Building scheme for AFS and BPH

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1. Periodic Building Unit:

AFS and BPH can be built using units of 14 T atoms (bold in Figure 1(a)). The T14-unit consists of two double 4-rings each missing one T atom or two 6*1 units. The two-dimensional Periodic Building Unit (PerBU) equals the hexagonal layer obtained by connecting T14-units through 4-rings around a 6-fold inversion axis as shown in Figure 1(b-d).

![Figure 1. (a): Linkage between T14-units within the PerBU in AFS and BPH seen along [110] (top) and along [100] (bottom); (b): PerBU seen along c, (c): Idem along [120] and (d): Idem along [210]. The layers depicted in Figure 1(c and d) are identical and related by a 60° rotation about the hexagonal plane normal c.](image-url)
2. Connection mode:

Neighboring layers can be connected along the PerBU plane normal parallel to $c$ through 8-rings in two different ways:

(1): the lateral shift of the top layer along $a$ and $b$ is zero before connecting it to the bottom layer.

(2): the top layer is rotated over $60^\circ$ about $c$ before connecting it to the bottom layer.

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3. Projections of the unit cell content: See Figure 3.

Pure AFS and BPH are obtained when neighboring PerBUs are exclusively related by translation along $c$ or by a rotation of $60^\circ$ about $c$, respectively.
4. Channels and/or cages:

The channel intersection is depicted in Figure 4 together with the pore descriptor. The channel intersection is topologically equivalent to the intersection in AFY. Channel intersections are connected into channels along <100>, along <210> and along [001] as illustrated in Figure 5.

The intersections in both frameworkypes have the same pore descriptor:
\{3 [41\[86\]12\]} <100> (8-ring), <210> (8-ring), [001] (12-ring)\}

Figure 4. Channel intersections in AFS (top) and BPH (bottom) in perspective view along (from left to right) <100>, <210> and [001].

Figure 5. Connection of intersections parallel to [001] in AFS (left) and BPH (right) viewed along <100> (left and right) and along [001] (middle top and bottom). [Fig.5 is continued on next page]
5. Supplementary information:

Other framework types containing (modified) double 4-rings (D4Rs)
Double 4-rings (D4Rs) can be connected in several other 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.
In the INTRO pages links are given to a detailed description of a sub-set of framework types that contain (modified) D4Rs (choose: Double 4-rings). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: Appendix; Figure 5).