Building scheme for CON and IWR

Periodic Building Unit – 2. Connection mode – 3. Parallel projections of the unit cell
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1. Periodic Building Unit:

CON and **IWR** can be built using chains parallel to *c* constructed from units of 14 T atoms (bold in Figure 1) that are related by pure translations along *c*. The two-dimensional Periodic Building Unit (PerBU) is equal to the *bc* layer composed of parallel chains, related by a 180° rotation about *b* (or *c*), depicted in Figure 2.[Compare this PerBU with those in the **Beta-like framework types**]



Figure 1. T14-units (one in bold), consisting of two 1-5-1 units (see Alternative description) and related by pure translations along c, are connected into chains. The chain at the right is rotated over 90° about c with respect to the left one.











Figure 2. (a): PerBU, constructed from chains, viewed along a (one T14-unit in bold); (b) and (c): PerBU viewed along b. The PerBUs, depicted in (b) and (c) are identical and related by a rotation of 180° about b (or by a mirror operation perpendicular to the plane normal; or by an origin shift of $\frac{1}{2}b$); (d): PerBU viewed along c.

2. Connection mode:

Neighboring PerBUs, related by a mirror operation perpendicular to the plane normal n, can be connected along n through 4-rings in two different ways:

(1): the lateral shift of neighboring layers along *c* is zero;

(2): the lateral shift of neighboring layers along c is +1/3c, as illustrated in Figure 3.



Connection mode 2

Figure 3: Connection mode (1) in IWR (top) and connection mode (2) in CON (bottom) viewed along *b*. Fused 4-6-6 ring sequences and fused 5-5-6 ring sequences are formed in connection mode (1) and (2), respectively. The parallel projections are shown at the right. [Compare these connection modes with the ones in *BEA and BEC]

3. Projections of the unit cell content:

Pure **IWR** and **CON** are obtained when neighboring PerBUs, related by a mirror operation perpendicular to the plane normal n, are connected along n by applying a lateral shift along c of zero or 1/3c, respectively, as shown in Figure 4 on next page. There is no difference in the projection of the structure of **IWR** and **CON** along c.



Figure 4: Cell content of **IWR** (top) and **CON** (bottom) viewed in perspective along b (left) and in projection along b (middle) and along c (right). The projection along c is the same for both framework types.

4. Channels and/or cages:

10-Ring channels are parallel to b and 12-ring channels are parallel to c. The channels are depicted in Figure 4 on next page together with their **pore descriptor**. The 12-ring channels in **CON** and **IWR** parallel to c are topologically equivalent to those in ***BEA** and **BEC**, respectively [Compare the present Figure 5(a) with Figure 4 in ***BEA** and **BEC**]. The 10-ring channels parallel to b are equivalent in **CON** and **IWR**. The fusion of channels is illustrated in Figure 6. Diffusion along the 12-ring channel parallel to a is obstructed as can be seen from the drawings of the (fused) channels at the bottom of Figure 5 and Figure 6 on next pages.



Figure 5. (a): 12-Ring channel in **CON** (left) and **IWR** (right) viewed along *c* (top), *b* (middle) and *a* (bottom); (b): 10-Ring channel in both framework types viewed along *b* (top left), *c* (top right) and along *a* (bottom). [Figure 6 is on next page]



Figure 6. Fusion of channels in **CON** (left) and in **IWR** (right) viewed along c (top), along b (middle) and along a (bottom).

5. Supplementary information:

Beta-like framework types

Beta-like framework types can be constructed using two types of chains.

In the **INTRO** pages links are given to a description of the framework types that contain these chains (choose: **Beta-family**). There is also a link provided to a summary of the chains and PerBUs used in the building schemes of the framework types (choose: **Appendix**; **Figure 9**).

Alternative description using (modified) 5-rings

Several framework types, like **CON** and **IWR**, 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**).