The Beta Family

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

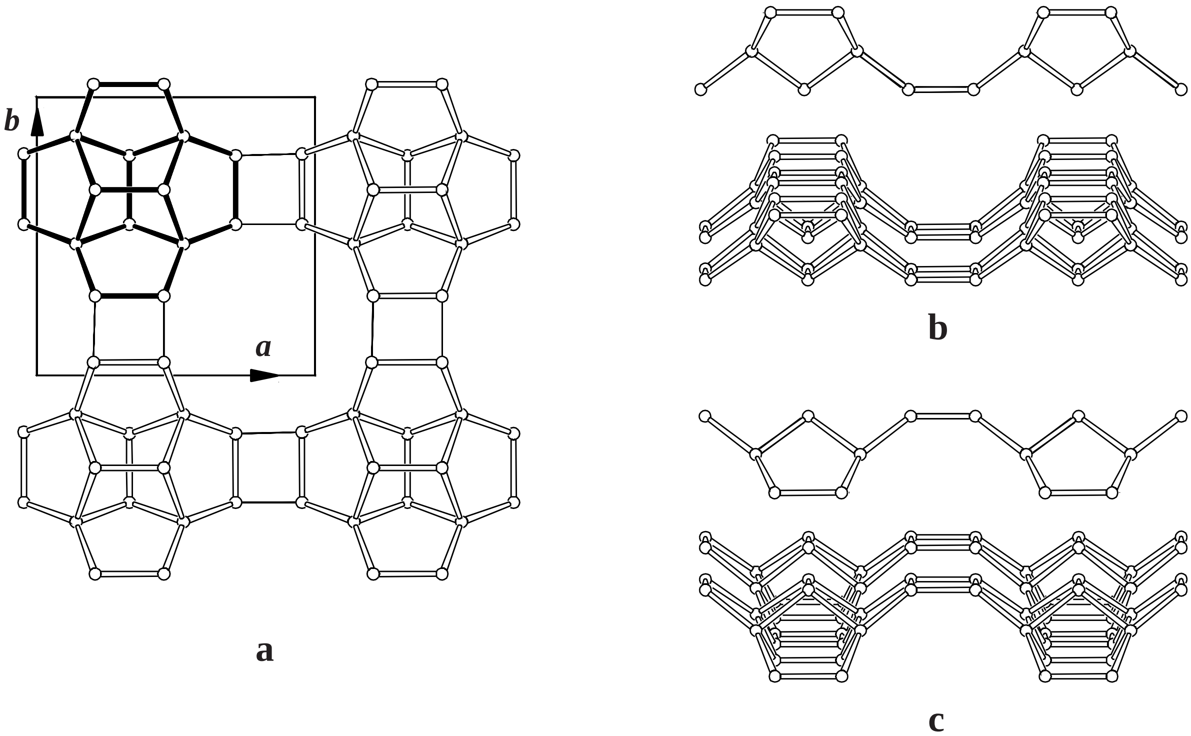

Figure 1: The PBU of the beta family shown parallel to ***c*** (a) and perpendicular to ***c*** (b and c)

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 $^{1}/_{3}$ ***a*** or $^{1}/_{3}$ ***b***,

c) the lateral shift of the top layer is **-** $^{1}/_{3}$ ***a*** or **-** $^{1}/_{3}$ ***b***,

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

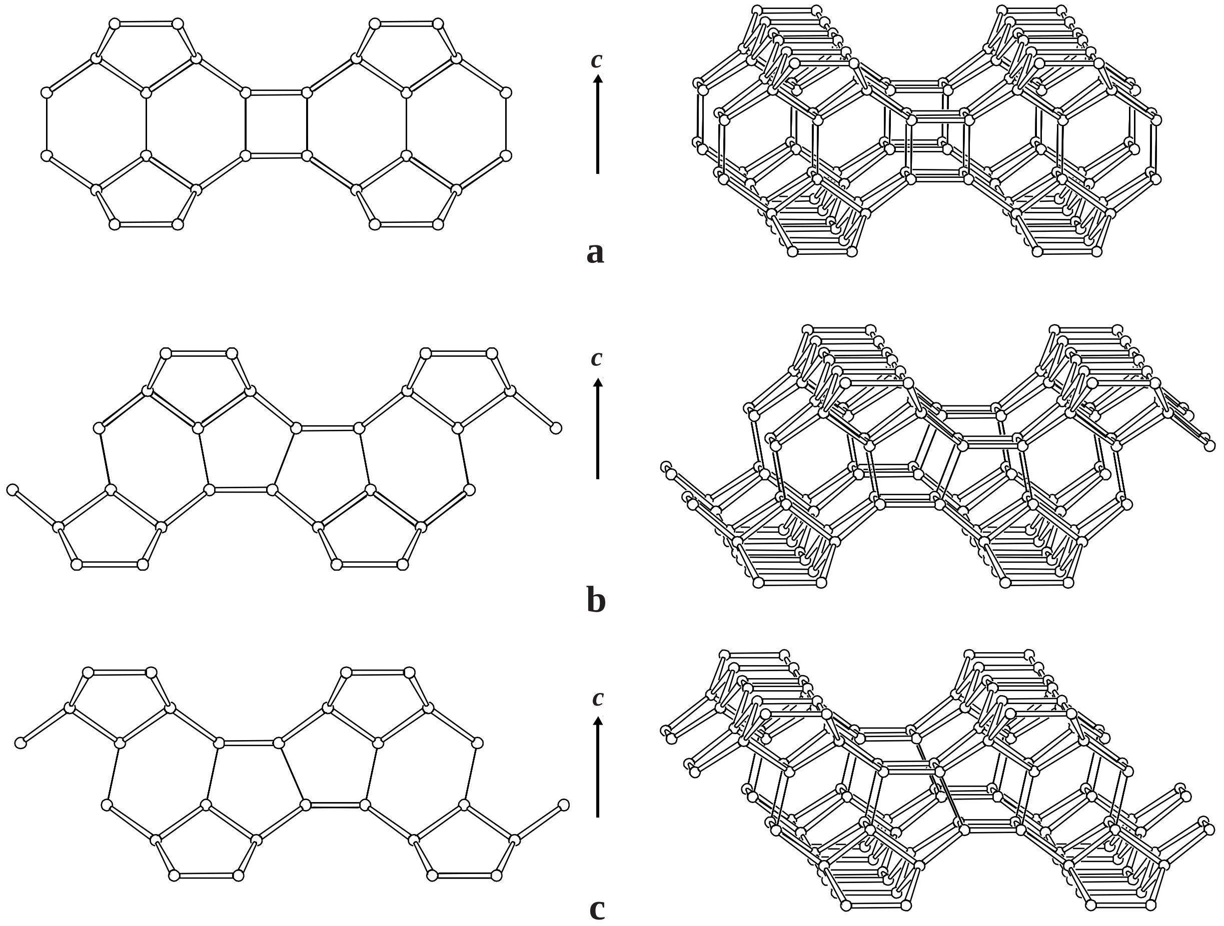

Figure 2: Connectivity of neighboring PBU's via 6MR-6MR-4MR (a) and 6MR-5MR-5MR (b and c), respectively

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.

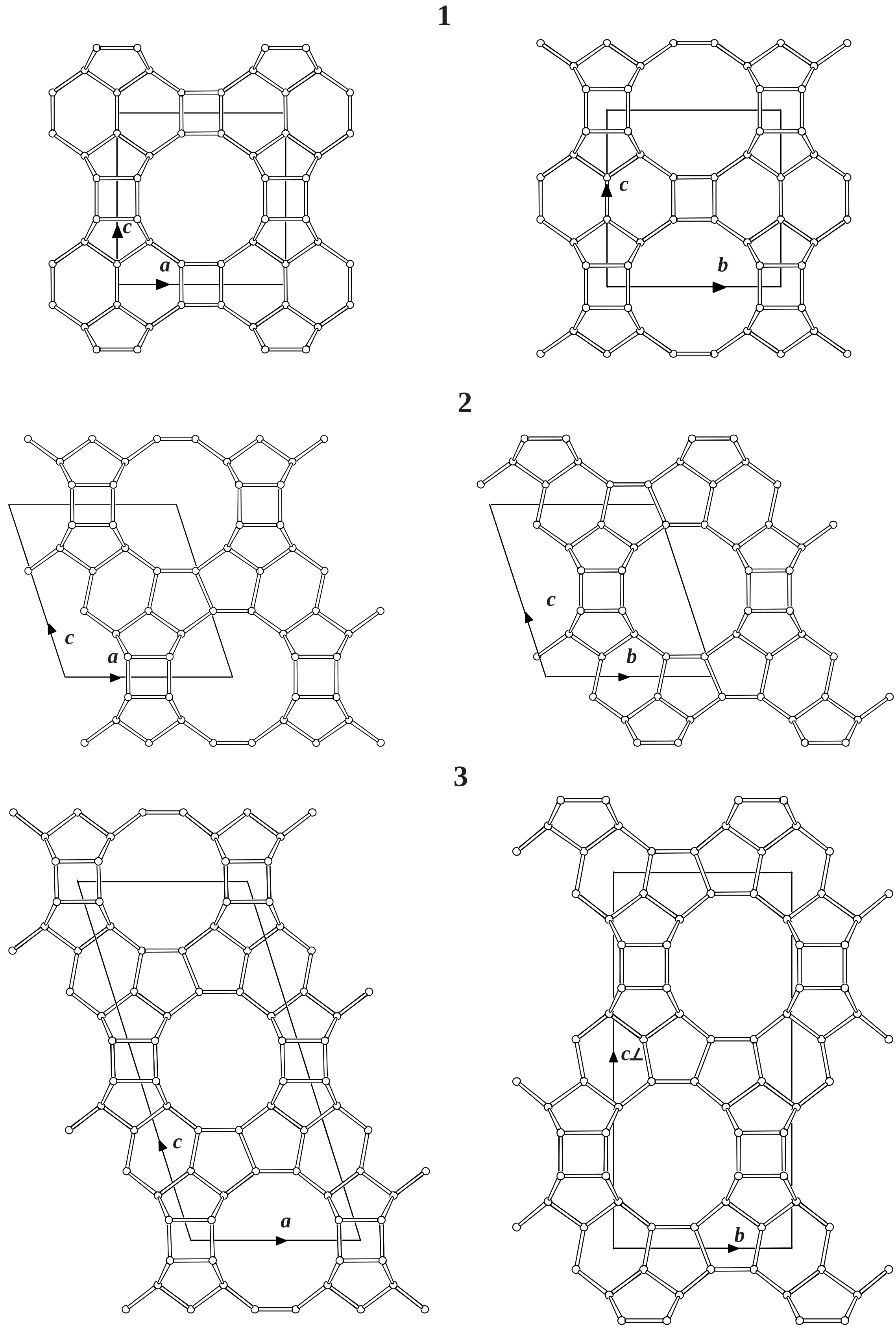

Figure 3: Projections of the structures of the simplest ordered end-members (cf. following table)

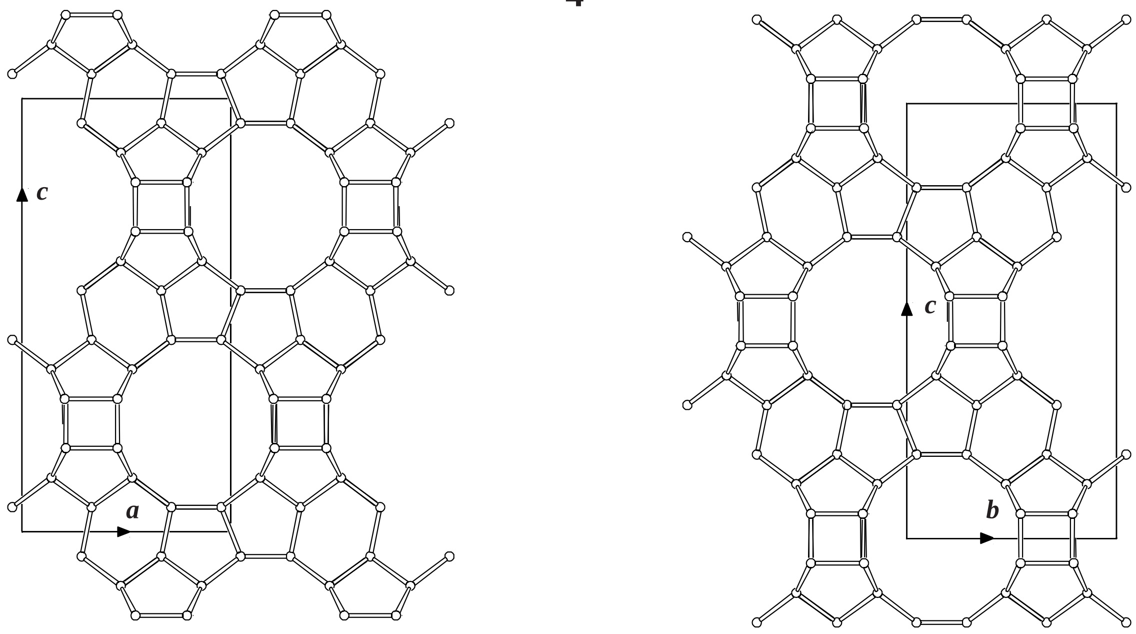

Figure 3cont.: Projections of the structures of the simplest ordered end-members (cf. following table)

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.

End-Member	***Lateral shifts between subsequent PBU's along [001]; shifts are in fractions of (a, and b)***					***Space group***
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	$(-{}^{1}/_{3},0)$;	$(0,-{}^{1}/_{3})$;	$(+{}^{1}/_{3},0)$;	$(0,+{}^{1}/_{3})$;	$(-{}^{1}/_{3},0)$;.....	$P4_122$ **
5	$(+{}^{1}/_{3},0)$;	$(0,-{}^{1}/_{3})$;	$(-{}^{1}/_{3},0)$;	$(0,+{}^{1}/_{3})$;	$(+{}^{1}/_{3},0)$;.....	$P4_322$ $

@ 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 $P4_322$ the coordinates in $P4_122$ 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‘

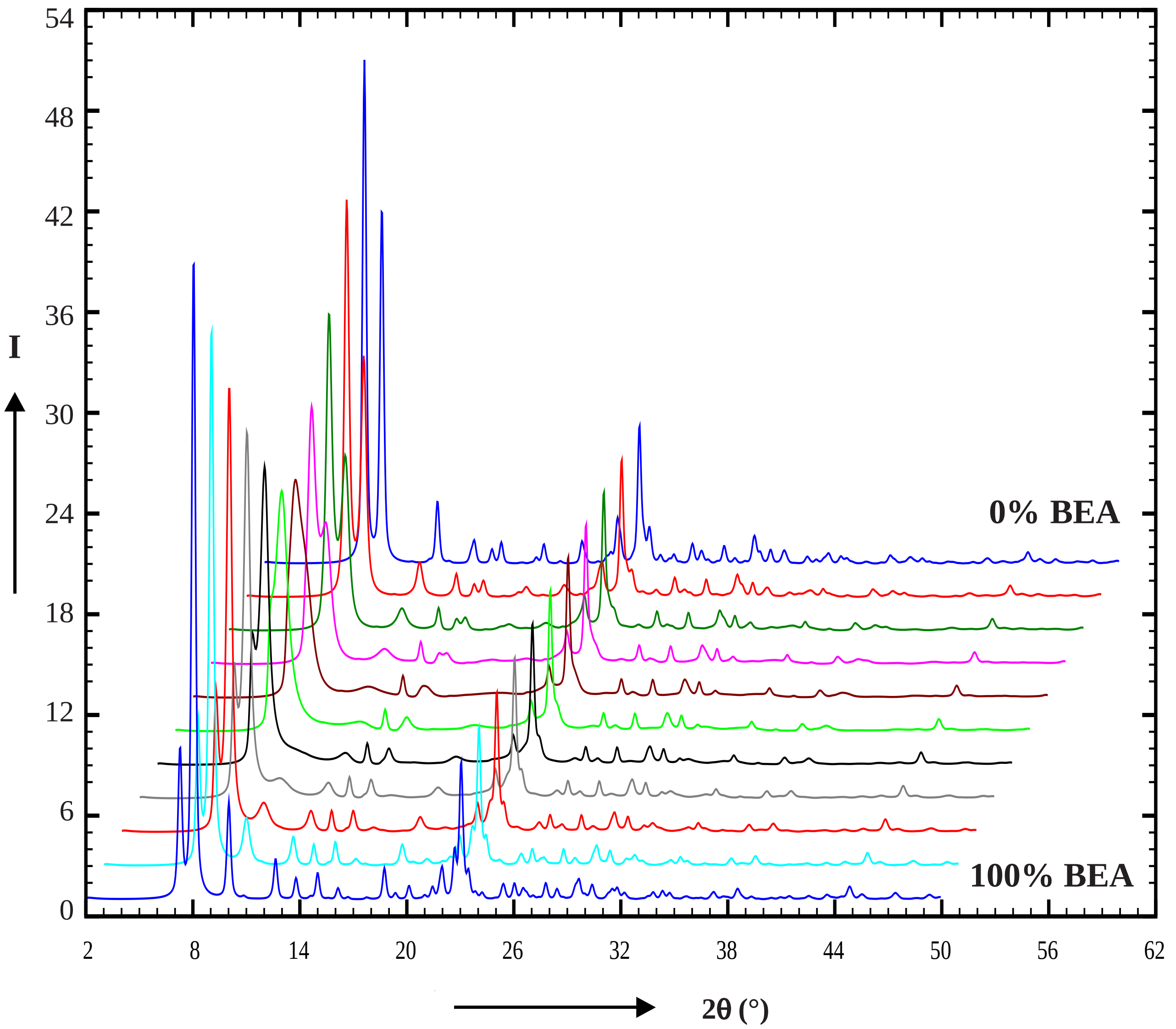

Figure 4: Intensity (**I,** a.u.) of simulated powder patterns versus diffraction angle (**2θ**) of the BEA-‘Polymorph B‘ series in steps of 10% intergrowth. The stacking sequences number **2** and **4** (cf. Table 1) are disordered. The 0% BEA pattern corresponds to the 100% ‘Polymorph B‘ pattern.

8. References

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(7) R. C. Boggs, D. G. Howard, J. V. Smith and G. L. Klein, Am. Mineral. **78**, 822 (1993).