The Faujasite Family

1. The Periodic Building Unit (PerBU) is the hexagonal layer shown in Figure 1. This layer is built from T24 units, the sodalite cages (sod-cages), shown in Figure 2.

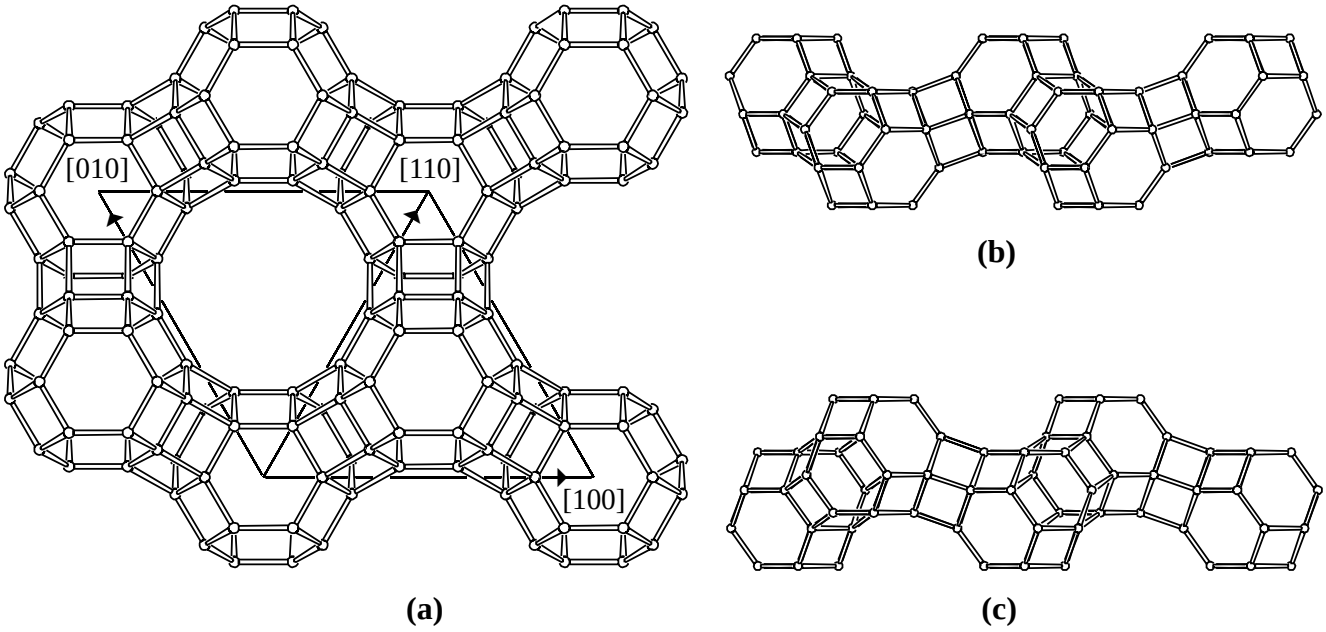

Figure 1: The PerBU in the Faujasite family of zeolite frameworks is composed of sod-cages which are linked through double T6-rings into a hexagonal layer. The PerBU corresponds to the (001) layer in hexagonal EMT and to the (111) layer in cubic FAU. Hexagonal axes are given. Views along [001] (a), [010] (b) and [110] (c) are shown. The layers, depicted in Figure 1b and 1c are identical and related by a 60º rotation about the (hexagonal) ***c***-axis or by a mirror operation perpendicular to ***c***

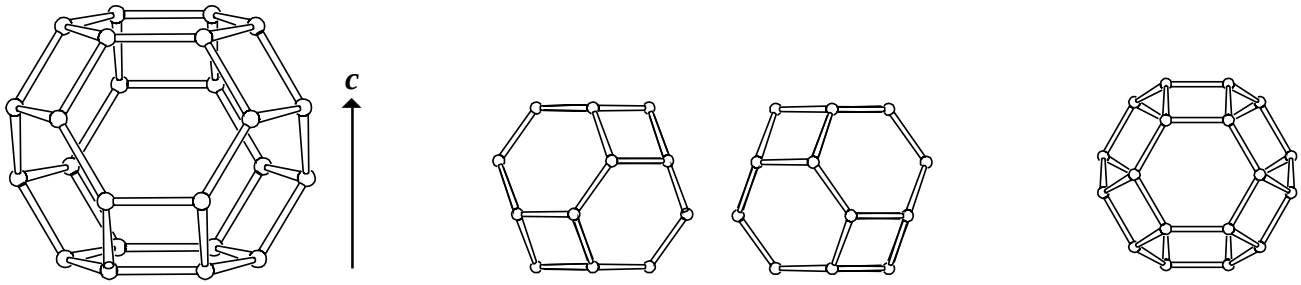

Figure 2: The sod-cage. From left to right: perspective view perpendicular to ***c***; parallel views perpendicular to ***c***, after rotation of +30º and -30º about ***c*** with respect to the most left drawing; and parallel view down ***c***. [Compare the packing of sod-cages in LTA and SOD]

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2. Type of Faulting: 1-dimensional stacking disorder of the PerBU's along [001].

3. The Layer Symmetry: the plane space group of the PerBU is P ($\bar{3}$) m 1.

4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's can be connected along [001] through double T6-rings in two different ways:
(a): the top layer is shifted over ⅓(-***a*** + ***b***) before connecting it to the bottom layer. The resulting connectivity exhibits inversion symmetry (**i**: o) between successive layers.
(b): the top layer is rotated over 60° about [001] (followed by the shift vector ⅓(-***a*** + ***b***)) before connecting it to the bottom layer. The connectivity now shows mirror symmetry (**m**:|) between successive layers (see also Fig.1b and 1c).

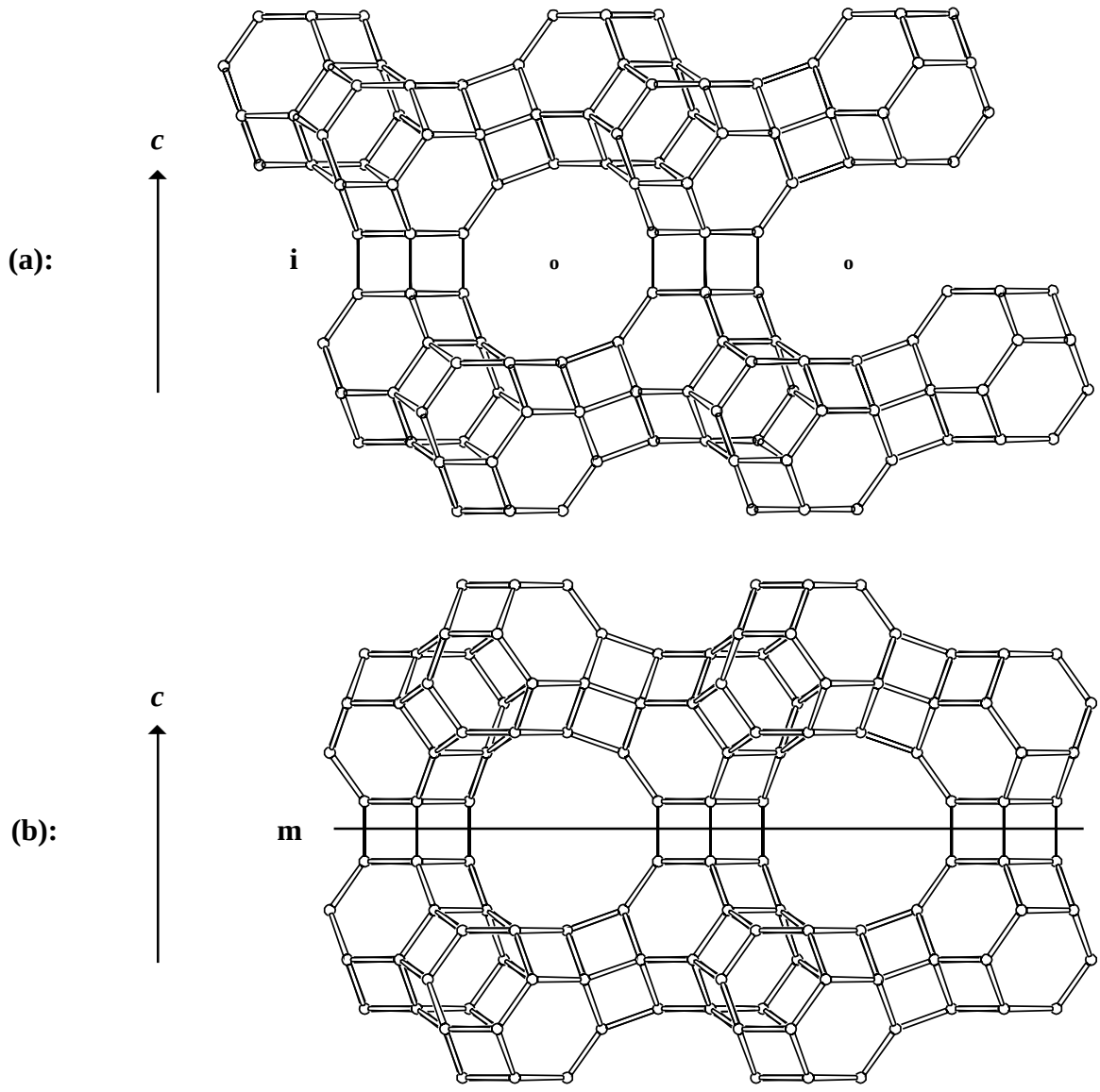

Figure 3: Parallel projection along [010] of the connection modes **(a)** and **(b)** in the Faujasite family of zeolite frameworks

Once the distribution of the symmetry elements **i** and **m** between the layers stacked along [001] is known, the 3-dimensional structure is defined.

An example of an intermediate structure in the Faujasite family of zeolite frameworks [hexagonal as well as cubic axes have been indicated] is shown in Figure 4:

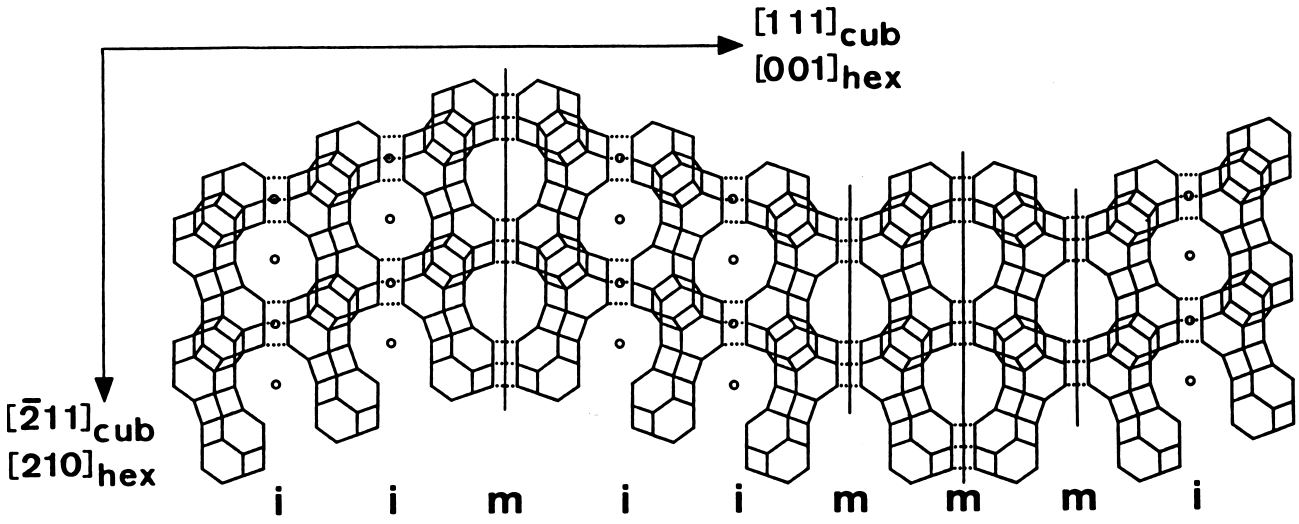

Figure 4: Connectivity sequence of PerBU's with **m** and **i** as symmetry elements

5. The Simplest Ordered End-Members in the Faujasite family are presented in Figure 5:

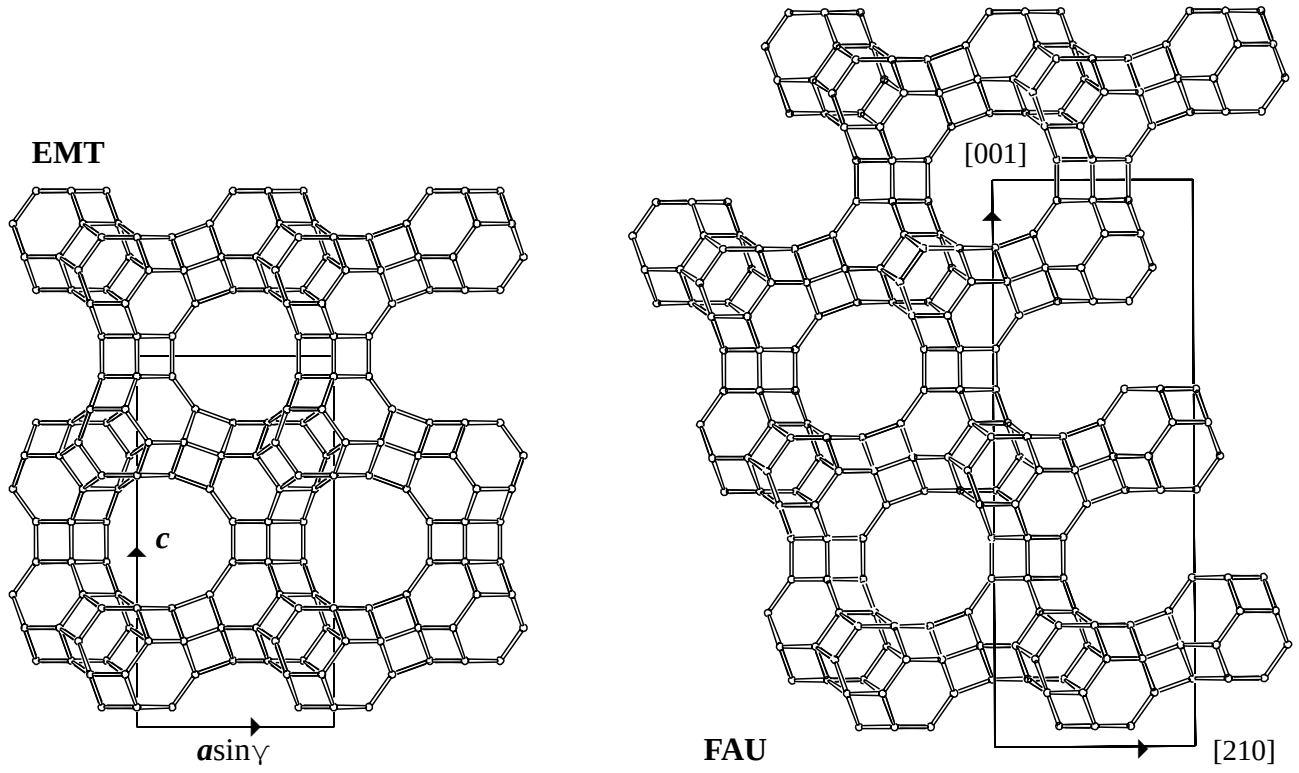

Figure 5: Projection of the unit cell content along the hexagonal [010] axis of the two simplest ordered end-members in the Faujasite family: EMT (left) and FAU (right)

Pure EMT(1,2) and FAU(3,4) are obtained when neighbouring PerBU's along the (hexagonal) [001] axis are exclusively related by **m** and **i**, respectively.

6. Disordered Materials Synthesized and Characterized to Date:

CSZ-1 (5,6); CSZ-3 (5,7); ZSM-3 (5,8); ZSM-20 (5,9); ECR-30 (5,10).

7. Supplementary Information

7.1 *Comparison with LTA:*

In LTA, each sodalite(sod)-cage is connected to six nearest neighbouring sod-cages through double T4-rings (Fig.6). [In FAU/EMT each sod-cage is connected to four nearest neighbouring sod-cages through double T6-rings]. Eight sod-cages in a cubic packing enclose a RHO-cage (Fig.7).
[For more details: see the building scheme of LTA in 'Schemes for Building Zeolite Framework Models' on http://www.iza-structure.org/databases/].

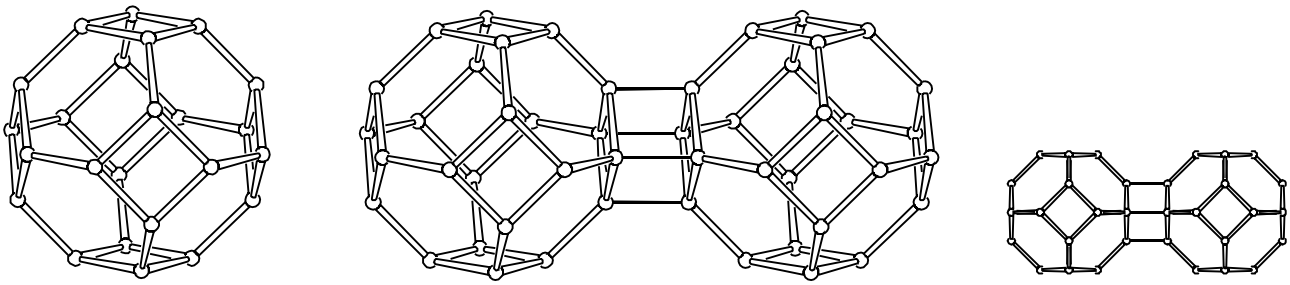

Figure 6: Sod-cage (left) connected through a double T4-ring to one of its nearest neighbours in perspective view (middle) and in parallel projection (right)

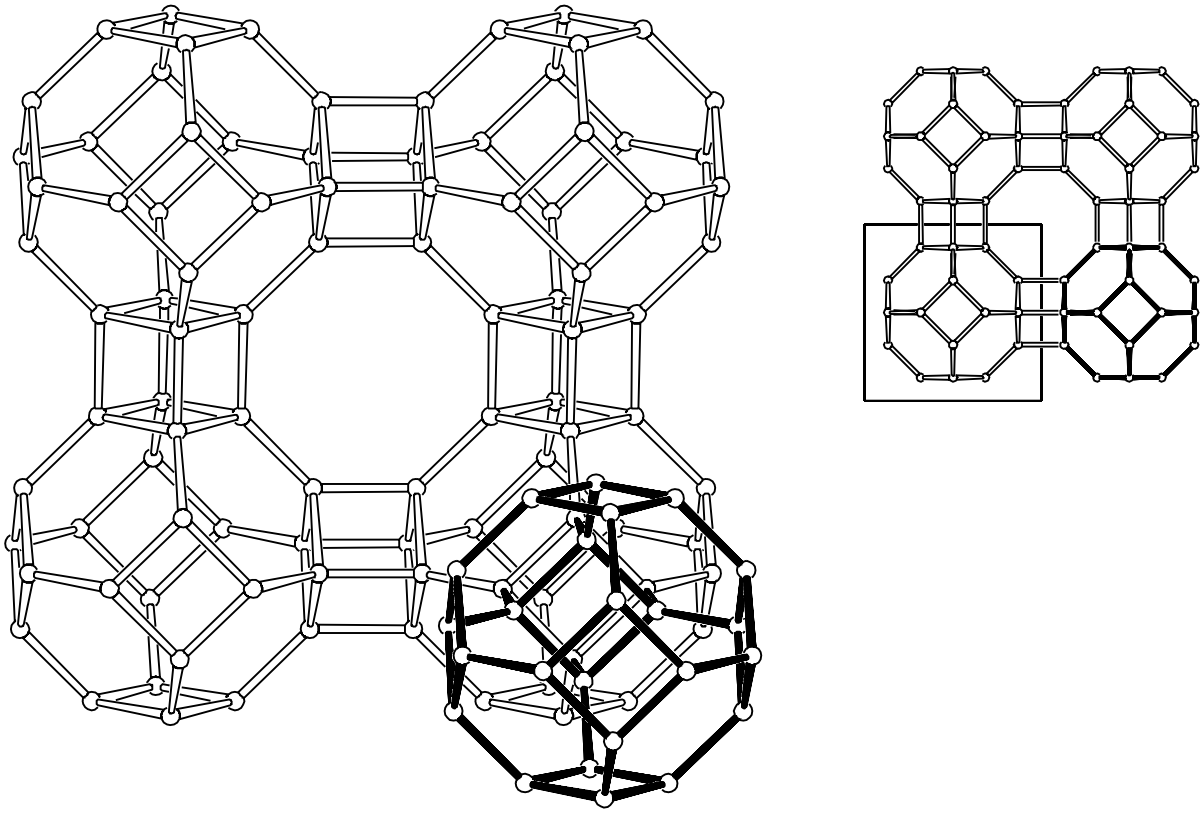

Figure 7: Cell content seen along a cube axis in perspective view (left) and in parallel projection (top right). For clarity, only one additional sod-cage along the viewing direction has been drawn (in bold)

7.2 *Comparison with SOD:*

In SOD, each sod-cage is connected to six nearest neighbouring sod-cages through common T4-rings (Fig.8). Eight (fused) sod-cages in a cubic packing enclose 'new' sod-cages. [For more details: see the building scheme of SOD in 'Schemes for Building Zeolite Framework Models' on: http://www.iza-structure.org/databases/].

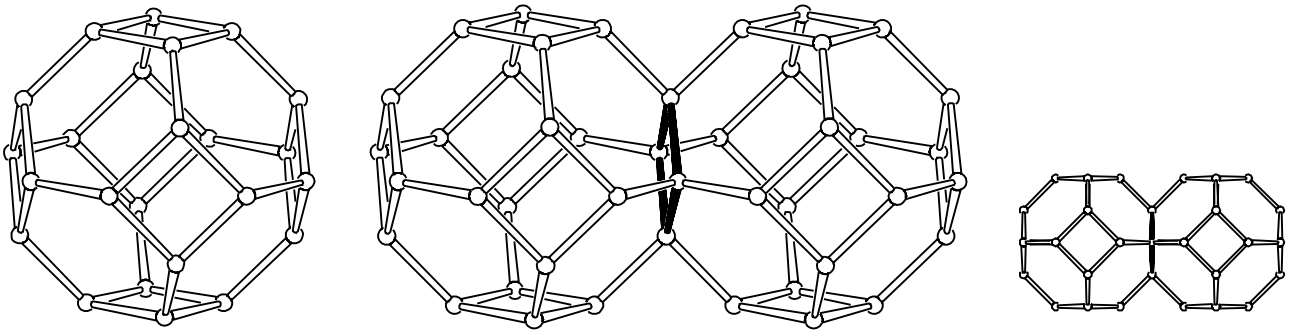

Figure 8: Sod-cage (left) connected through a common T4-ring (in bold) to one of its nearest neighbours in perspective view (middle) and in parallel projection (right)

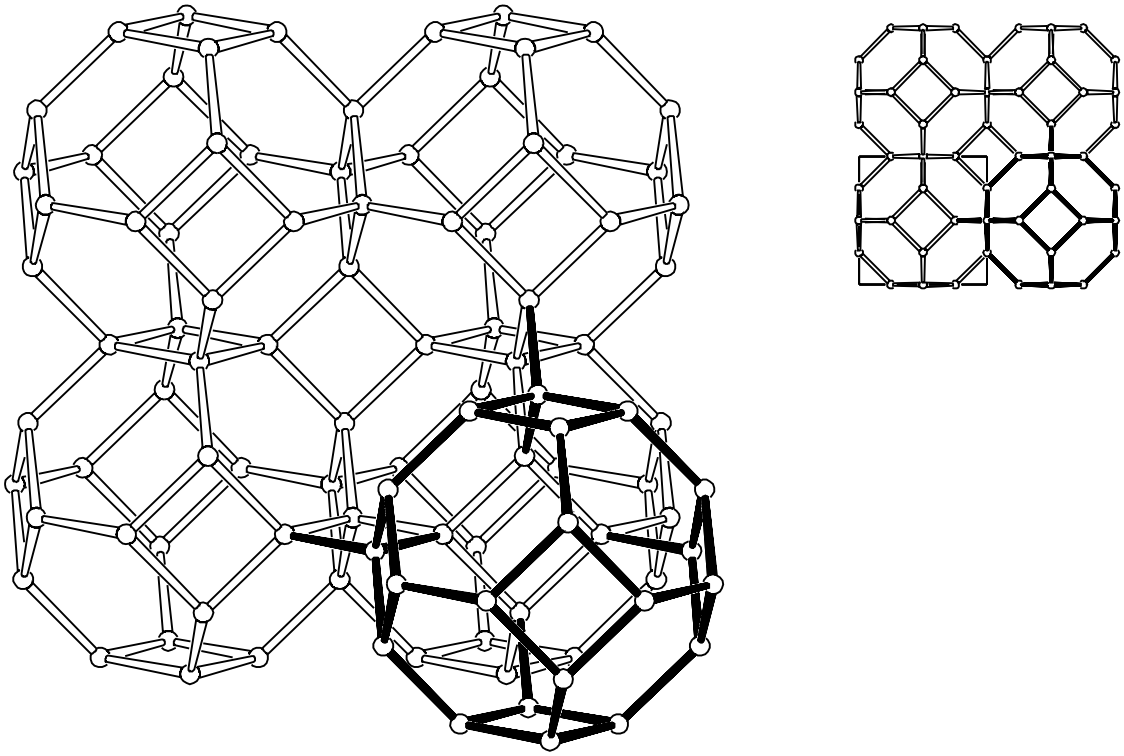

Figure 9: Cell content seen along a cube axis in perspective view (left) and in parallel projection (right). For clarity, only one additional sod-cage along the viewing direction has been drawn (in bold)

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8. References

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