

The AFS/BPH Family

1. The periodic Building Unit (PerBU) - 2. Type of Faulting - 3. The Layer Symmetry
4. Connectivity Pattern - 5. Ordered End-Members - 6. Disordered Materials synthesized to date
7. Supplementary Information - 8. References

1. The Periodic Building Unit (PerBU) is the hexagonal layer shown in Figure 1. This layer is built from T14-units consisting of two connected ‘capped’ T6-rings shown in Figure 2.

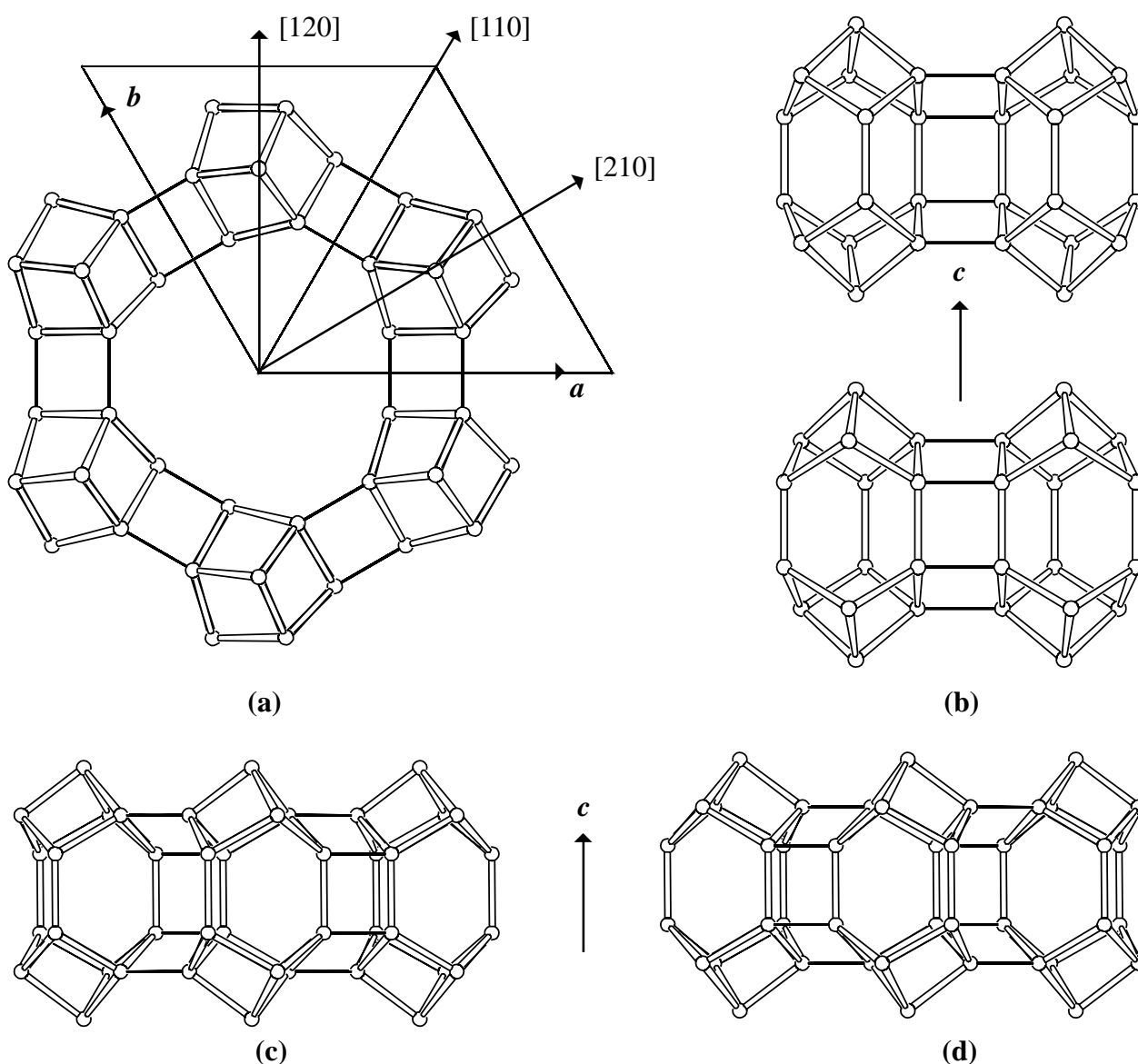


Figure 1. (a): The Periodic Building Unit of the AFS/BPH family seen along c consisting of linked T14-units; (b): Linkage between the T14 units within the layer as seen along $[110]$ (top) and along $[100]$ (bottom); (c): PerBU as seen along $[120]$; (d): PerBU as seen along $[210]$

The linkage within the layer is illustrated in Figure 1b. The PerBU's depicted in Figure 1c and 1d are identical and related by a 60° rotation about the hexagonal plane normal c .

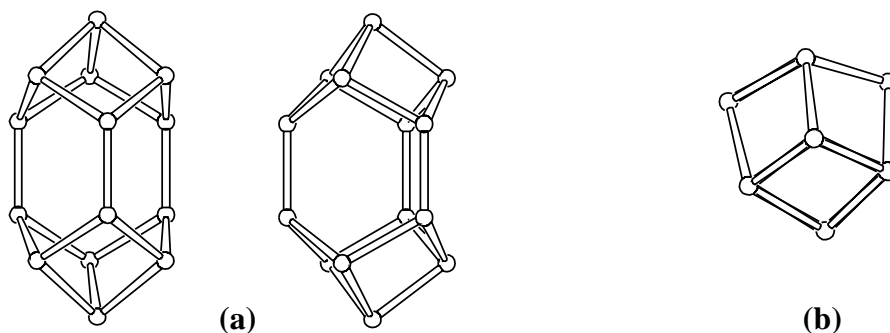


Figure 2. (a): T14-unit seen along [110] (left) and along [120] (right); (b): T14-unit seen down c ▲

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

3. The plane space group of the PerBU is $P(3)1m$.

4. Connectivity pattern of the PerBU: ▲

Neighbouring PerBU's can be connected via O-bridges along [001] in two different ways:

(a): the lateral shift of the top layer along a and b is zero before connecting it to the bottom layer. The resulting connectivity shows mirror symmetry (m ;|) between successive layers.

(b): the top layer is rotated over 60° about [001] before connecting it to the bottom layer. The connectivity now exhibits inversion symmetry (i ; o) between successive layers.

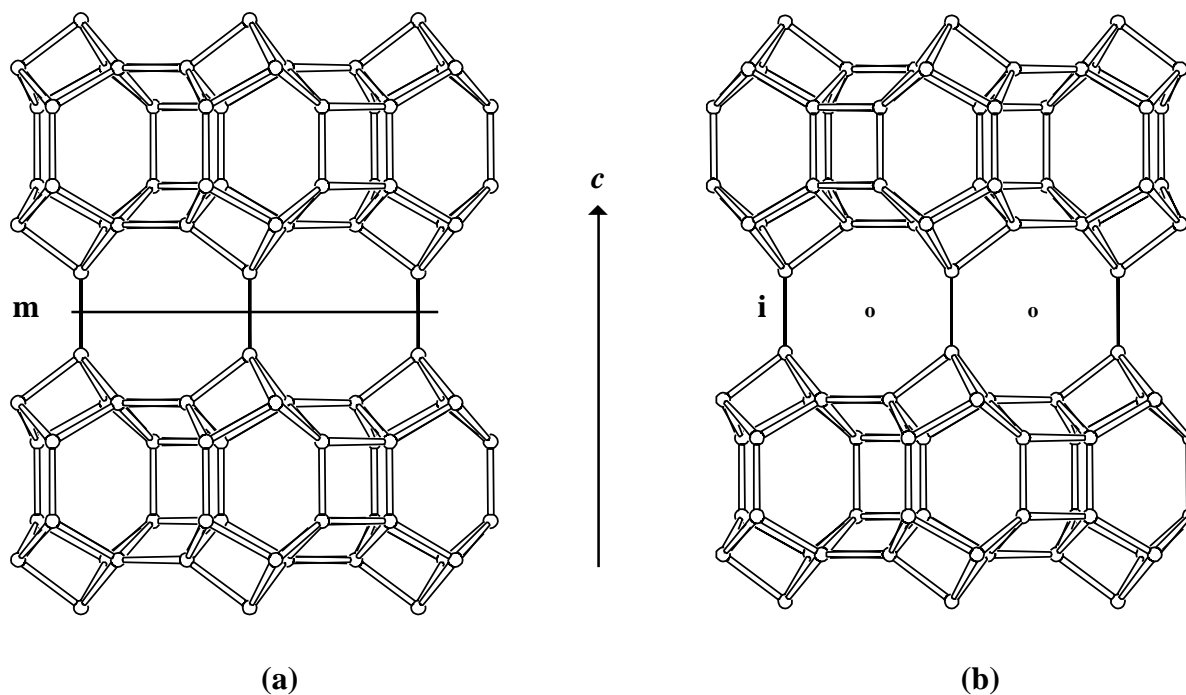


Figure 3: Parallel projection along [120] of the connection modes (a) and (b) in the AFS/BPH family of framework types ▲

5. The simplest ordered end-members in the AFS/BPH family are shown in Fig. 4:

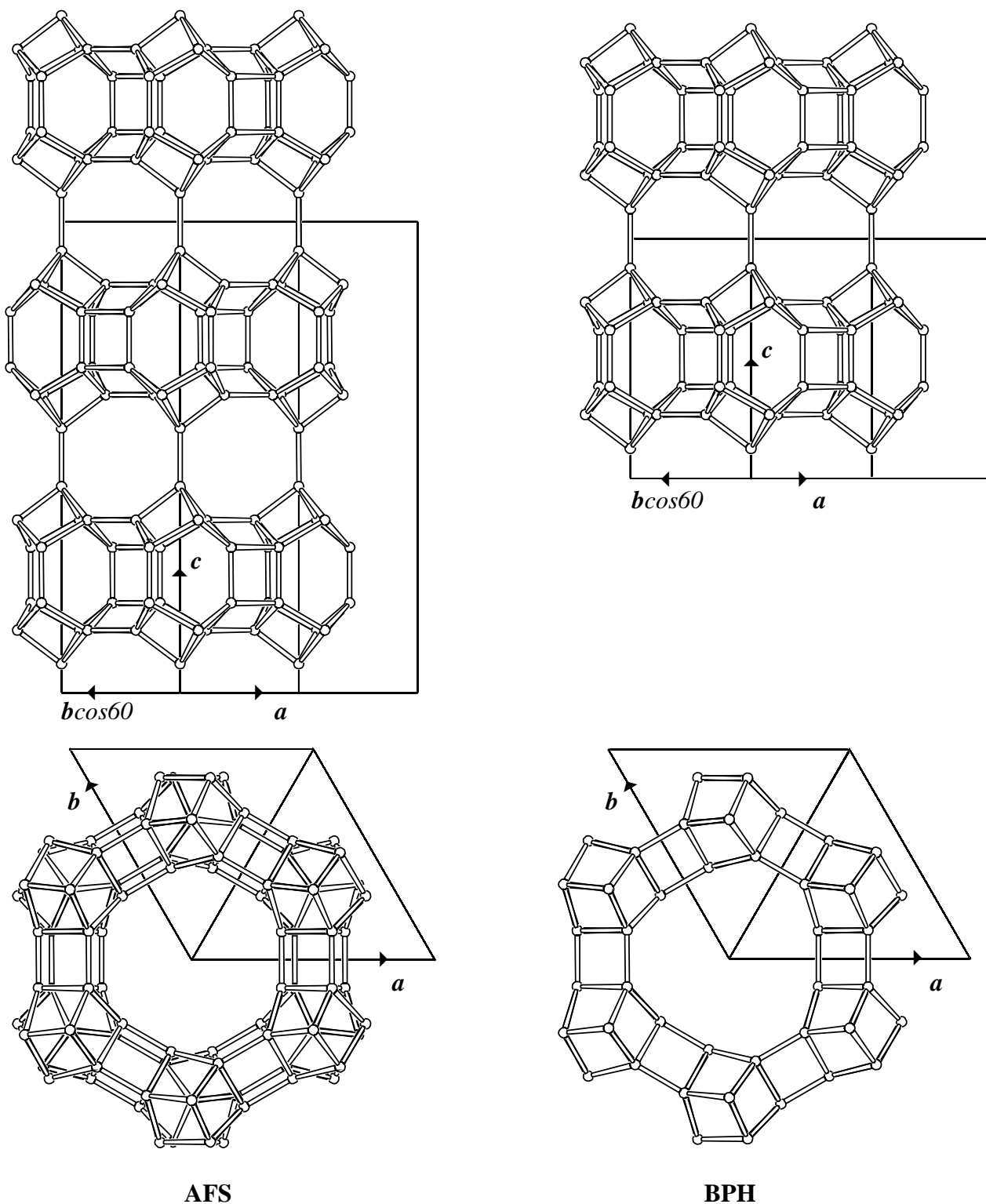


Figure 4: Parallel projections of the cell content along [120] (top) and along [001] (bottom) of the two simplest ordered end-members in the AFS/BPH family: AFS (left) and BPH (right)

Pure AFS (1) and BPH (2,3) are obtained when neighbouring PerBU's along [001] are exclusively related by a 60° rotation about c and by a pure translation along c , respectively. ▲

6. Disordered materials synthesized and characterized to date:

to be added

7. Supplementary material

to be added

8. References

- (1) J.M. Bennett and B.K. Marcus, *Stud. Surf. Sci. Catal.* **37**, 269 (1988).
- (2) G. Harvey, *Z. Kristallogr.* **182**, 123 (1988).
- (3) G. Harvey, Ch. Baerlocher and T. Wroblewski, *Z. Kristallogr.* **201**, 113 (1992).

