Building scheme for *BEA and BEC

1. Periodic Building Unit:

The Periodic Building Unit (PerBU) in tetragonal ***BEA** and **BEC** equals the beta layer shown in Figure 1. The PerBU is composed of T16 units: four fused 6-rings or eight fused 5-rings (in bold) related by pure translations along the cell edges *a* and *b*. [Compare this PerBU with those in the **Beta-like framework types**; for a different PerBU in **BEC**: see **Alternative description**]

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Figure 1. PerBU viewed along the plane normal *c* (left), along *b* (or *a*) (top right), and along *a* (or *b*) (bottom right). The depicted PerBUs at the right are related by a rotation of 90º about *c*.

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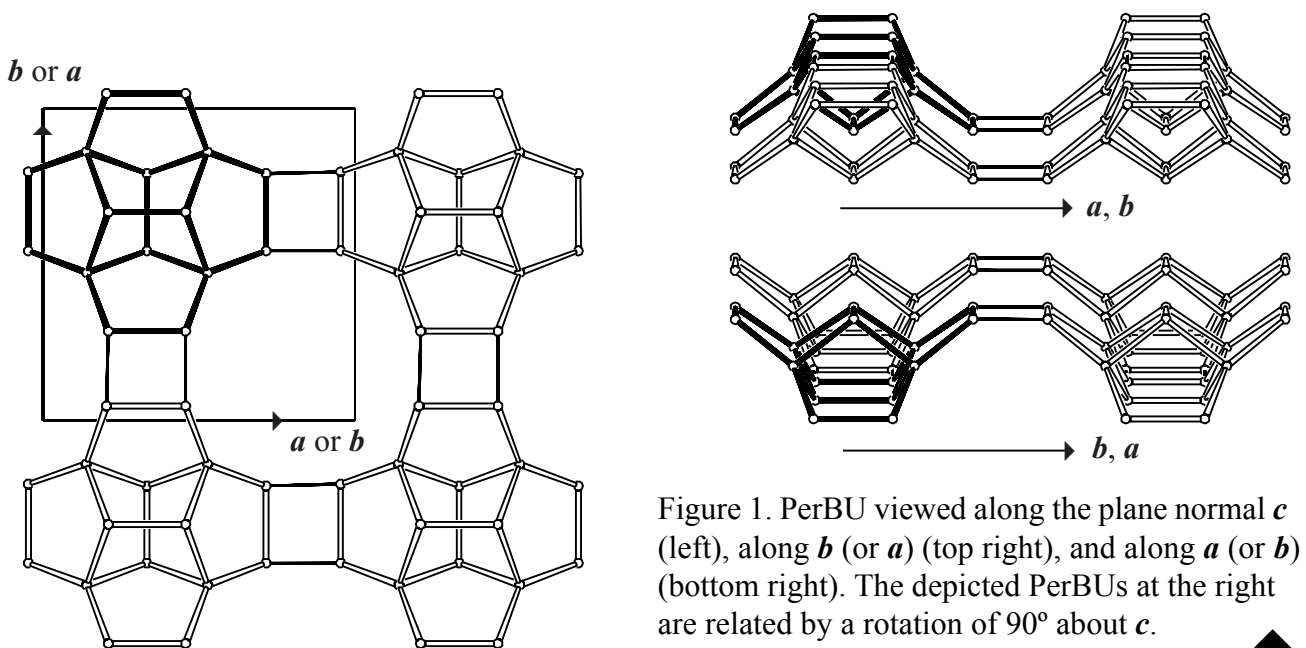
2. Connection mode:

Neighboring PerBUs, related by a 90º rotation about the plane normal, are connected along *c* in different ways:
(1): the lateral shift of the top layer is 1/3*a* or 1/3*b*; denoted as (1/3,0) or (0,1/3), respectively;
(2): the lateral shift of the top layer is -1/3*a* or -1/3*b*; denoted as (-1/3,0) or (0, -1/3), respectively;
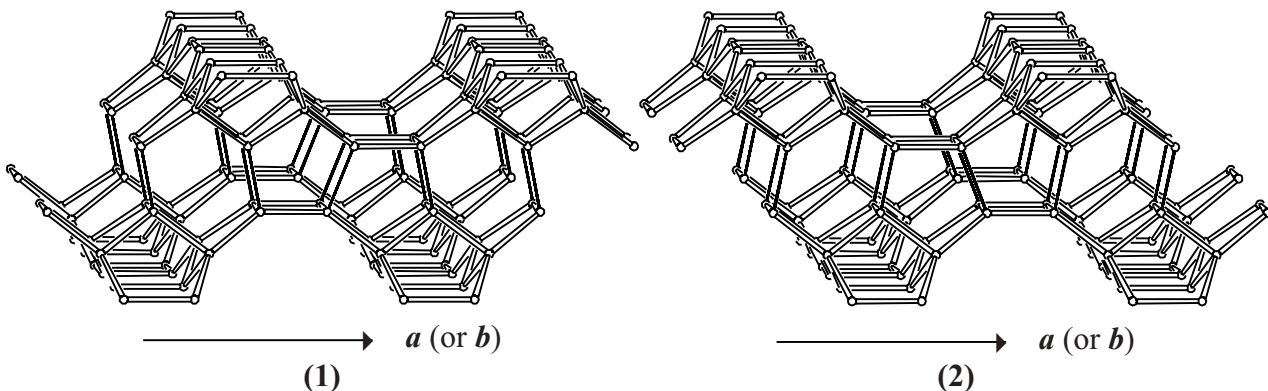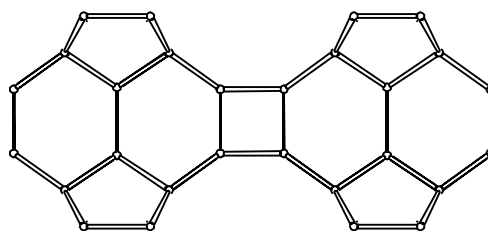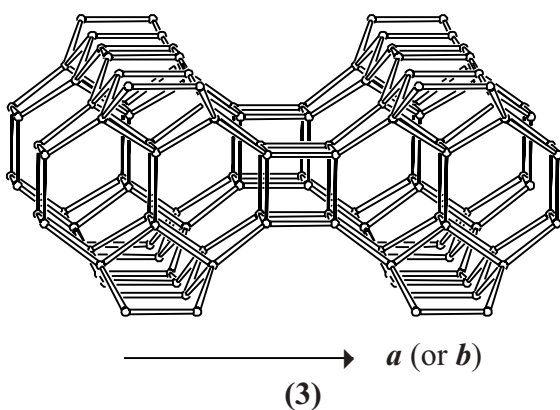**(3):** the lateral shift of the top layer along *a* and *b* is zero; denoted as (0,0).

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(1)   **(2)**

Figure 2. Connection modes **(1)** and **(2)** in ***BEA** through fused 6-5-5-ring sequences. Between these ring sequences single 4 rings are formed. [Figure 2 is continued on next page]

Connection mode **(3)** in **BEC** through fused 4-6-6-ring sequences. Between these ring sequences single- and double-4 rings are formed. The parallel projection is shown at the right. ▲

a (or **b**)

(3)

3. Projections of the unit cell content:

Neighboring PerBUs in the tetragonal unit cells of ***BEA** and **BEC** are related by a rotation of 90° about **c**. The required lateral shifts are given in Figure 3. [The enantiomorph of ***BEA** (not drawn) has a lateral shift sequence of: (1/3,0); (0, -1/3); (-1/3,0); (0,1/3); (1/3,0); etc..]
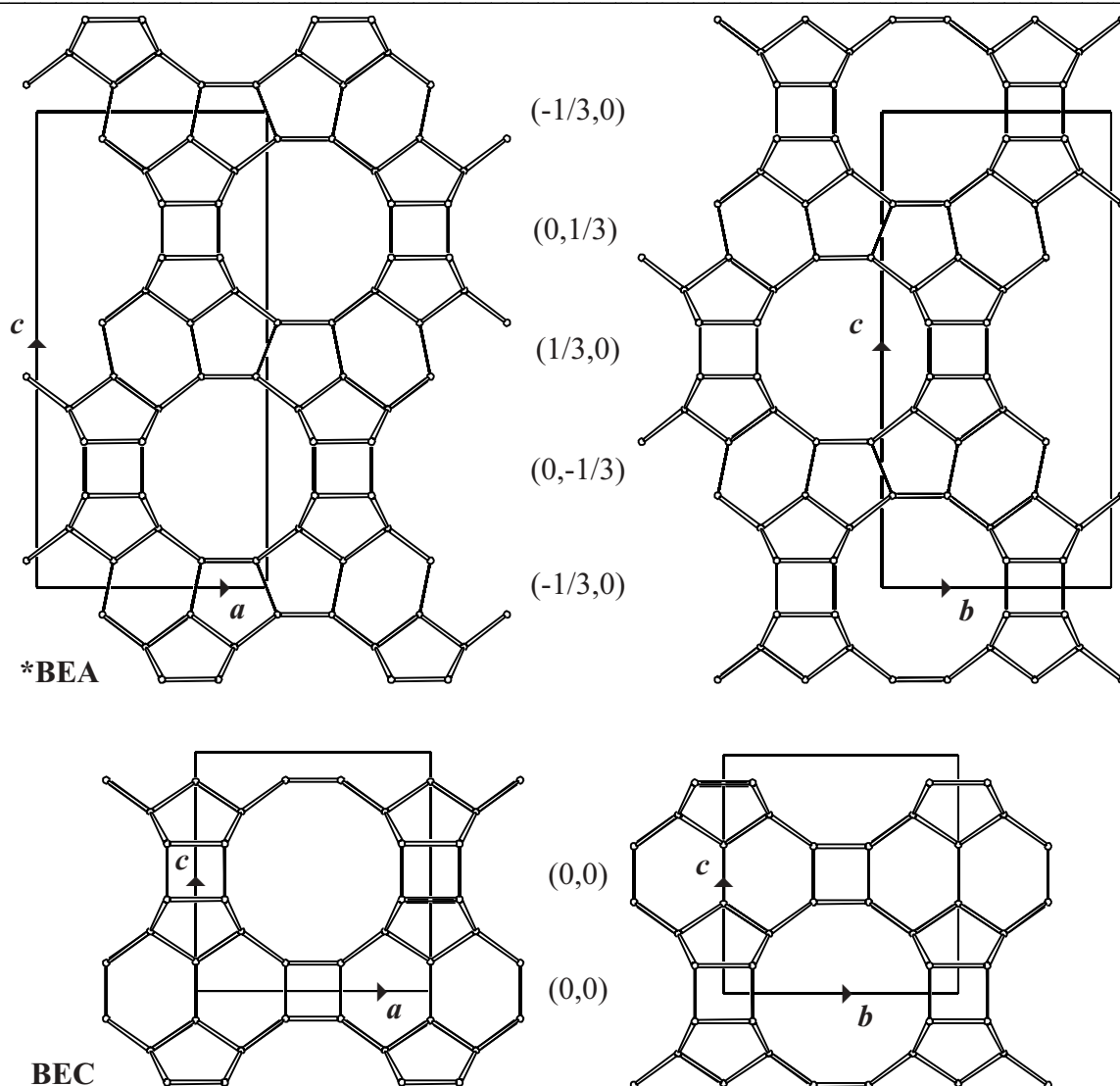

(-1/3,0)

(0,1/3)

(1/3,0)

(0,-1/3)

(-1/3,0)

*BEA

(0,0)

(0,0)

BEC

Figure 3. Parallel projections of the unit cell content in ***BEA** (top) and **BEC** (bottom) viewed along **b** (left), and along **a** (right). The lateral shifts are indicated. ▲

4. Channels and/or cages:

12-Ring channels are parallel to <100> and [001]. The channels are depicted in Figure 4 together with their **pore descriptor**. The channels in ***BEA** and **BEC** parallel to <100> are topologically equivalent to those in **CON** and **IWR**, respectively [Compare the present Figure 4 with Figure 5(a) in **CON** and **IWR**]. The fusion of channels is illustrated in Figure 5. Diffusion along the 12-ring channel in ***BEC** parallel to [001] is obstructed as can be seen from the drawings of the (fused) channels at the bottom of Figure 4 and Figure 5.
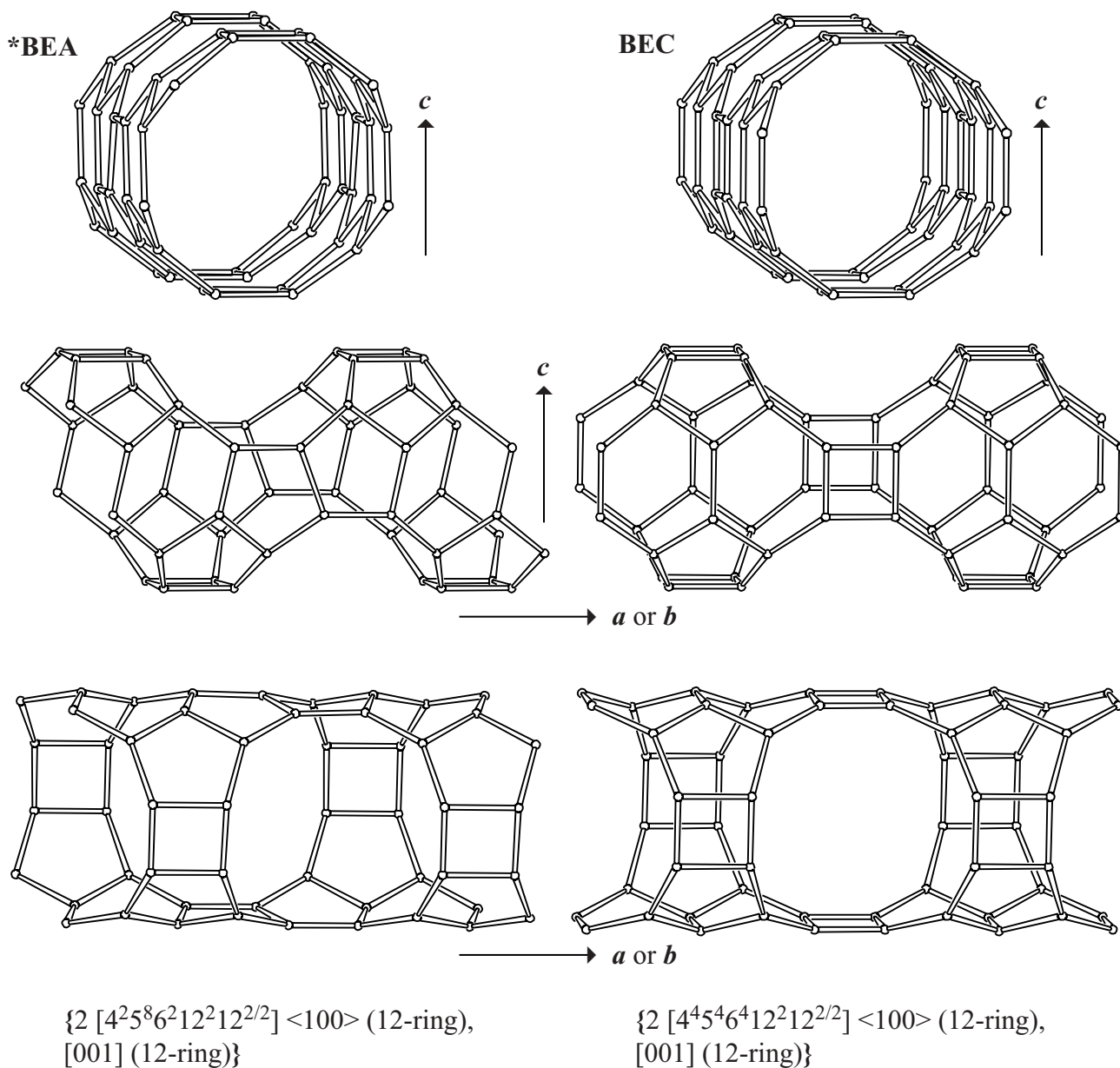

$\{2\ [4^2 5^8 6^2 12^2 12^{2/2}]$ <100> (12-ring),
[001] (12-ring)$\}$

$\{2\ [4^4 5^4 6^4 12^2 12^{2/2}]$ <100> (12-ring),
[001] (12-ring)$\}$

Figure 4. 12-Ring channels in ***BEA** (left) and **BEC** (right) viewed perpendicular to the tetragonal *c* axis (top and middle), and down the tetragonal axis (bottom).
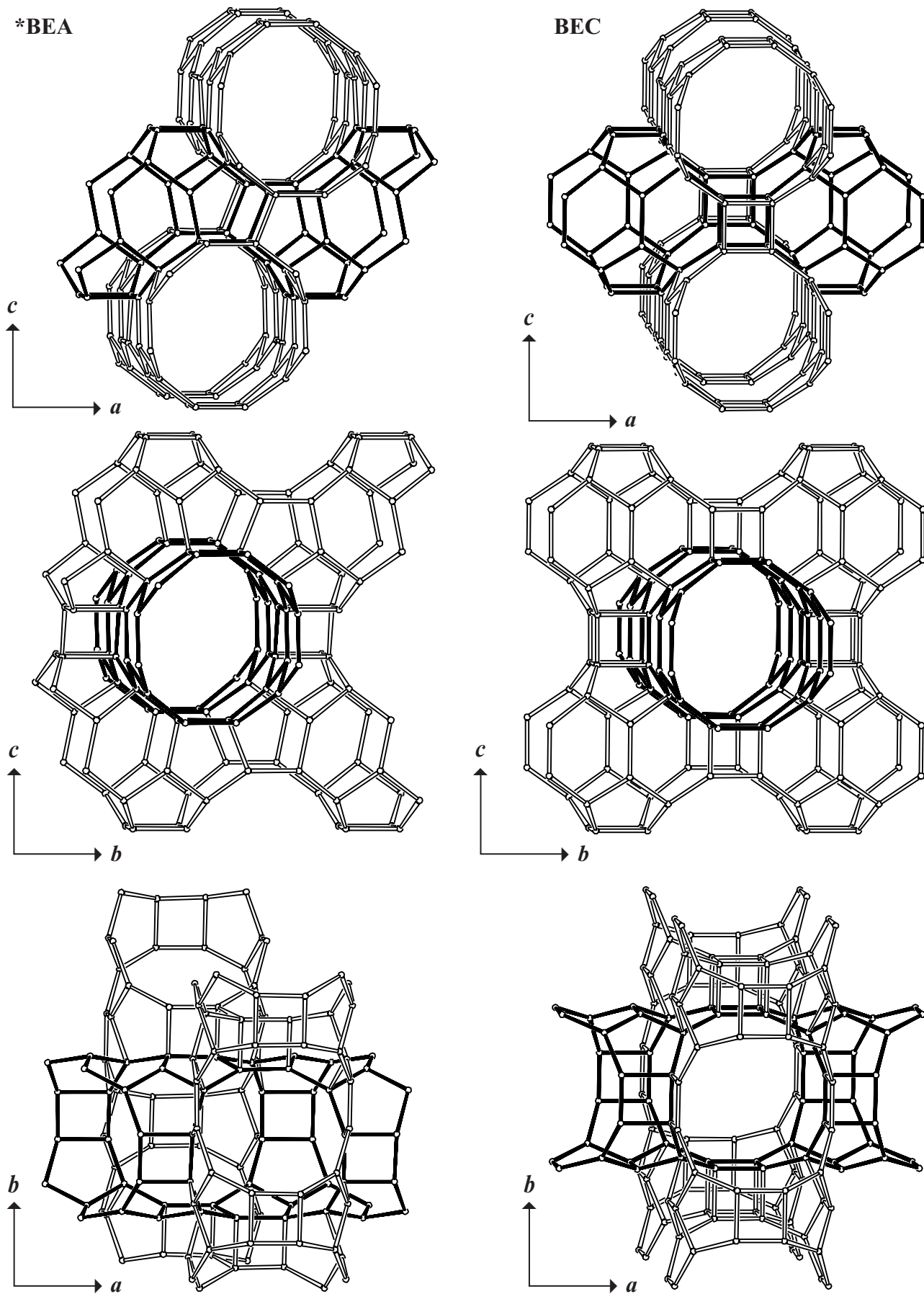[Figure 5 is on next page]

*BEA

BEC

Figure 5. Fusion of channels in ***BEA** (left) and in **BEC** (right) viewed along **b** (top), along **a** (middle), and along **c** (bottom).

5. Supplementary information:

Alternative description of BEC
An alternative description of **BEC** using different PerBUs (also one using 6-2 units) is presented in the building scheme of **ISV**.

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**).