. **TOP**

ABC-6 FAMILY

A large number of framework types can be constructed using a hexagonal PerBU consisting of an array of non-connected 6-rings. They all belong to the so-called ABC-6-family. In these framework types the unit cell dimension along the hexagonal axis is about (n*)2.55 Å (n=number of PerBUs along the hexagonal axis). A detailed description of the framework types is given in the building schemes of **AFG**, **AFT**, **AFX**, **CAN**, **CHA**, **EAB**, **ERI**, **FRA**, **GIU**, **GME**, **LEV**, **LIO**, **LOS**, **MAR**, **OFF**, **SAT** and **SOD**.
For a description of the PerBU: click **ABC**. **TOP**

BETA-(like) FAMILY

The framework types ***BEA**, **BEC**, **CON**, **ISV**, **ITH**, **IWR** and **IWW** can be built using chains that resemble each other.
For a summary of the chains: click: **BET**. **TOP**

CLATHRASILS

The famework types **DDR**, **DOH**, **MEP** and **MTN** belong to the clathrasil family and can be built using units that consist of 30 T-atoms. These T30-units can be connected in a periodic manner in 2-dimensions to form layers. Additional 6-ring layers are sometimes needed.
composed of units of 30 T atoms.
For a summary of the PerBUs: click **CLAT**. **TOP**

CAGES

A polyhedron whose maximum window is a 6-ring is called a cage. All other polyhedra are called cavities. Cages or cavities can be connected in several ways. A detailed description of the framework types obtained is given in the building schemes of (in alphabetic order): **AST**, **ATN**, **AWW**, **-CLO**, **DDR**, **DOH**, **EMT**, **FAU**, **KFI**, **LTA**, **LTN**, **MEP**, **MER**, **MTN**, **PAU**, **RHO**, **SBE**, **SBS**, **SBT**, **SOD** and **TSC**.
For a summary of the PerBUs: click **CAGES**. **TOP**

MISCELLANEOUS

A detailed description of the miscellaneous framework types is given in the building schemes of **ANA**, **CZP**, **SFG**, **UFI**, **UTL**,
For a summary of the PerBUs: click **MISCEL**. **TOP**

The database presents a mainly pictorial description of how to build the framework types using the PerBUs summarized in the **APPENDIX**. All drawings are prepared using the ORTEP program of Carroll K. Johnson [12]. The topological symmetry and unit cell data of the zeolites are obtained from the Atlas [1]. Only T atoms are drawn. Oxygen atoms are about midway between T atoms.

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REFERENCES

1. Ch. Baerlocher, W.M. Meier and D.H. Olson. Atlas of Zeolite Framework Types, 5th rev. ed., Elsevier, London, 2001.
2. W.M. Meier, in Molecular Sieves, Soc. of Chem. and Ind., London, 1968, pp. 10-27.
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12. C.K. Johnson. ORTEP. Report ORNL-3794, revised June 1970. Oak Ridge National Laboratory, Tennessee, USA.

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CREDITS

"Schemes for Building Zeolite Framework Models" is compiled by Henk van Koningsveld and is provided as a service to the zeolite community by the Structure Commission of the International Zeolite Association. The web-pages are maintained by Christian Baerlocher. We welcome corrections, comments and suggestions (email: h.vankoningsveld@tnw.tudelft.nl).

If you would like to give a reference to "Schemes for Building Zeolite Framework Models" in a publication, we suggest:

H. van Koningsveld
"Schemes for Building Zeolite Framework Models"
http://www.iza-structure.org/databases/
Published on behalf of the Structure Commission of the International Zeolite Association.

Although several documents are still incomplete, the author felt that the information should be made available to the zeolite community. Efforts are underway to complete the "Schemes" as soon as possible.

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APPENDIX

Figures 1-12 on next pages summarize the PerBUs used in building several groups of zeolite framework types:

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Figure 1: PerBUs containing zigzag chains

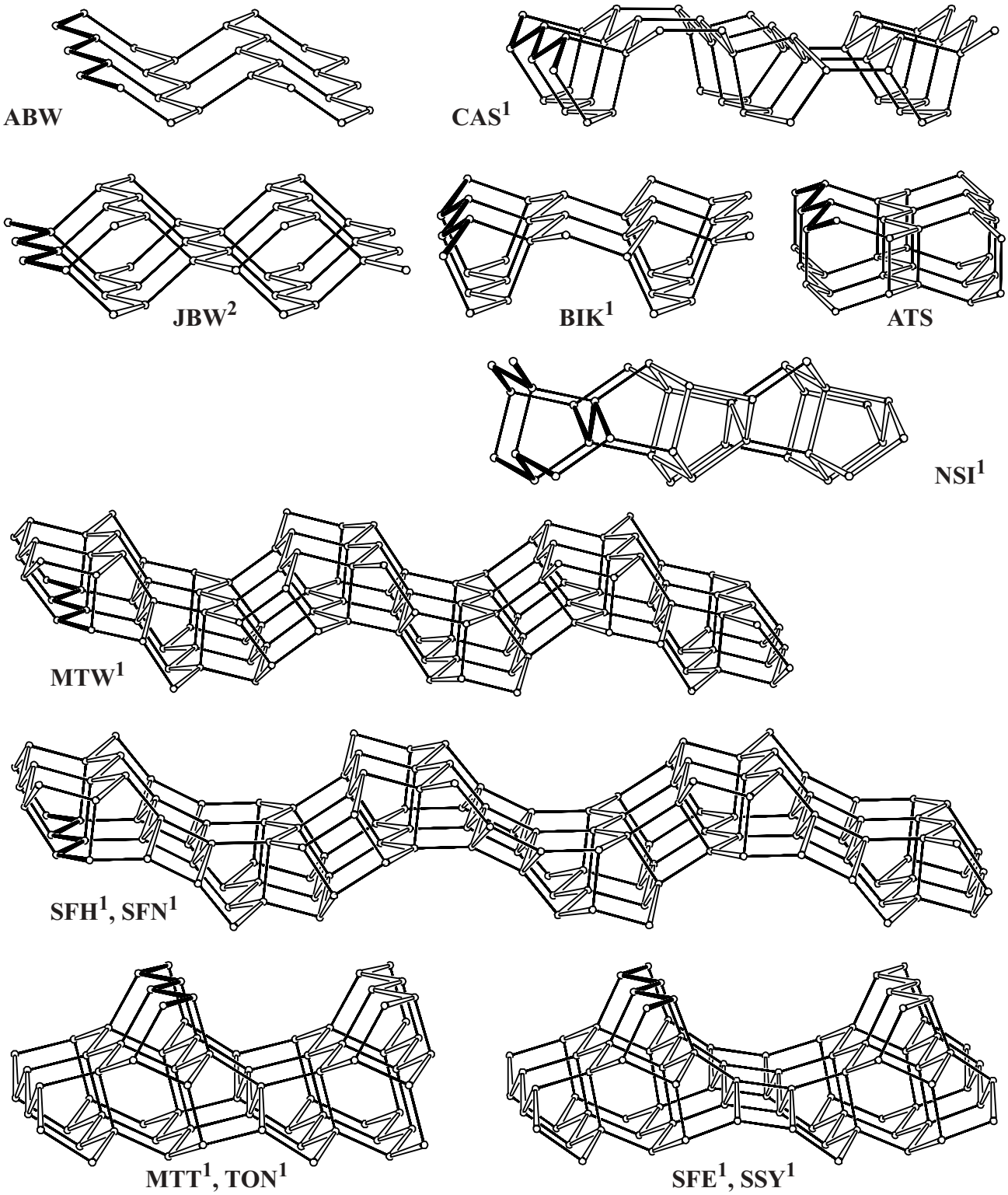
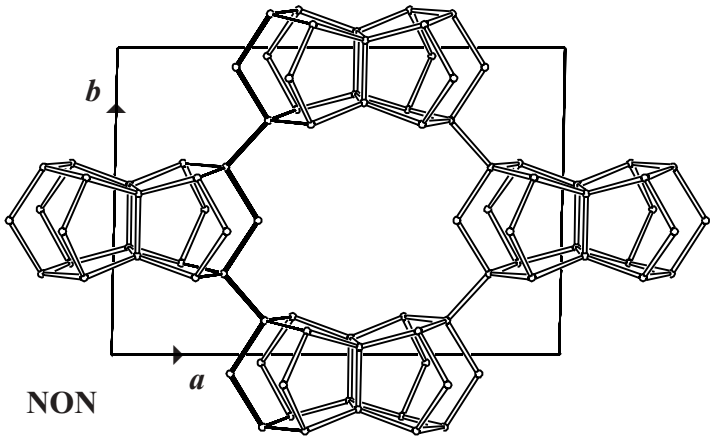
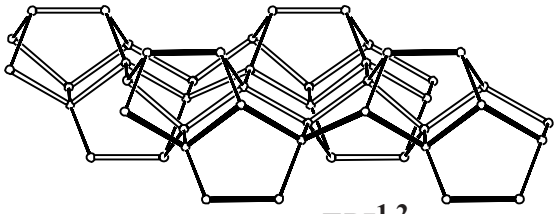


Figure 1. Summary of PerBUs containing zigzag chains (in bold). All PerBUs consist of (double) layers of (corrugated) fused 6-rings decorated with additional zigzag chains or 4-rings, of isolated zigzag chains connected to 4-rings, or of tubular pores of fused 6-rings. The PerBUs are arranged accordingly. [Fig.1 is continued on next page]

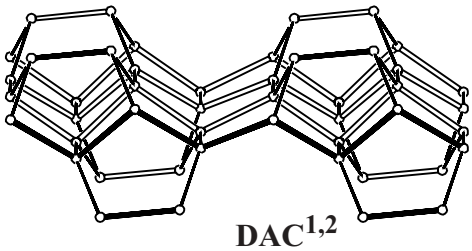
Figure 1 [Continued]



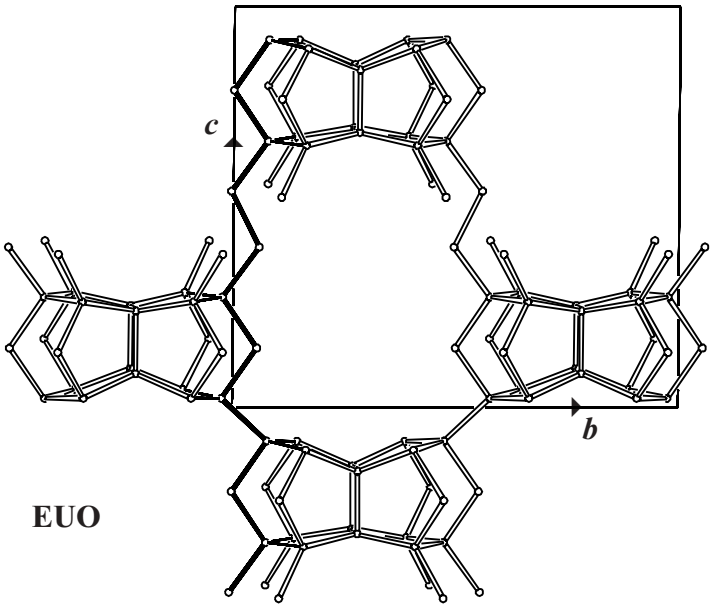
NON



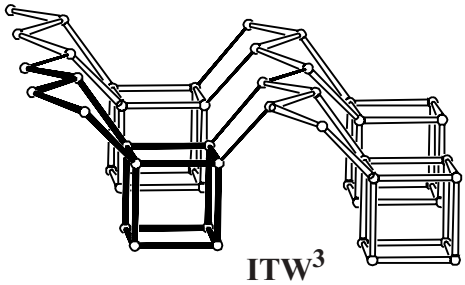
EPI[1,2]



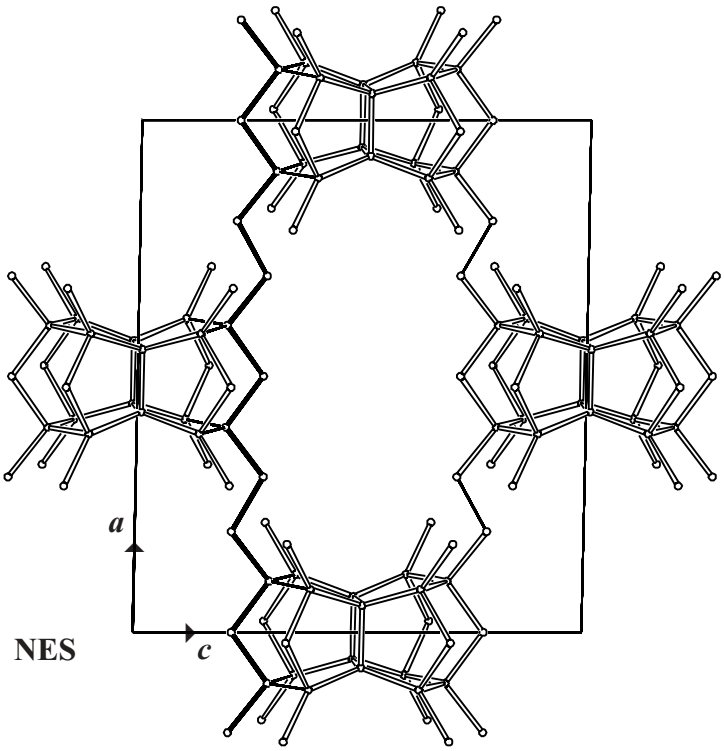
DAC[1,2]



EUO



ITW[3]



NES

Figure 1 [Cont'd]. Summary of PerBUs containing zigzag chains (in bold). All PerBUs consist of (double) layers of (corrugated) fused 6-rings decorated with additional zigzag chains or 4-rings, of isolated zigzag chains connected to 4-rings, or of tubular pores of fused 6-rings. The PerBUs are arranged accordingly. [Fig.1 is continued on next page]

Figure 1 [Continued]

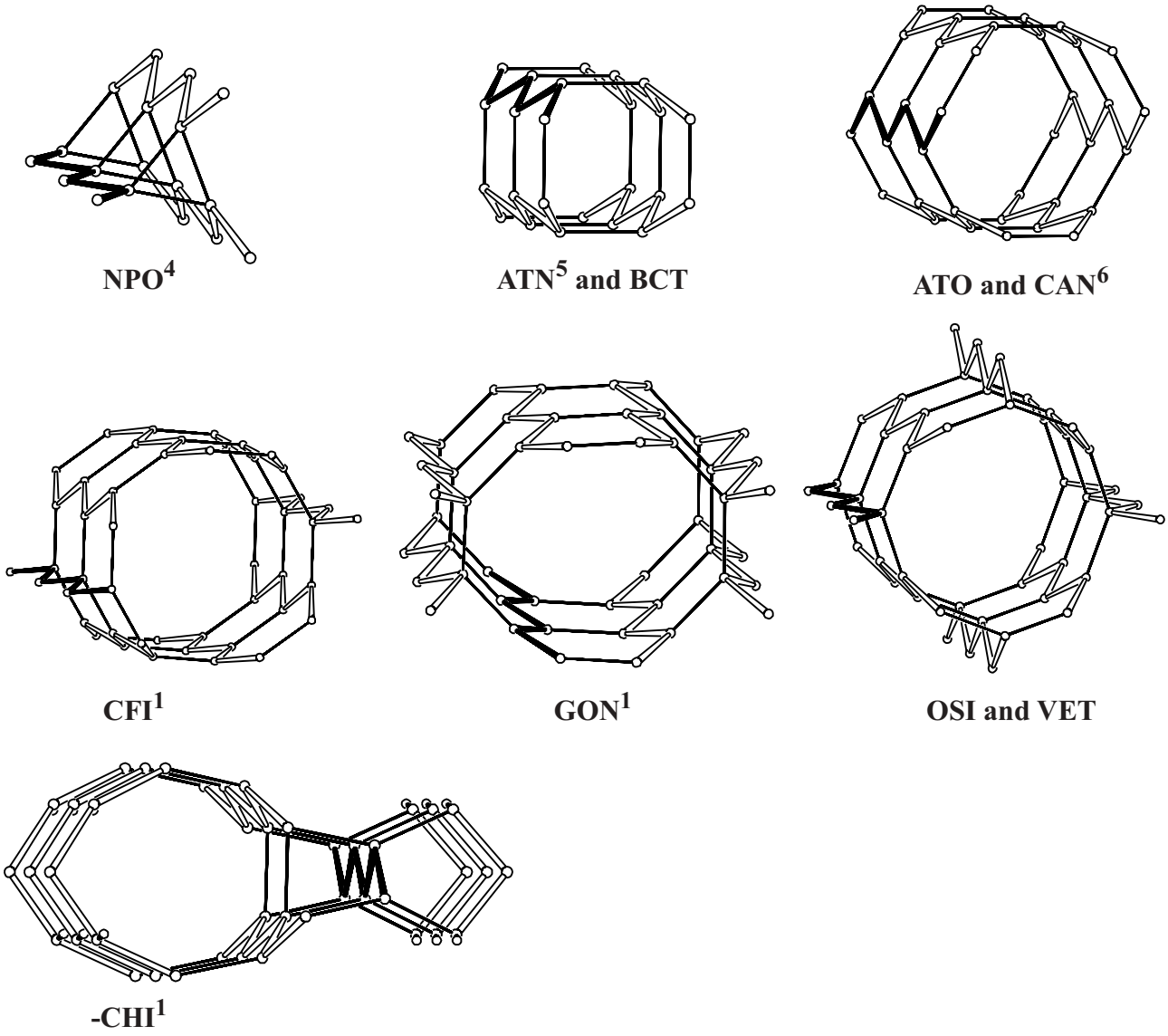


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Figure 1 [Continued]

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[1] **BIK, CAS, CFI, -CHI, DAC, EPI, GON, MTT, MTW, NSI, SFE, SFH, SFN, SSY** and **TON** can also be constructed using (modified) 5-rings (**5RINGS**).
[2] **JBW, DAC** and **EPI** can also be constructed using saw chains (**SAW**).
[3] **ITW** can also be constructed using (not fully-connected) double 4-rings (**D4R**).
[4] **NPO** can also be built using 3-rings (**S3/4R**)
[5] **ATN** can also be built using cages (**CAGES**).
[6] **CAN** belongs to the ABC-6 family (**ABC**).

Figure 1 [Final page]. Summary of PerBUs containing zigzag chains (in bold). All PerBUs consist of (double) layers of (corrugated) fused 6-rings decorated with additional zigzag chains or 4-rings, of isolated zigzag chains connected to 4-rings, or of tubular pores of fused 6-rings. The PerBUs are arranged accordingly.

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Figure 2: PerBUs containing saw chains

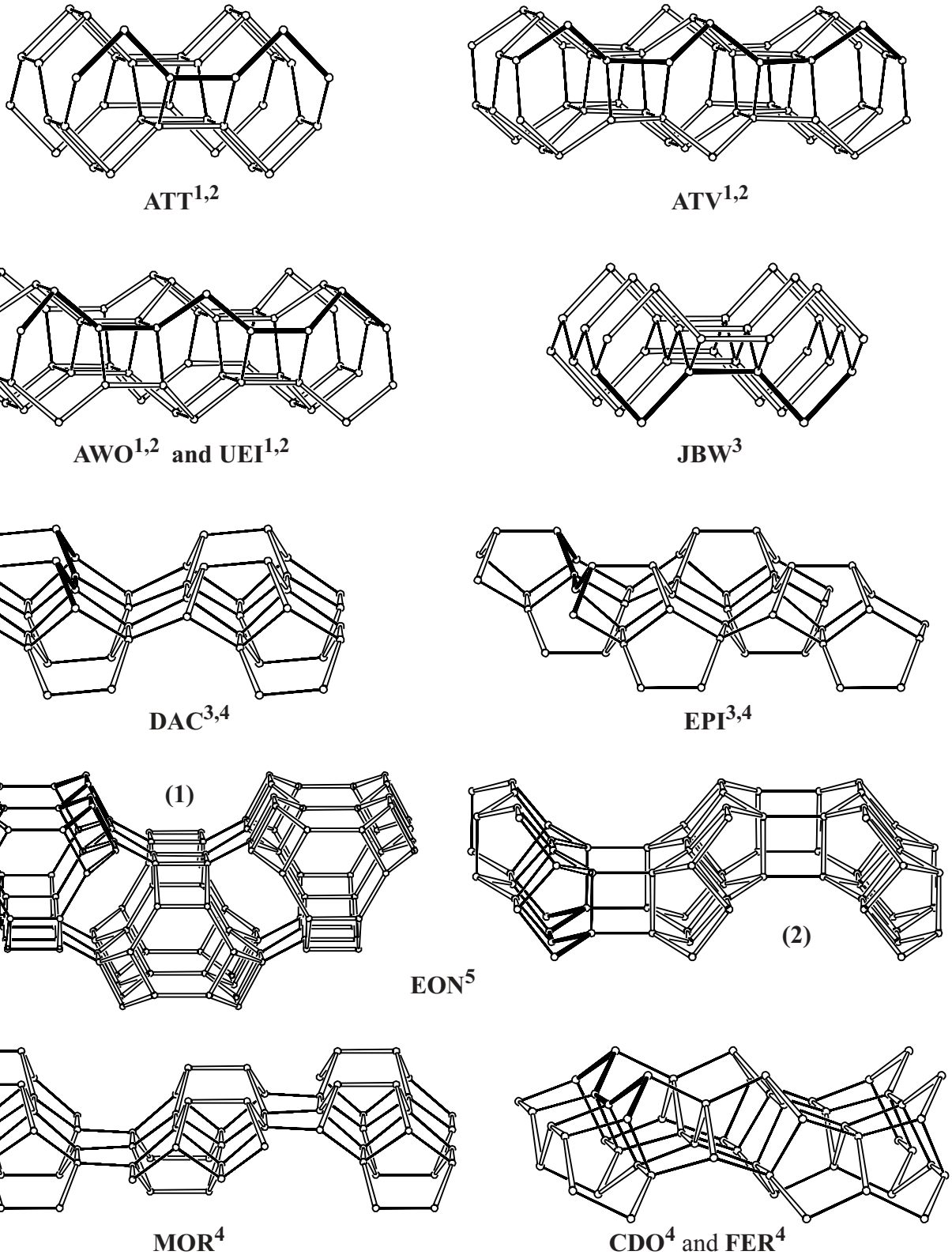
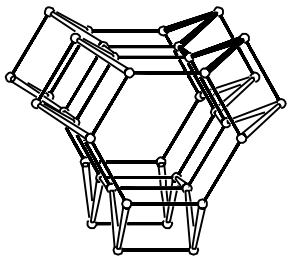
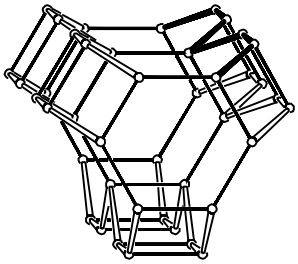


Figure 2. Summary of PerBUs containing (modified) saw chains (in bold). [Fig. 2 is continued on next page]

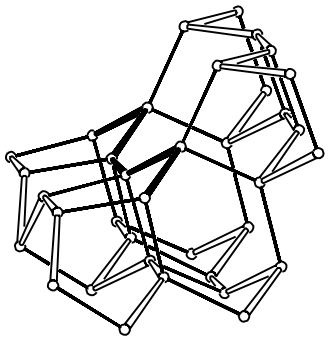
Figure 2 [Continued]



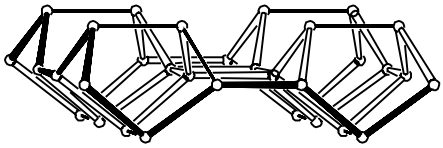
LTL and OFF[6]



MAZ



MFS[4]



RWR

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[1] **ATT, ATV, AWO** and **UEI** can also be constructed using crankshaft chains (**CRSHFT**).
[2] **ATT, ATV, AWO** and **UEI** can also be constructed using (not fully-connected) double 6-rings (**D6R**).
[3] **JBW, DAC** and **EPI** can also be constructed using zigzag chains (**ZZ**).
[4] **CDO, DAC, EPI, FER, MFS** and **MOR** can also be constructed using (modified) 5-rings (**5RINGS**).
[5] **EON** is an ordered intergrowth of **MAZ** layers (**1**) and **MOR** layers (**2**).
[6] **OFF** belongs to the ABC-6 family (**ABC**).

Figure 2 [Final page]. Summary of PerBUs containing (modified) saw chains (in bold).

Back to: **SAW-chains** - **APPENDIX** - **TOP**

Figure 3: PerBUs containing crankshaft chains

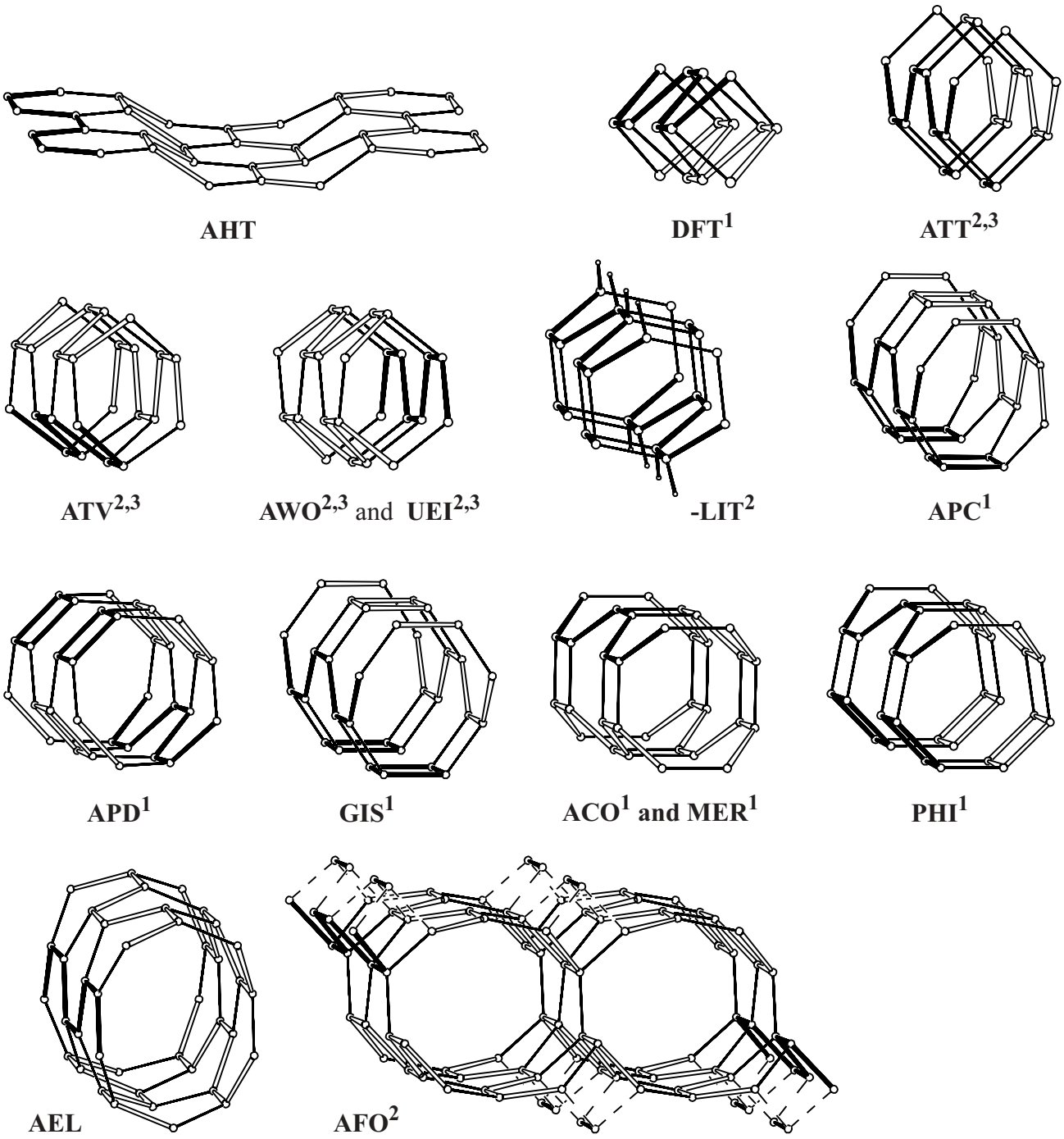

Figure 3. Summary of PerBUs of framework types in which the repeat distance along the pore axis is between 8.3 and 9.9 Å indicating the presence of crankshaft chains. The PerBUs consist of a layer of fused 6-rings, or of pores with a 4-, 6-, 8-, 10-, 12-, 14- or 18-ring window. In some cases additional crankshaft chains or 4-rings are needed. The PerBUs are arranged accordingly. [Fig.3 is continued on next page]

Figure 3 [Continued]

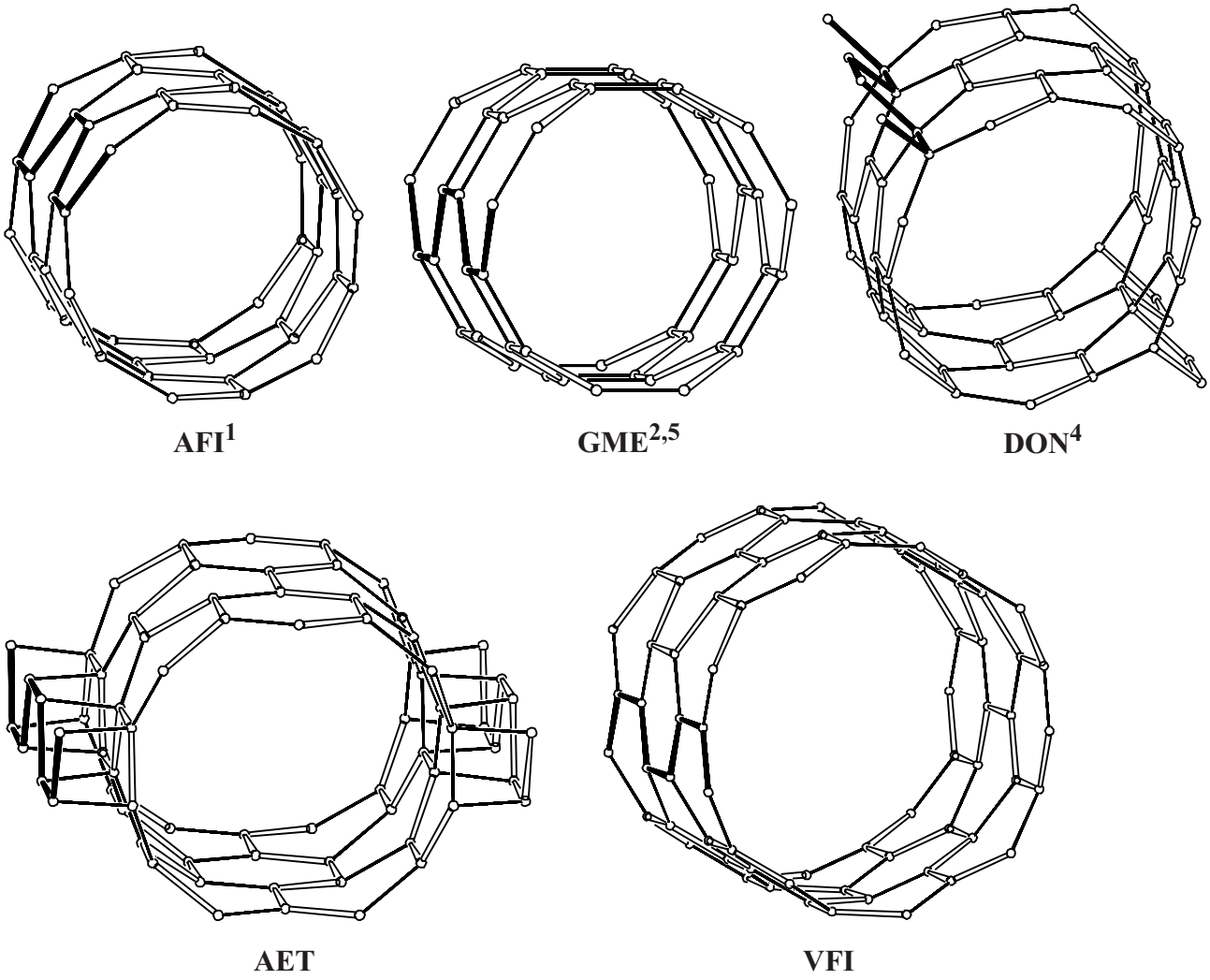

Figure 3 [Cont'd]. Summary of PerBUs of framework types in which the repeat distance along the pore axis is between 8.3 and 9.9 Å indicating the presence of crankshaft chains. The PerBUs consist of a layer of fused 6-rings, or of pores with a 4-, 6-, 8-, 10-, 12-, 14- or 18-ring window. In some cases additional crankshaft chains or 4-rings are needed. The PerBUs are arranged accordingly.
[Fig.3 is continued on next page]

Figure 3 [Continued]

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[1] **ACO, AFI, APC, APD, DFT, GIS, MER and PHI** can also be constructed using (not fully-connected) double 4-rings (**D4R**).
[2] **AFO, ATT, ATV, AWO, GME, -LIT and UEI** can also be constructed using (not fully-connected) double 6-rings (**D6R**).
[3] **ATT, ATV, AWO** and **UEI** can also be constructed using (twisted) saw chains (**SAW**).
[4] **DON** can also be constructed using (modified) 5-rings (**5RINGS**).
[5] **GME** belongs to the ABC-6 family (**ABC**).

Figure 3 [Final page]. Summary of PerBUs of framework types in which the repeat distance along the pore axis is between 8.3 and 9.9 Å indicating the presence of crankshaft chains. The PerBUs consist of a layer of fused 6-rings, or of pores with a 4-, 6-, 8-, 10-, 12-, 14- or 18-ring window. In some cases additional crankshaft chains or 4-rings are needed. The PerBUs are arranged accordingly.

Back to: **CRSHFT-chains** - **APPENDIX** - **TOP**

Figure 4. PerBUs containing single 3- and/or 4-rings

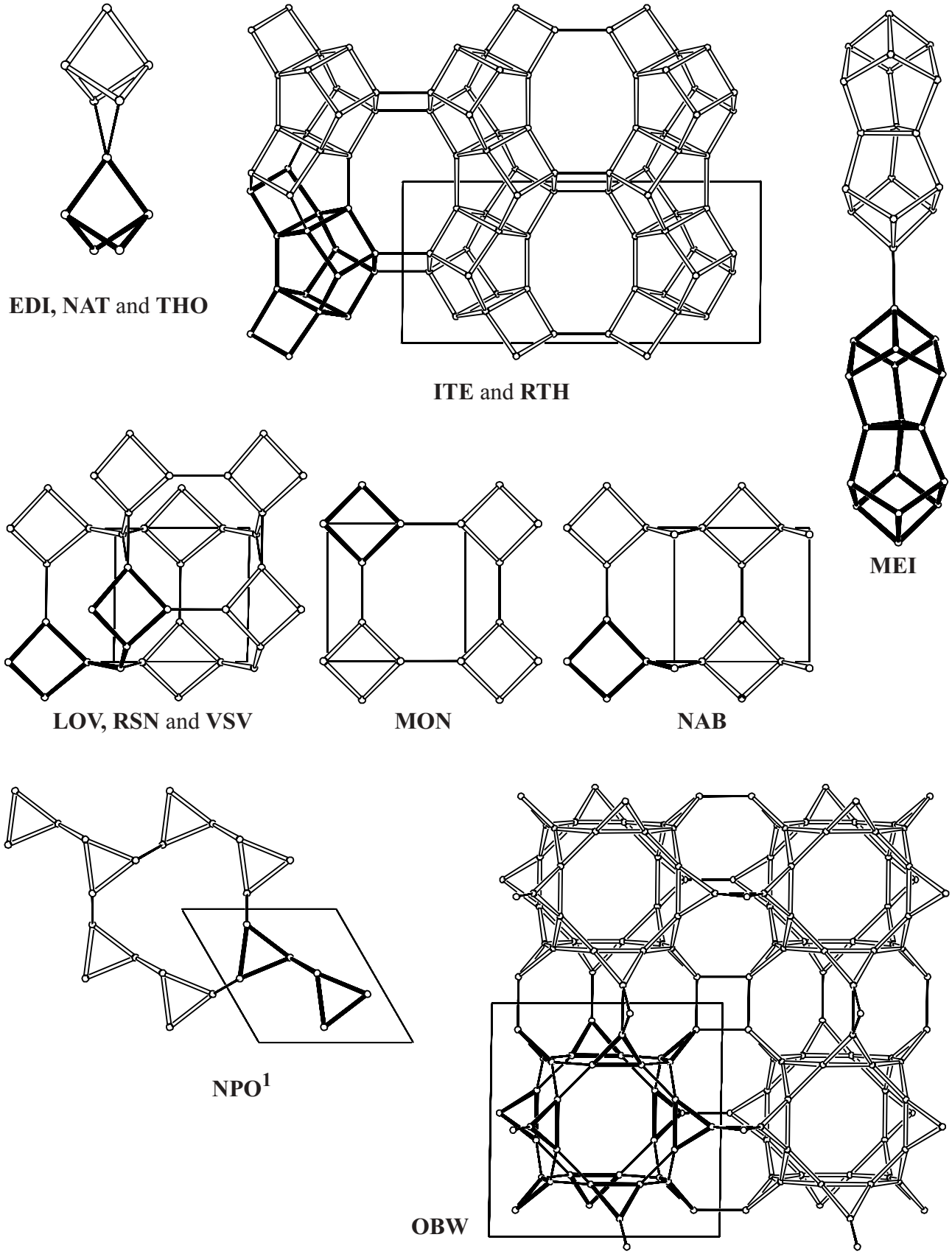


Figure 4. Summary of PerBUs containing (modified) 3- and/or 4-rings (in bold). References are on final page. [Figure 4 is continued on next page]

Figure 4 [Continued]

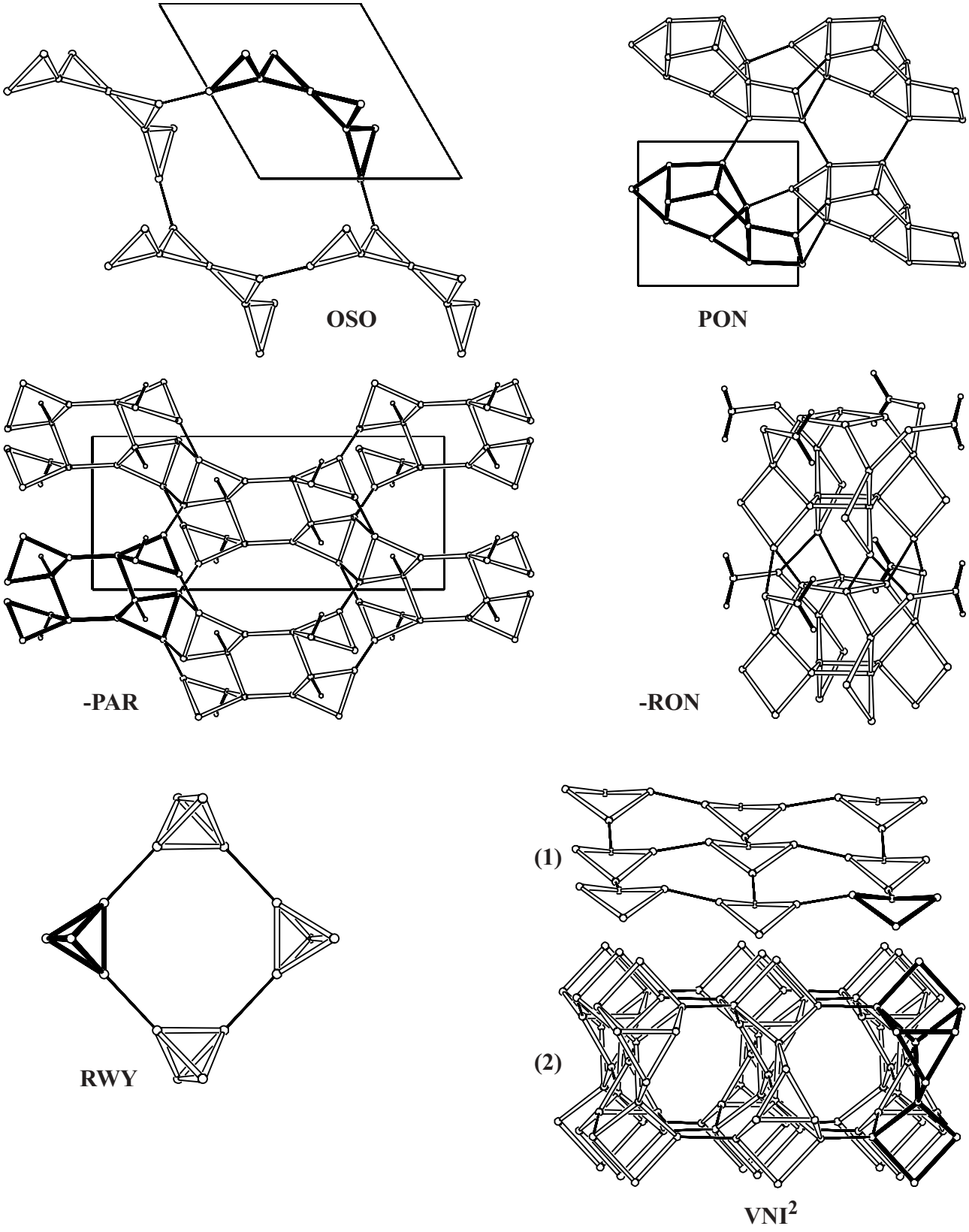
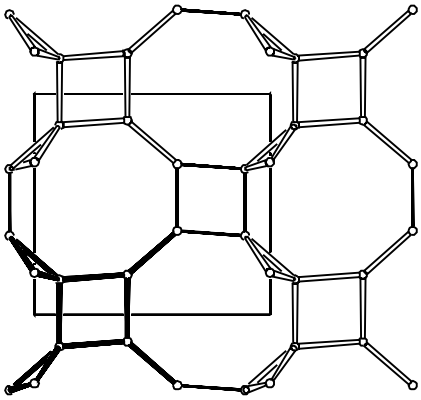


Figure 4 [Cont'd]. Summary of PerBUs containing (modified) 3- and/or 4-rings (in bold). References are on final page. [Figure 4 is continued on next page]

Figure 4 [Continued]



WEI[3]

---

[1] **NPO** can also be built fiom zigzag chains (**ZZ**).
[2] In **VNI** the PerBU is composed of two building units: **(1)** and **(2)**. **(1)** is composed of 4-rings and **(2)** of 4-rings and 3-rings**.**
[3] **WEI** is the only framework type that can also be constructed using spiro-5 rings (**WEI**).

Figure 4 [Final page]. Summary of PerBUs containing (modified) 3- and/or 4-rings (in bold).

Back to: **S3/4R** - **APPENDIX** - **TOP**

Figure 5. PerBUs containing double 4-rings (D4Rs)

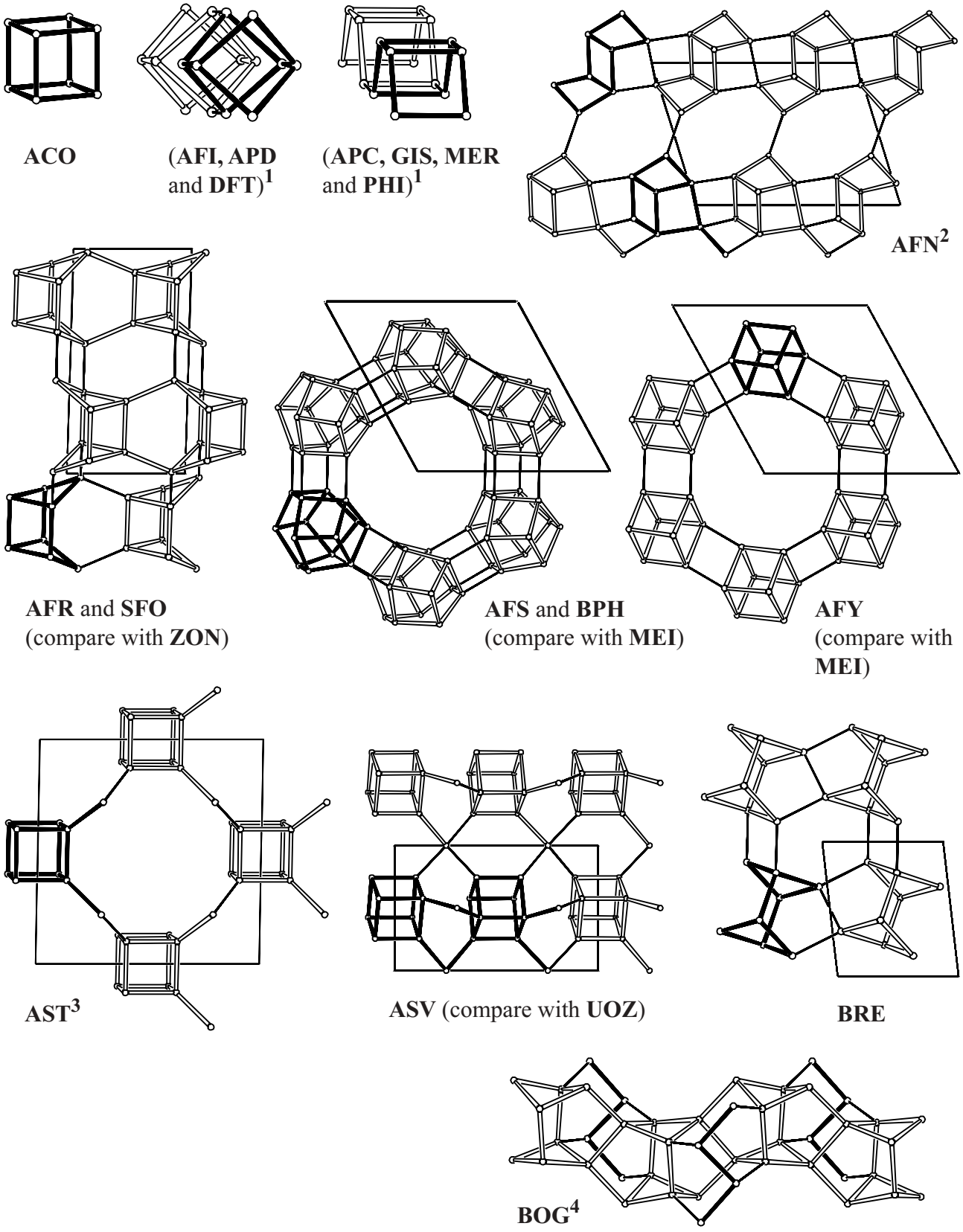


Figure 5. Summary of PerBUs containing (substituted) D4Rs (in bold). References are on final page.
[Figure 5 is continued on next page]

Figure 5 [Cont'd]

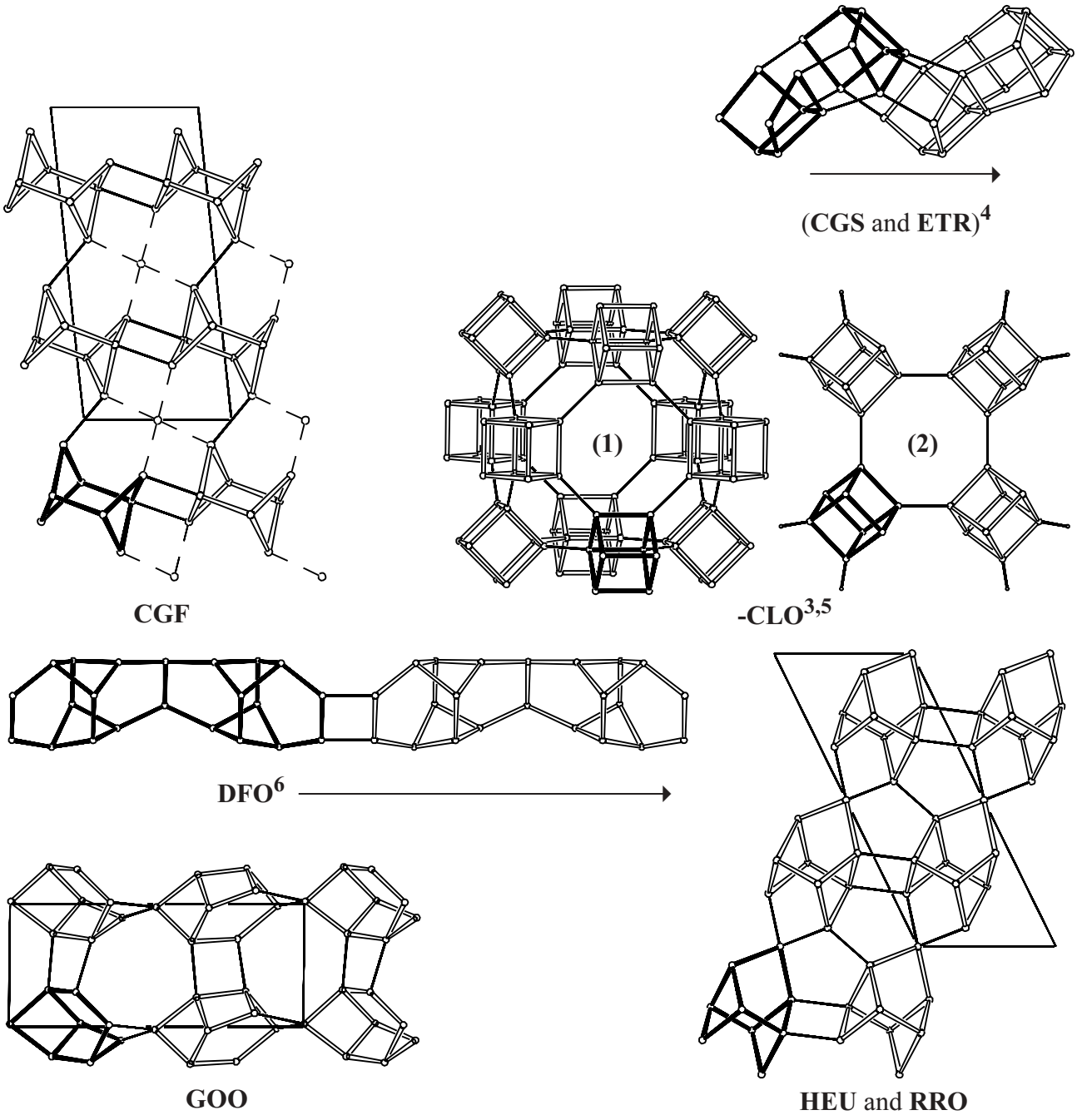
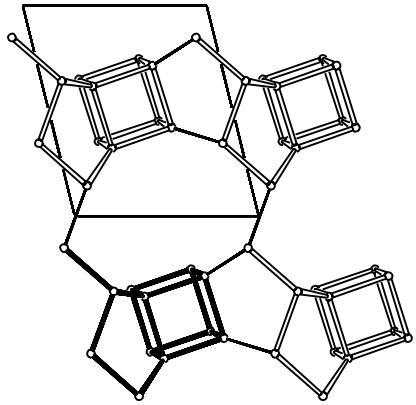
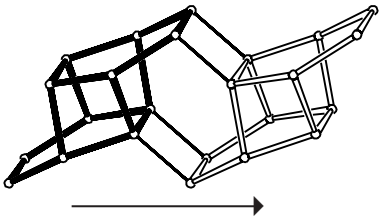


Figure 5 [Cont'd]. Summary of PerBUs containing (substituted) D4Rs (in bold). References are on final page. [Figure 5 is continued on next page]

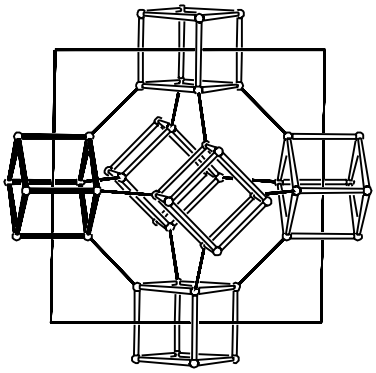
Figure 5 [Cont'd]



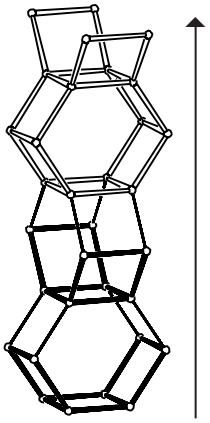
ITW



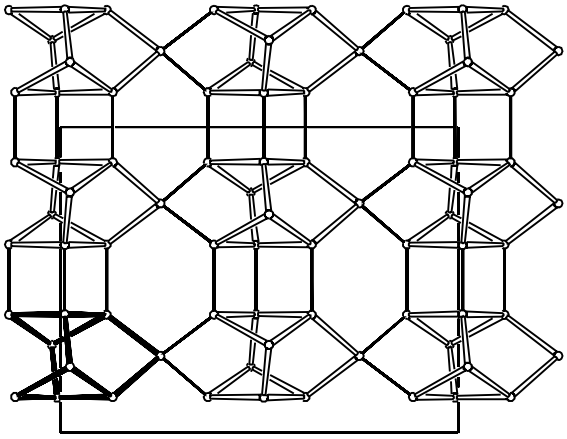
LAU[4]



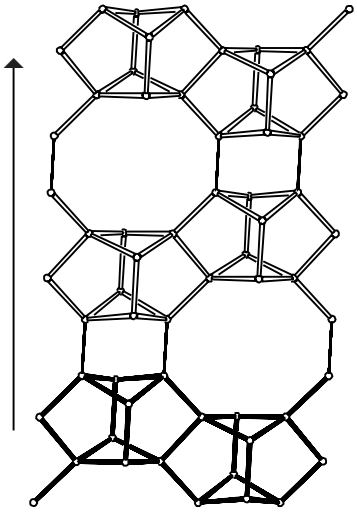
LTA[3,7]



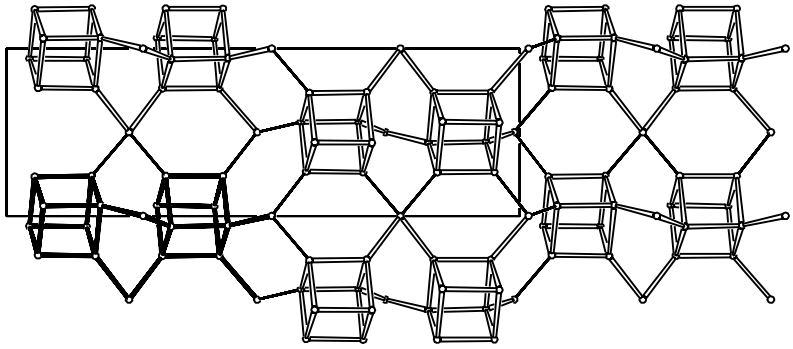
SAS[4]



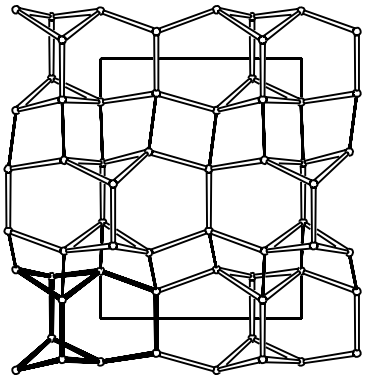
STI



TER



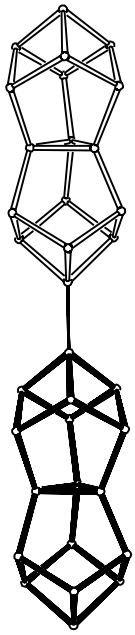
UOZ (compare with **ASV**)



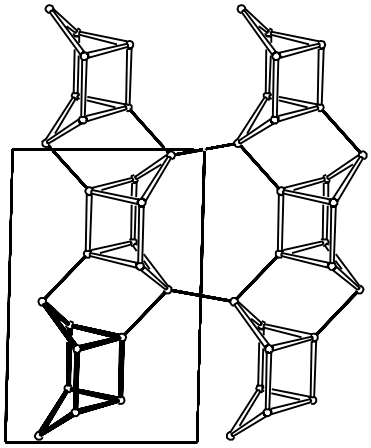
USI

Figure 5 [Cont'd]. Summary of PerBUs containing (substituted) D4Rs (in bold). References are on next page. [Figure 5 is continued on next page]

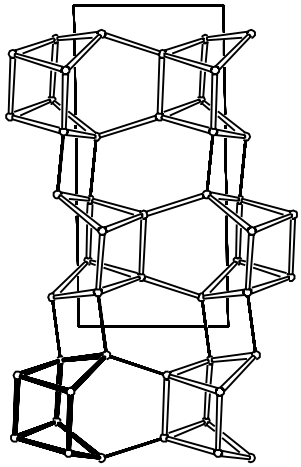
Figure 5 [Cont'd]



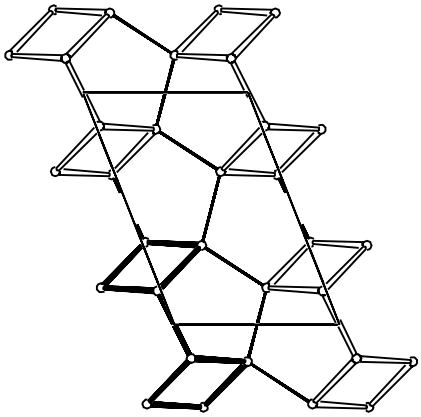
MEI
(compare with
AFS, **BPH** and **AFY**)



OWE



ZON
(compare with **AFR** and **SFO**)



YUG

Figure 5 [Cont'd]. Summary of PerBUs containing (substituted) D4Rs (in bold). References are on next page. [Figure 5 is continued on next page]

Figure 5 [Cont'd]

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[1] **AFI, APD, APC, DFT, GIS, MER** and **PHI** can also be constructed using (double) crankshaft chains (**CRSHFT**)

[2] **AFN** can be built using a not fully connected double 4-ring or, alternatively, using T8-units composed of three fused 4 rings.

[3] **AST**, **-CLO** and **LTA** can also be built using cages (**CAGES**).

[4] **BOG**, **CGS**, **ETR**, **LAU** and **SAS** can also be constructed using (substituted) double 6-rings (**D6R**s).

[5] In **-CLO** the PerBU is composed of two building units: **(1)** and **(2)**. **(1)** is obtained when all twelve 4-rings in an α-cavity (compare **KFI**, **LTA**, **LTN**, **PAU**, **RHO**, **TSC**, and **UFI**) are replaced by D4Rs. **(2)** equals a slice of **(1)** and consists of four D4Rs connected around a 4-fold axis. In each of the four D4Rs there are two terminal oxygen atoms where the framework is not fully connected.

[6] Chains, like the one shown, are connected in **DFO** parallel around a 6-fold axis to form a tubular PerBU.

[7] **LTA** can be built using the D4R as the PerBU. Each 4-ring in the D4Rs is one of the six 4-rings that form β-cages (or sodalite cages; compare **SOD**, **EMT**, **FAU** and **LTN**).

Figure 5 [Final page]. Summary of PerBUs containing (substituted) D4Rs (in bold).

Back to: **D4R** - **APPENDIX** - **TOP**

Figure 6: PerBUs containing (modified) 5-rings

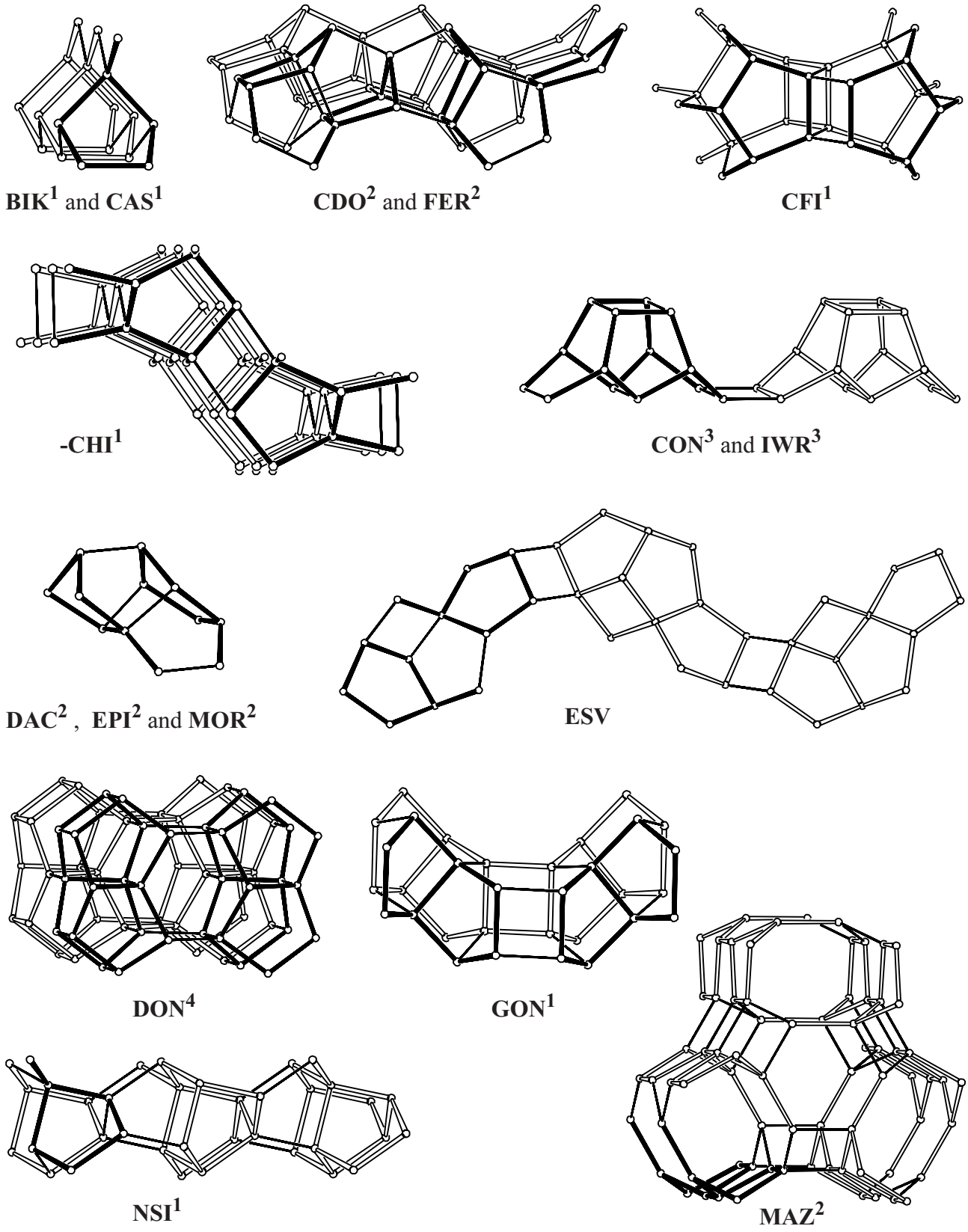


Figure 6. Summary of PerBUs built from (modified) 5-rings (in bold). Footnotes are on final page.
[Figure 6 is continued on next page]

Figure 6 [Continued]

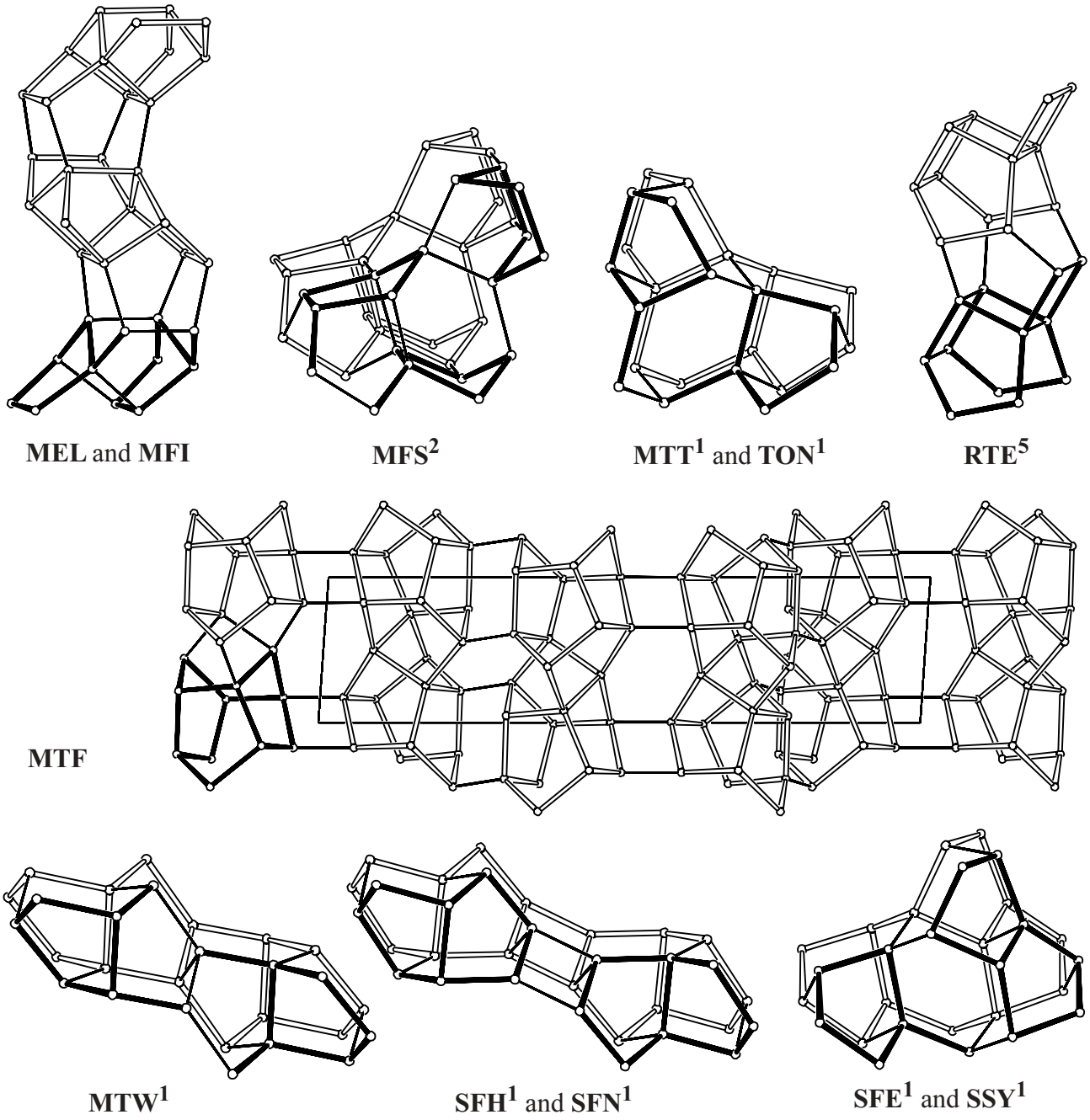
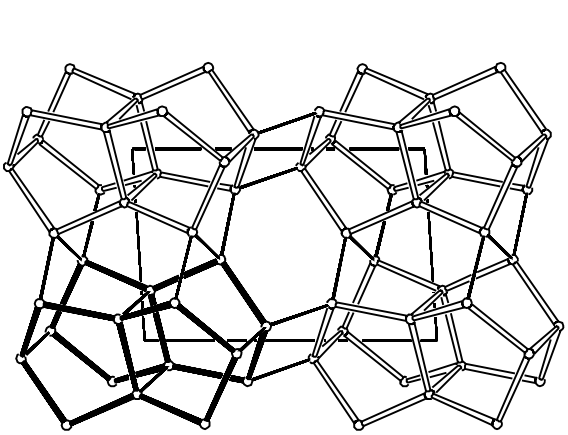
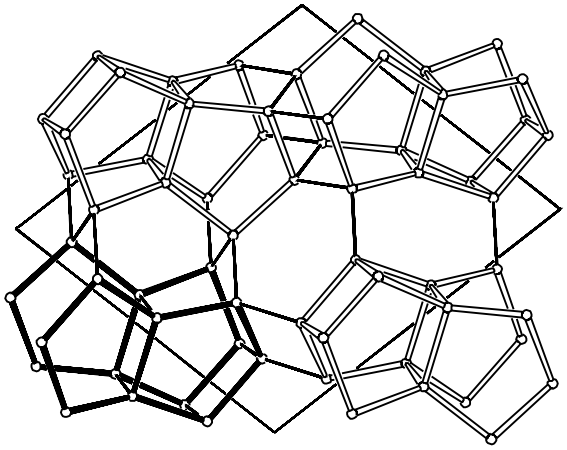


Figure 6 [Cont'd]. Summary of PerBUs built from (modified) 5-rings (in bold). Footnotes are on final page. [Figure 6 is continued on next page]

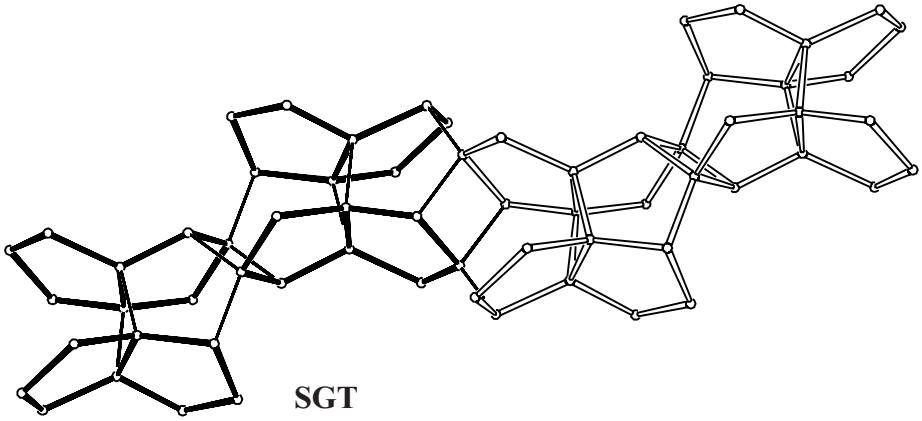
Figure 6 [Continued]



SFF and **STF**



STT



SGT

Figure 6 [Cont'd]. Summary of PerBUs built from (modified) 5-rings (in bold). Footnotes are on final page. [Figure 6 is continued on next page]

Figure 6 [Continued]

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[1] **BIK**, **CAS**, **CFI**, **-CHI**, **GON**, **MTT**, **MTW**, **NSI**, **SFE**, **SFH**, **SFN**, **SSY** and **TON** can also be built using zigzag chains (**ZZ**).
[2] **CDO**, **DAC**, **EPI**, **FER**, **MFS**, **MAZ** and **MOR** can also be built using (distorted) saw chains (**SAW**).
[3] **CON** and **IWR** are also described in the beta-like family (**BET**).
[4] **DON** can also be built using crankshaft chains (**CRSHFT**).
[5] **RTE** can also be built using (double) 6-rings (**D6R**).

Figure 6 [Final page]. Summary of PerBUs built from (modified) 5-rings (in bold).

Back to: **5RINGS - APPENDIX - TOP**

Figure 7: PerBUs containing double 6-rings (D6Rs)

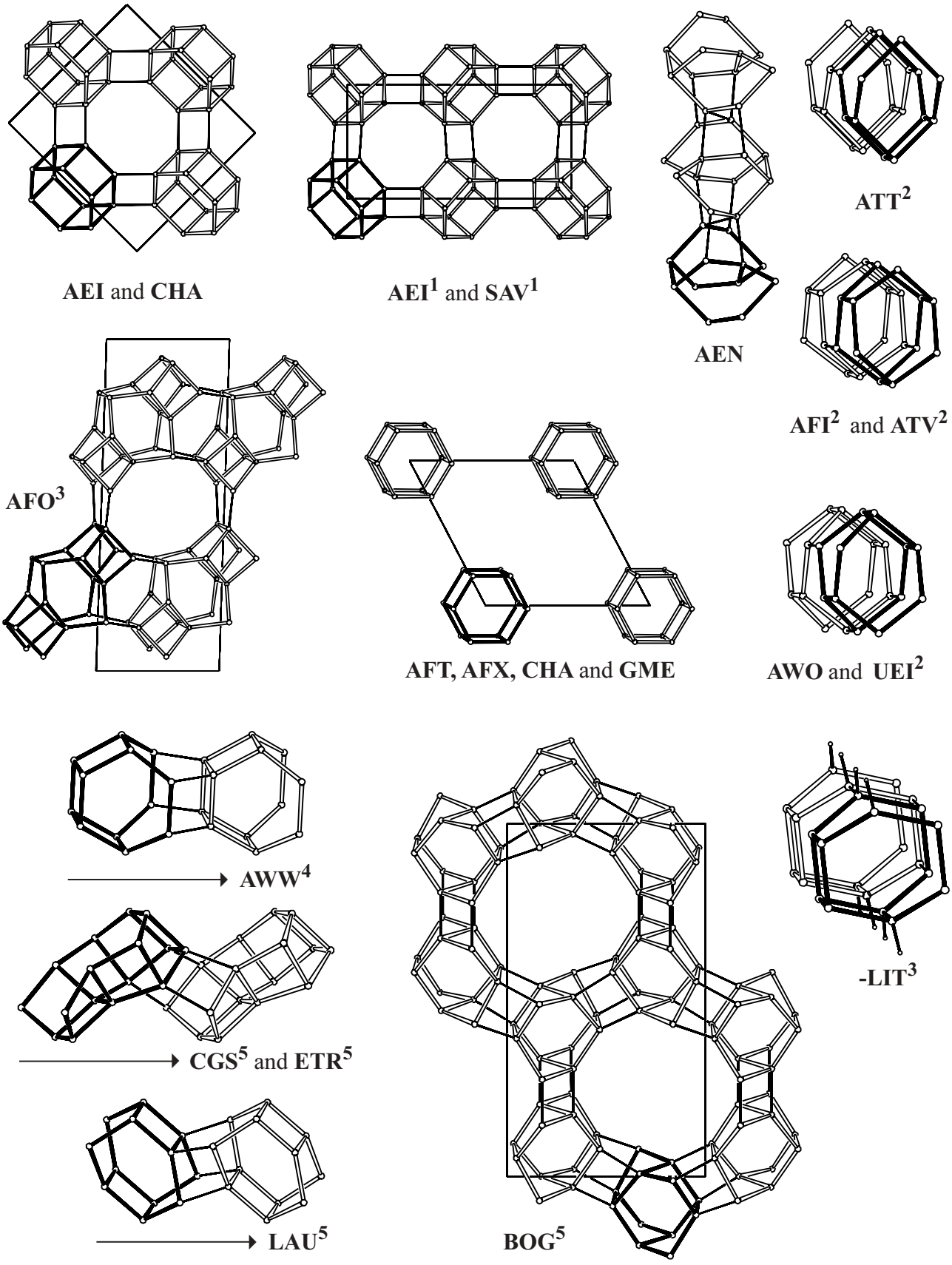

Figure 7. Summary of PerBUs built from (not fully connected) D6Rs (in bold). [Figure 7 is continued on next page]

Figure 7 [Cont'd]

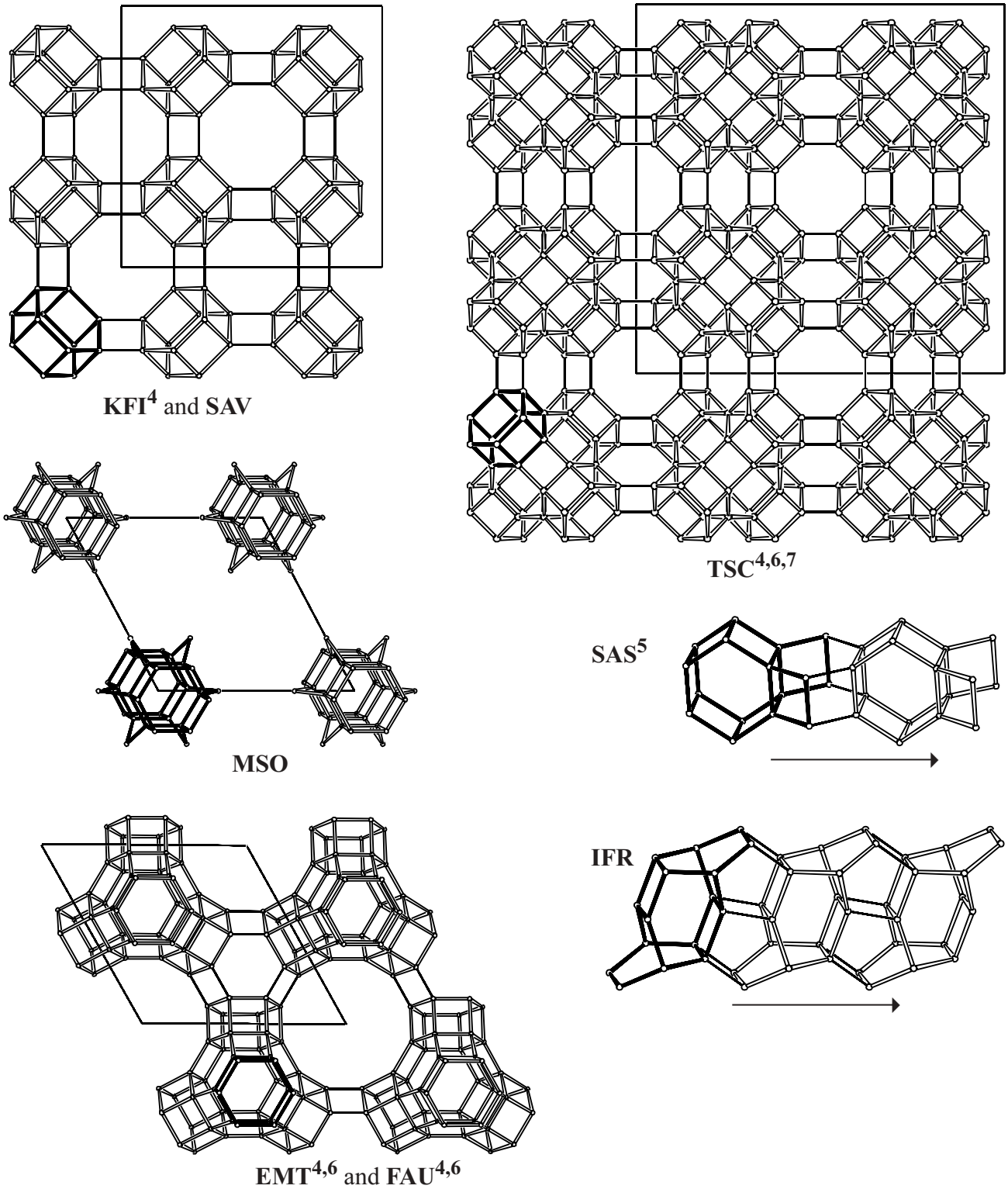

Figure 7 [Cont'd]. Summary of PerBUs built from (not fully connected) D6Rs (in bold). [Figure 7 is continued on next page]

Figure 7 [Cont'd]

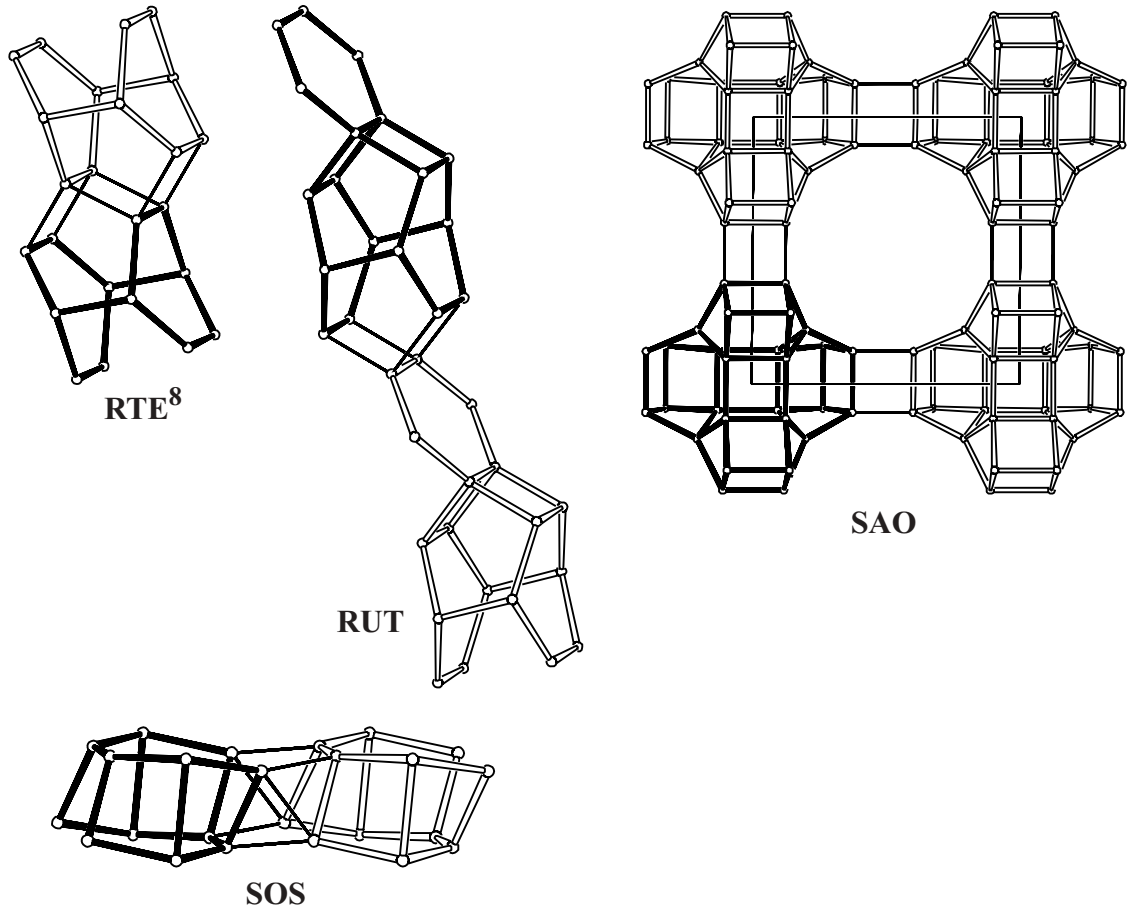

Figure 7 [Cont'd]. Summary of PerBUs built from (not fully connected) D6Rs (in bold). [Figure 7 is continued on next page]

Figure 7 [Cont'd]

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[1] A building scheme of **AEI** and **SAV** using this PerBU is given in the schemes of **AEI** and **SAV**.
[2] **ATT**, **ATV**, **AWO** and **UEI** can also be constructed from crankshaft chains (**CRSHFT**) or saw chains (**SAW**).
[3] **AFO** and **-LIT** can also be constructed from crankshaft chains (**CRSHFT**).
[4] **AWW**, **EMT**, **FAU**, **KFI** and **TSC** can also be built using cages (**CAGES**).
[5] **BOG**, **CGS**, **ETR**, **LAU** and **SAS** can also be constructed using (substituted) double 4-rings (**D4R**s).
[6] In **EMT**, **FAU** and **TSC** four D6Rs are tetrahedral coordinated around the center of a β-cage (or sodalite cage; compare **SOD** and **LTN**) formed by connecting the D6Rs. The cluster of four D6Rs exhibits 4-fold inversion symmetry
[7] In **TSC** clusters of four tetrahedral coordinated D6Rs are connected along the cube axes to form α-cages (compare **KFI**, **LTA**, **LTN**, **PAU**, **RHO** and **UFI**).
[8] **RTE** can also be built using (modified) 5-rings (**5RINGS**).

Figure 7 [Final page]. Summary of PerBUs built from (not fully connected) D6Rs (in bold).

Back to: **D6R** - **APPENDIX** - **TOP**

FIGURE 8. PerBU consisting of an hexagonal array of non-connected 6-rings

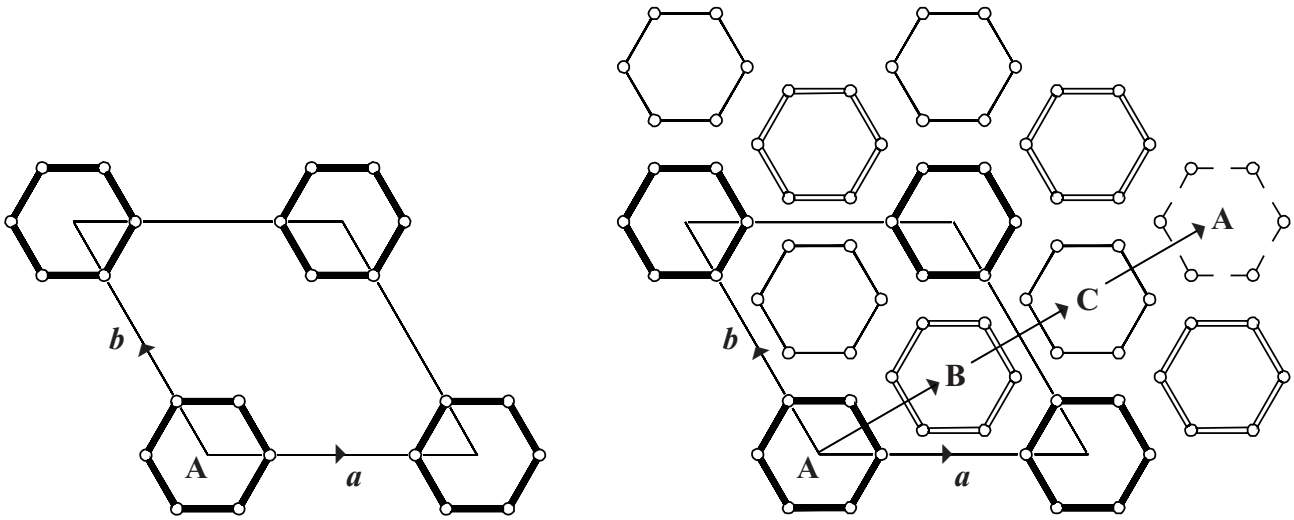


Figure 8. The two-dimensional Periodic Building Unit (PerBU) in the ABC-6-family consists of an hexagonal array of non-connected planar 6-rings (bold in Figure 1), which are related by pure translations along ***a*** and ***b***. The 6-rings are centered at (0,0) in the ***ab*** layer. This position is usually called the A position. Neighboring PerBUs are connected through tilted 4-rings along the hexagonal ***c*** axis. The distance between two neighboring PerBUs, measured along ***c*** is about 2.55 Å. The Figure shows the PerBU in the ABC-6-family (left) and illustrates the definition of the 6-ring positions in neighboring PerBUs with respect to each other (right).

Back to: **ABC** - **APPENDIX** - **TOP**

Figure 9. Chains and PerBUs in the Beta-like family

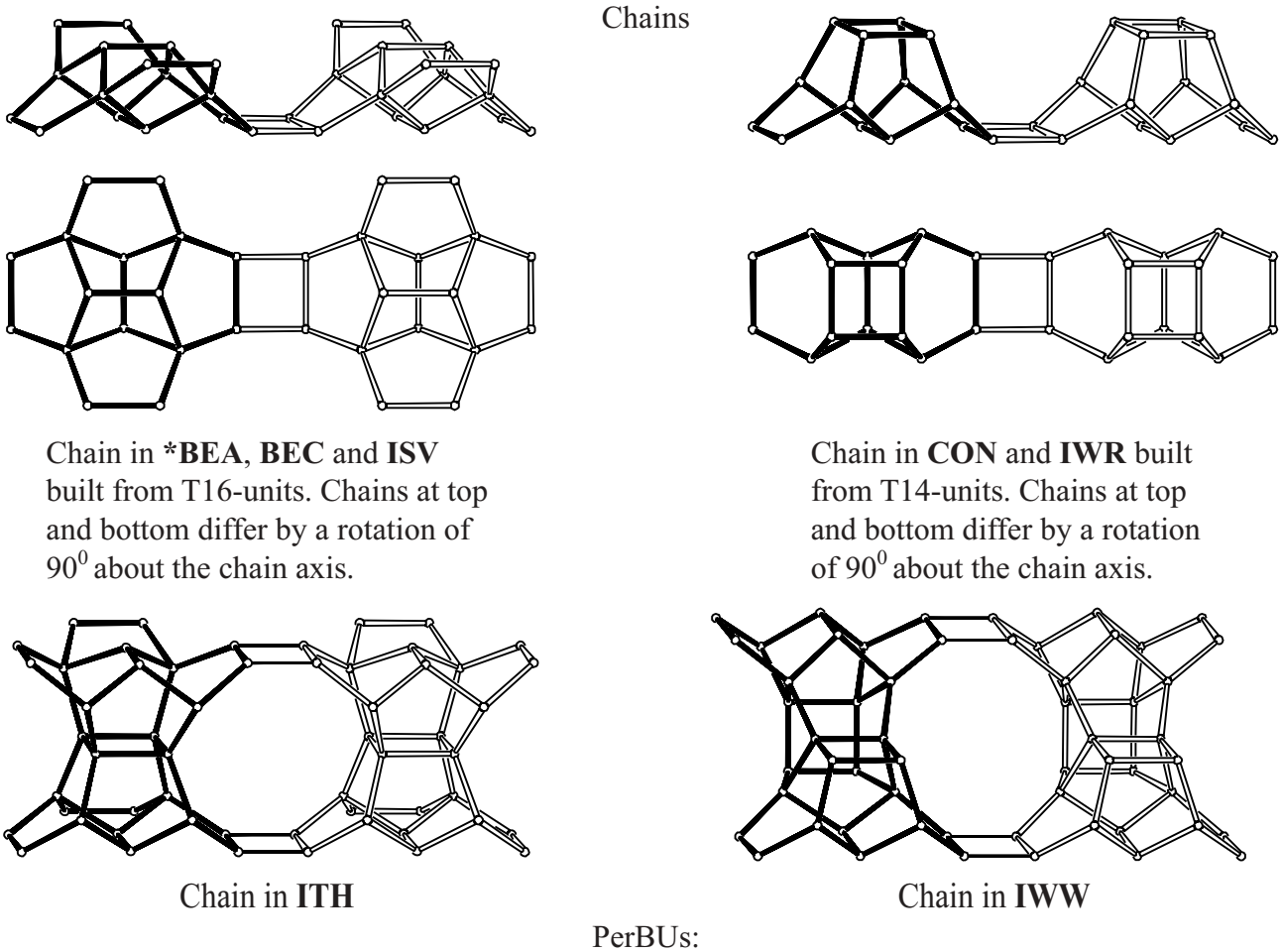
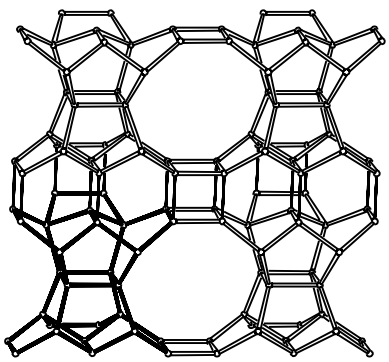
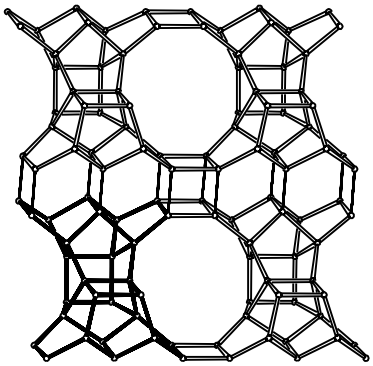


Figure 9. Summary of chains and PerBUs in beta-like framework types.
[Figure 9 is continued on next page]

Figure 9 [Cont'd]



ITH



IWW

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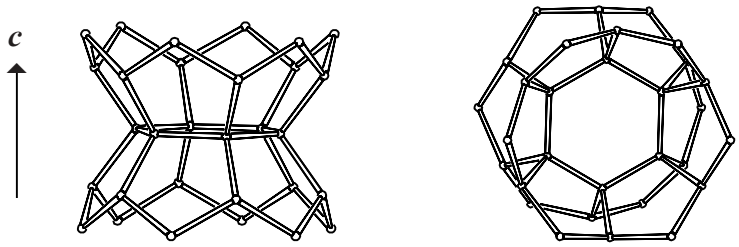
[1] **CON** and **IWR** can also be built using (modified) 5-rings (**5RINGS**).

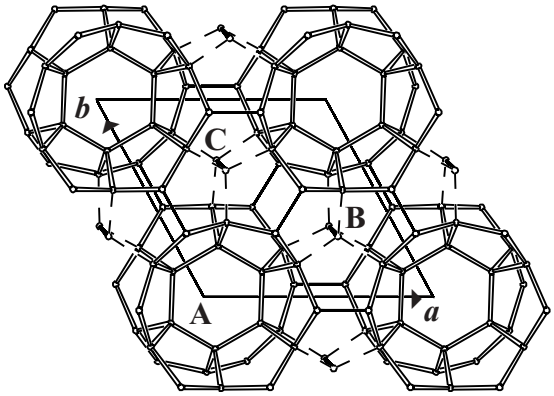
Figure 9 [Final page]. Summary of chains and PerBUs in beta-like framework types.

Back to: **BET** - **APPENDIX** - **TOP**

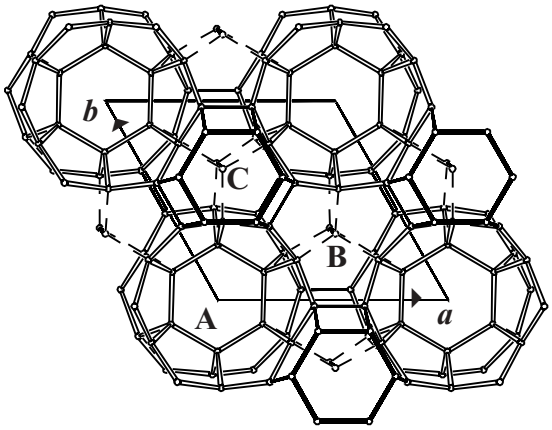
Figure 10. PerBUs in the Clathrasils[1]



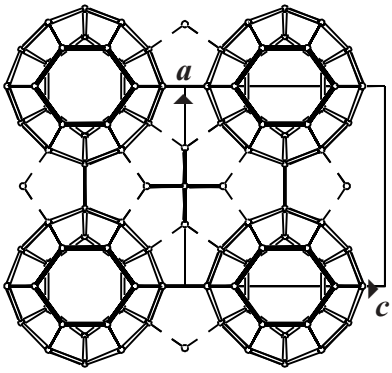
T30-unit viewed perpendicular to ***c*** (left)and along ***c*** (right)



DOH and MTN



DDR



MEP

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[1] The clathrasils can also be built using cages (**CAGES**)

Figure10. Summary of T30-unit and PerBUs in the clathrasils.

Back to: **CLAT** - **APPENDIX** - **TOP**

Figure 11. PerBUs built from cages

Figure 11. Summary of PerBUs built from cages.[**to follow]**

Back to: **CAGES** - **APPENDIX** - **TOP**

Figure 12. PerBUs in the miscellaneous group

Figure 12. Summary of PerBUs in the miscellaneous group. [**to follow**]

Back to: **MISCELLANEOUS** - **APPENDIX** - **TOP**

END OF APPENDIX

Back to: **APPENDIX** - **TOP**