Building scheme for OBW



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1. Periodic Building Unit:

Tetragonal **OBW** can be built using units of 38T atoms. The T38-unit consists of twelve 3-rings that are connected around a 4-fold axis parallel to c and two additional T atoms (Be). Six (fused) 8-rings are formed. A two-dimensional Periodic Building Unit (PerBU) is obtained when T38-units are connected along a, and b after pure translations. The two additional T atoms connect the PerBUs in three dimensions.



Figure 1. PerBU viewed along *c* (left) and along *a* (or *b*) (right). The Be atoms (4 per unit cell), connecting the PerBU to its neighboring PerBUs (See 2. Connection mode), are also shown.

2. Connection mode:

Neighboring PerBUs, related by a shift of $\frac{1}{2}(a + b + c)$, are connected along *c* through spiro-5 rings (with the Be atom as the central atom) as illustrated in Figure 2.



Figure 2. Connection mode in **OBW** viewed along *a*. The PerBUs are connected along *c* through spiro-5-rings with Be atoms as central atoms.

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



Figure 3. Parallel projections of the unit cell content along *c* (left) and along *a* (or *b*) (right).

4. Channels and/or cages:

8-Ring channels are parallel to <100> and 10-ring channels are parallel to <110>. The channel systems interconnect through common 8-rings. The two types of channel intersections are shown in Figure 4. The **pore descriptor** is added. The fusion of cavities is illustrated in Figure 5.



Figure 4. Channel intersection 1 (left) viewed along a (or b; top), and along the same view direction (bottom) after a rotation of 45° about b (or a) has been applied; channel intersection 2 viewed along a (or b; middle), and along <110> (right).



Figure 5. Fusion of channel intersections along b (or a) and along c viewed along a (or b; left), along the 8-ring channel axis parallel to b (or a; right), and along the 10-ring channel axis parallel to <110> (see next page). [Figure 5 is continued on next page]



Figure 5 [Cont'd]. Fusion of channel intersections along *b* (or *a*) and along *c* viewed along the 10-ring channel axis parallel to <110>.

5. Supplementary information:

Other framework types containing (modified) single 3- and/or 4-rings

Single 3- and/or 4-rings can be connected in several other ways. In several cases 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) single 3- and/or 4-rings (choose: **Single 3- and/or 4-rings**). There is also a link to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 4**).