

The Beta Family



1. The Periodic Building Unit (PBU) – 2. Type of Faulting – 3. The Layer Symmetry – 4. Connectivity Pattern –
5. Ordered End-Members – 6. Disordered Materials synthesized so far – 7. Supplementary Information
8. References

1. The Periodic Building Unit (PBU) equals the layer shown in Fig.1 (a - c):

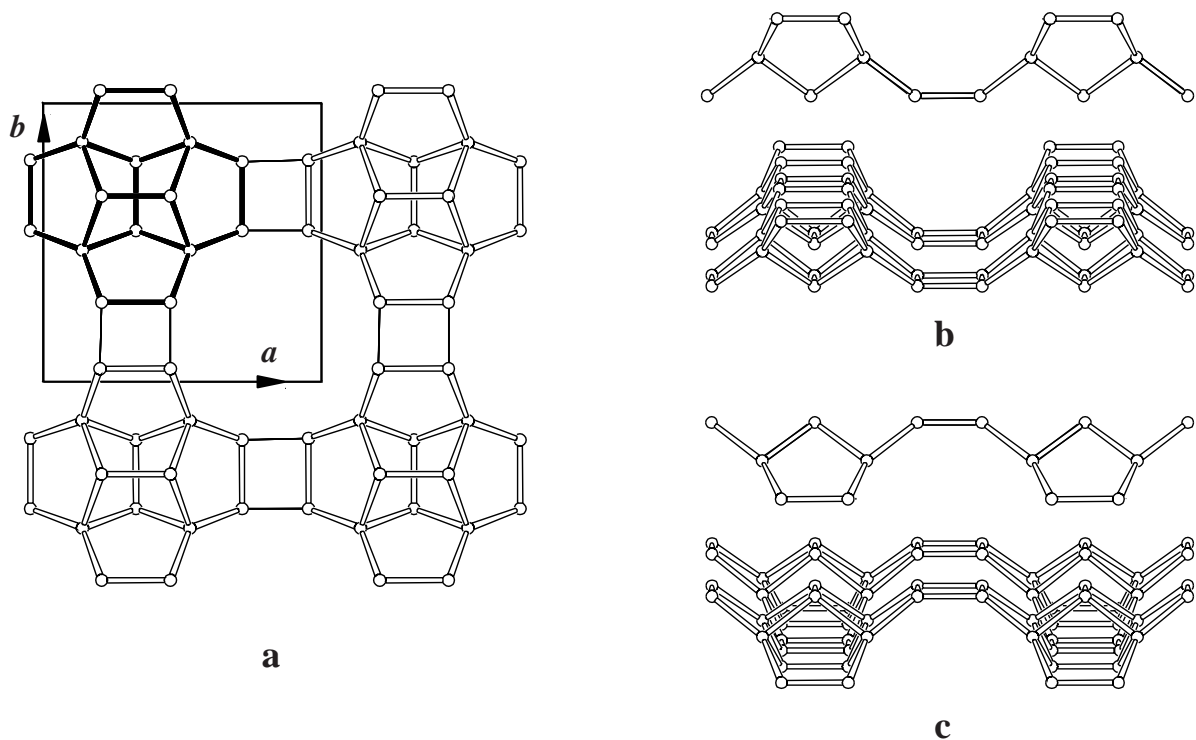


Figure 1: The PBU of the beta family shown parallel to c (a) and perpendicular to c (b and c)

The PBU of the beta family of structure types, the tetragonal beta layer (a), is composed of T16 units (in bold) related by pure translations along a and b . Views along $[001]$ (a), $[010]$ (b) and $[100]$ (c) are shown. The layers depicted in (b) and (c) (In parallel projection (top) and in perspective view (bottom)) are identical and related by a 90° rotation about the plane normal or by a mirror operation perpendicular to the plane normal.



2. Type of faulting: 1-dimensional stacking disorder of the PBU's along $[001]$.



3. The planar space group symmetry of the PBU is $P(\bar{4})m2$.



4. Connectivity pattern of the PBU:

Neighbouring PBU's, related by a mirror operation, can be connected along [001] via O-bridges in three different ways:

a) the lateral shift of the top layer along a or b is zero, (this connection mode has not been observed yet)

b) the lateral shift of the top layer is $\frac{1}{3} a$ or $\frac{1}{3} b$,

c) the lateral shift of the top layer is $-\frac{1}{3} a$ or $-\frac{1}{3} b$,

denoted as a): (0,0); b): $(+\frac{1}{3},0)$ or $(0,+\frac{1}{3})$; c): $(-\frac{1}{3},0)$ or $(0,-\frac{1}{3})$.

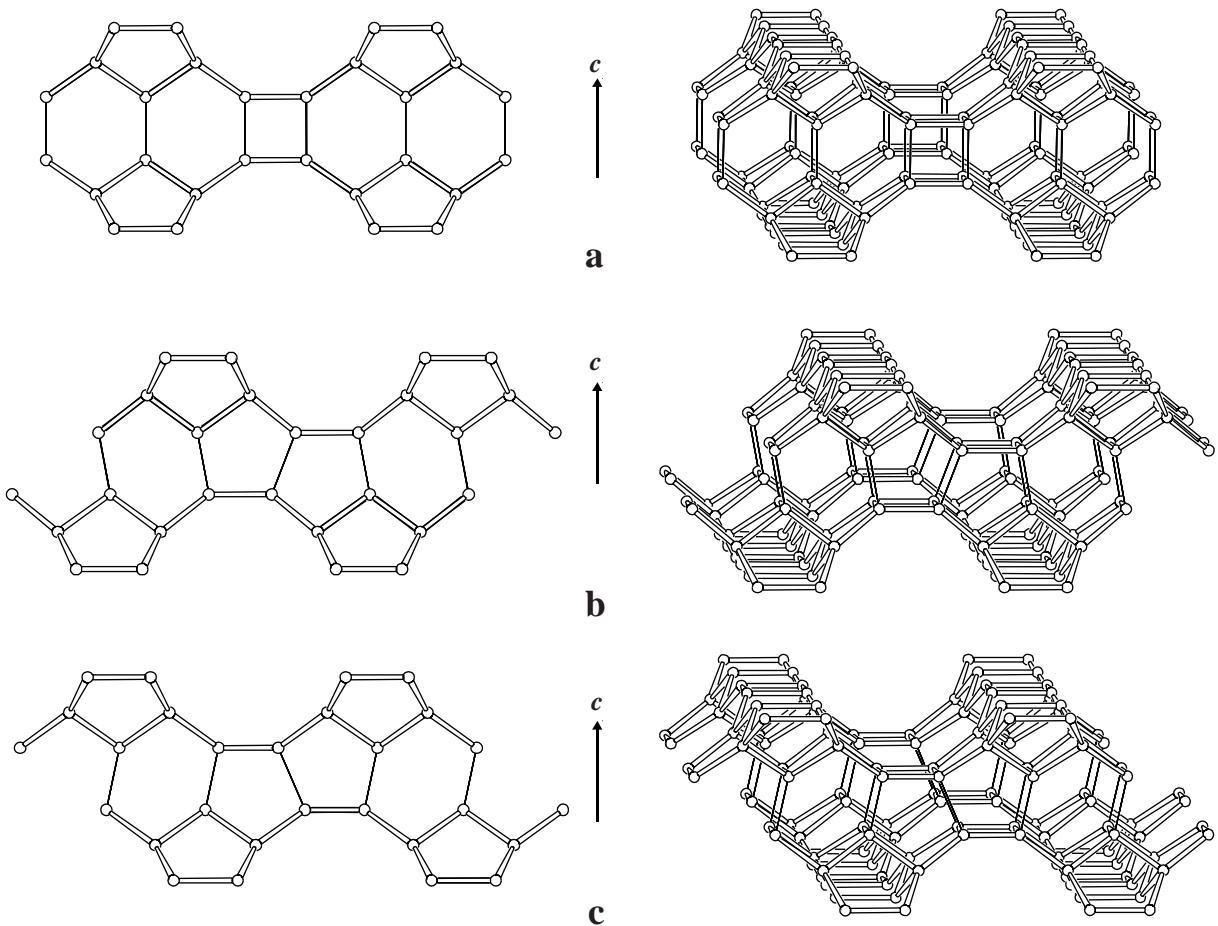


Figure 2: Connectivity of neighboring PBU's via 6MR-6MR-4MR (a) and 6MR-5MR-5MR (b and c), respectively

Once the distribution of the lateral shifts between the layers stacked along [001] is known, the 3-dimensional structure is defined.



5. The simplest ordered end-members in the beta family are given below. None of them has been observed yet as pure single crystal material.

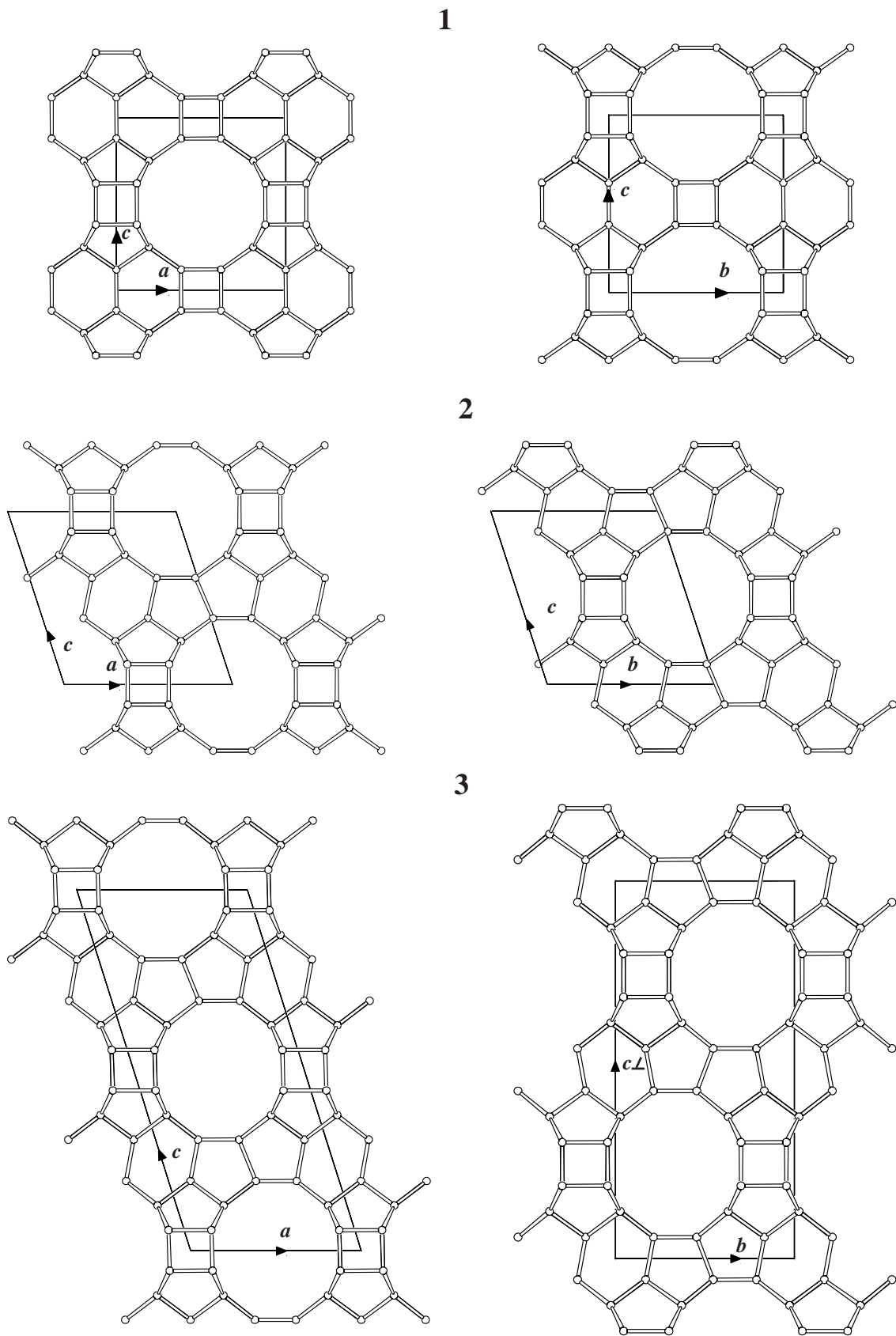


Figure 3: Projections of the structures of the simplest ordered end-members (cf. following table)

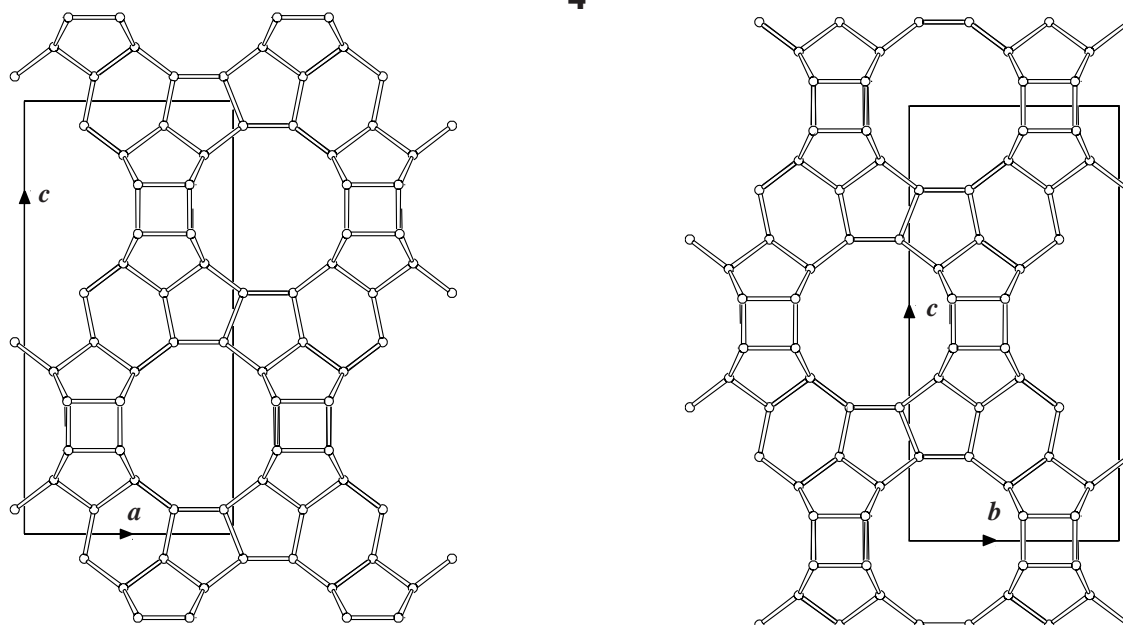


Figure 3cont.: Projections of the structures of the simplest ordered end-members (cf. following table)

Table 1: Stacking sequences of PBU for the simplest ordered end-members in the beta family. The end-member number refers to the structure plots 1-4 on the previous and this pages.

<i>End-Member</i>	<i>Lateral shifts between subsequent PBU's along [001]; shifts are in fractions of (a, and b)</i>					<i>Space group</i>
1	(0,0);	(0,0);	(0,0);.....			$P4_2/mmc$
2	$(0, -1/3)$;	$(-1/3, 0)$;	$(0, -1/3)$;		$P\bar{1} @*$
3	$(0, -1/3)$;	$(-1/3, 0)$;	$(0, +1/3)$;	$(-1/3, 0)$;	$(0, -1/3)$;	$P2/c @$
4	$(-1/3, 0)$;	$(0, -1/3)$;	$(+1/3, 0)$;	$(0, +1/3)$;	$(-1/3, 0)$;	$P4_1 22 **$
5	$(+1/3, 0)$;	$(0, -1/3)$;	$(-1/3, 0)$;	$(0, +1/3)$;	$(+1/3, 0)$;	$P4_3 22 \$$

@ Space group is centrosymmetric and the same structure is obtained by reversing the signs of all lateral shifts.

* For comparison reasons the maximum topological symmetry of end-member number 2 has been transformed from $C2/c$ to $P\bar{1}$.

** This is the end-member with structure type code *BEA.

\$ In $P4_3 22$ the coordinates in $P4_1 22$ are transformed to $x y \bar{z}$; end-member numbers 4 and 5 are enantiomorphs.



6. Disordered materials synthesized and observed so far:

Beta (1,2,3), Borosilicate *BEA (4,5), Gallosilicate *BEA (5), Tschernichite (6)



7. Supplementary material

Simulation of the stacking disorder in the beta family: BEA-‘Polymorph B’

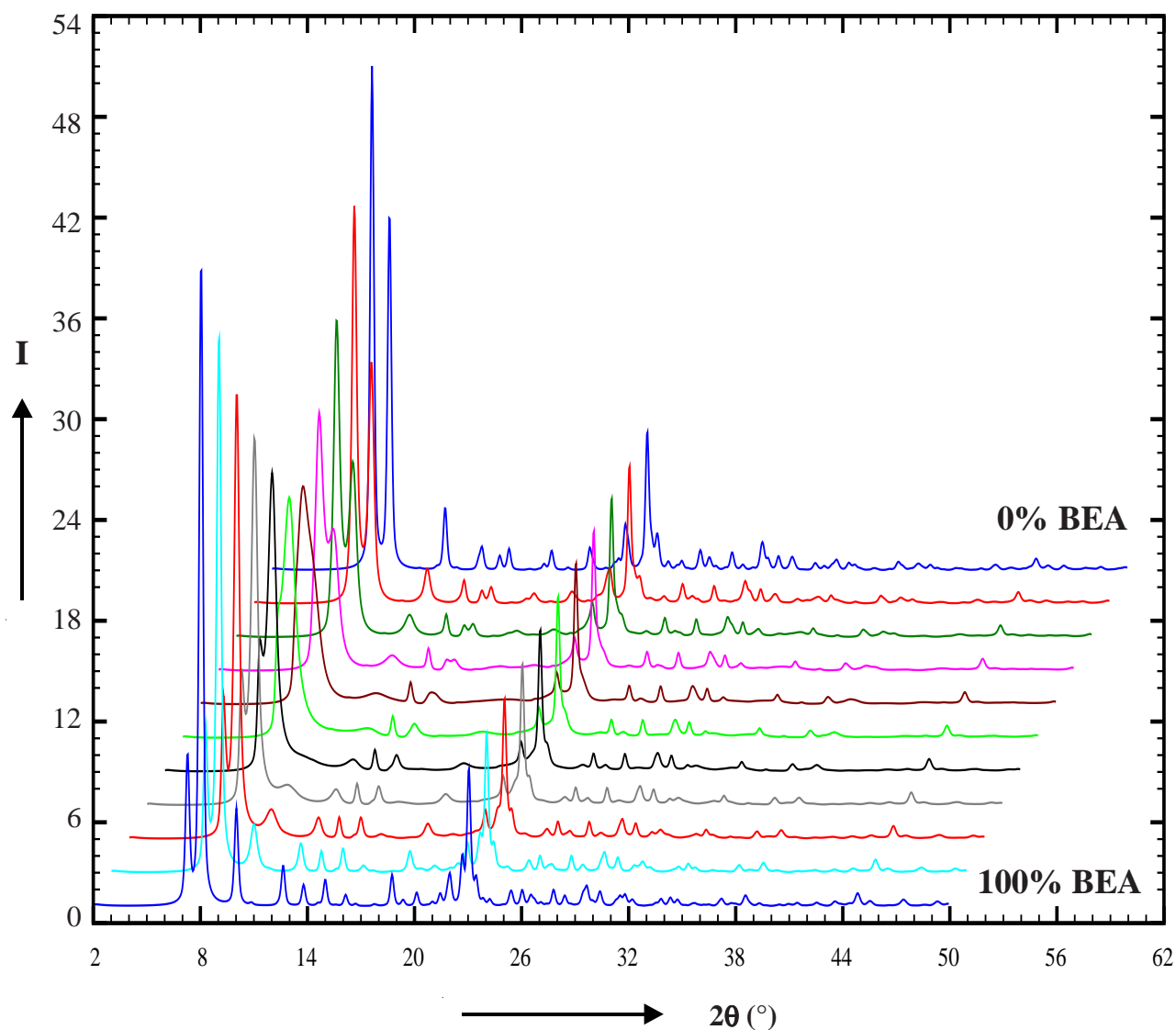


Figure 4: Intensity (**I**, a.u.) of simulated powder patterns versus diffraction angle (**2θ**) of the BEA-‘Polymorph B’ series in steps of 10% intergrowth. The stacking sequences number **2** and **4** (cf. Table 1) are disordered. The 0% BEA pattern corresponds to the 100% ‘Polymorph B’ pattern.



8. References

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- (3) J. M. Newsam, M. M. J. Treacy, W. T. Koetsier and C. B. de Gruyter, *Proc. R. Soc. Lond. A* **420**, 375 (1988).
- (4) J. B. Higgins, R. B. LaPierre, J. L. Schlenker, A. C. Rohrman, J. D. Wood, G. T. Kerr and W. J. Rohrbaugh, *Zeolites*, **8**, 446 (1988).
- (5) M. Marler, R. Boehme and H. Gies, *Proc. 9th IZC, Montreal, Butterworth-Heinemann* (1993) p. 425.
- (6) K. S. N. Reddy, M. J. Eapen, P. N. Joshi, S. P. Mirajkar and V. P. Shiralkar, *J. Incl. Phenom. Mol. Recogn. Chem.* **20**, 197 (1994).
- (7) R. C. Boggs, D. G. Howard, J. V. Smith and G. L. Klein, *Am. Mineral.* **78**, 822 (1993).

