Building scheme for CDO and FER



1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content 4. Channels and/or cages – 5. Supplementary information

1. Periodic Building Unit:

CDO and **FER** can be built using the saw (s) chain (bold in Fig.1 (a)) parallel to **z**. The repeat distance along the saw chain is about 7.5 Å and the repeat unit consists of 3 T atoms. Three s chains are connected into an infinite building unit. A two-dimensional Periodic Building Unit (PerBU) is obtained when infinite building units, related by a rotation of 180° about **y** and a shift of $\frac{1}{2}$ **z**, are connected along **y** into the **yz** layer depicted in Fig.1(b). The PerBU can be considered as a strongly corrugated layer of (fused) 6-ring boats with "handles" of three additional T atoms.



2. Connection mode:

Neighboring PerBUs can be connected along **x** in two different ways (see Figure 2 on next page): (1): PerBUs, related by a shift of $\frac{1}{2}(\mathbf{x} + \mathbf{z})$, are connected through 8-rings. (2): PerBUs, related by a shift of $\frac{1}{2}(\mathbf{x} + \mathbf{y} + \mathbf{z})$, are connected through 6-, 8- and 10-rings.

[In DAC, EPI and MOR corrugated 6-ring layers are connected through 4-rings]



Figure 2. Connection mode (1) in CDO (left) and mode (2) in FER (right) viewed along z.



3. Projections of the unit cell content:

Figure 3. Parallel projections of the unit cell content in CDO (left) along a and along c, and in FER (right) viewed along c and b. The projections along c (in CDO) and along b (in FER) are equal.

4. Channels and/or cages:

Interconnecting one-dimensional channel systems are parallel to a and c in CDO, and to b and c in FER. The channel intersection in CDO consists of 5-, 6- and 8-rings. The intersection of channels in FER, composed of 6-, 8- and 10-rings, is topologically equivalent to the channel intersection in DAC. For each intersection the **pore descriptor** is added in Figure 3. In FER 10-ring channels, parallel to c, are interconnected along b through common 8-rings of cavities composed of fused 5- and 6-rings that are part of the wall of an 8-ring channel parallel to b.





Figure 5. (a): Fusion of channel intersections in **CDO**. Fusion of intersections along c viewed along a (top left) and along c (top right), and fusion of intersections along a viewed along c (bottom left), and along a (bottom right); (b): Fusion of channel intersections in **FER**. Fusion of intersections along b viewed along c (top left) and along b (top right), and fusion of intersections along c viewed along c (bottom left) and along b (top right), and fusion of intersections along c viewed along c (bottom left) and along c (bottom right).

5. Supplementary information:

Other framework types containing saw chains

In several framework types at least one of the unit cell dimensions is about n*7.5 Å (where n = 1, 2, 3... etc.). In many cases this indicates the presence of saw chains.

In the **INTRO** pages links are given to descriptions of other framework types containing (twisted) saw chains (choose: **Saw chains**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 2**).

Alternative description using (modified) 5-rings

Several framework types, like **CDO** and **FER**, can be constructed using (modified) 5-rings. In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **5-Rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).