# Building scheme for ISV and BEC

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

#### 1. Periodic Building Unit:

Tetragonal **ISV** and **BEC** can be built using T16-units: four fused 6-rings or eight fused 5-rings (one in bold in Figure 1). T16-units, related by pure translations along **x**, are connected into chains parallel to **x**. Neighboring chains, related by a rotation of 180° about the chain axis, are connected along **y** through 4-rings into the Periodic Building Unit (PerBU) depicted in Figure 2. [Compare this PerBU with those in the **Beta-like framework types**; for a different PerBU in **BEC**: see **Alternative description**; for the PerBU in **ISV** and **BEC** built from 6-2 units: see **Figure 7**]



Figure 1. T16 units, related by pure translations along **x** are connected into chains along **x**. Chain viewed along **y** (left), and along **z** (right). The chains on the right differ by a rotation of 180° about **x**.



Figure 2. PerBU viewed along the plane normal z (left), down x (top right), and along y (bottom right). The PerBU's, depicted at the right, are identical and related by a rotation of 90° about z.

# 2. Connection mode:

Neighboring PerBUs are connected along z in two different ways:

(1): neighboring PerBUs, related by pure translations along z, are connected through double 4-rings. The connectivity exhibits mirror symmetry between successive layers.

(2): neighboring PerBUs, related by a rotation of 90° about z, are connected through double 4-rings. Successive layers are related by a  $4_2$  axis.



Figure 3. Connection mode (1) in BEC (left) and connection mode (2) in ISV (right) viewed along y.

## 3. Projections of the unit cell content: see Figure 4





Figure 4. Parallel projections of the unit cell content in **BEC** viewed along c (top left) and along a (bottom left), and parallel projections of the unit cell content in **ISV** viewed along b (middle) and along a (right). [Figure 4 is continued on next page]



#### 4. Channels and/or cages:

The pore system in **ISV** can be described using "double" cavities depicted in Figure 5 together with the **pore descriptor**. Fused cavities form 12-ring channels parallel to <100> and to [001] as shown in Figure 6. Diffusion through the 12-ring channel in **ISV** parallel to [001] is obstructed as can be seen from Figures 4, 5 and 6. For a description of the channels in **BEC**: see **BEC**.





## 5. Supplementary information:

#### Alternative description of BEC

An alternative description of **BEC** using a different PerBU is presented in the building scheme of **BEC**.

#### Beta-like framework types

Beta-like framework types can be constructed using chains that resemble the chain in the **BEA** framework type.

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**).

Figure 7.



Figure 7. PerBU built from 6-2 units. The 6-2 units farthest from the reader are in bold.