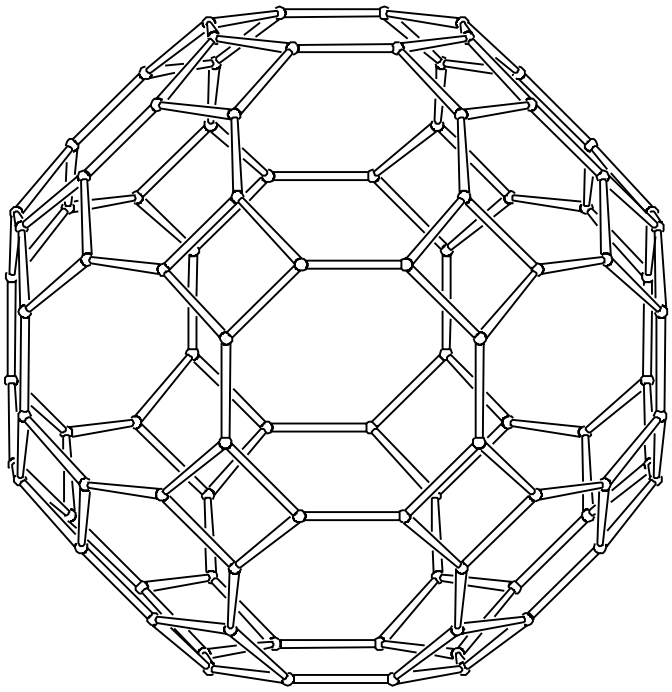
Building scheme for TSC

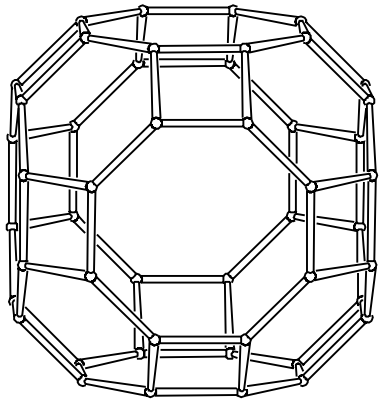
1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
4. Channels and/or cages – 5. Supplementary information

1. Periodic Building Unit:

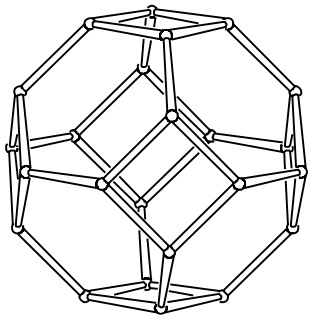
Cubic **TSC** can be built using the tschoertnerite (***tsch***) cavity consisting of twenty-four 4-rings (or twelf 8-rings) that are connected as shown in Figure 1 (left). A Periodic Building Unit (PerBU) is obtained when these cavites, related by translations of halve the cube face diagonals, are linked through double 8-rings (D8Rs) as illustrated in Figure 2(a). An alternative PerBU can be built when rho cavities (***rho*** cavities), consisting of twelf 4-rings (Figure 1 (top right)), and sodalite cages (***sod*** cages), consisting of 24 T atoms (Figure 1(bottom right)) are connected through double 6-rings (D6Rs) as shown in Figure 2(b).



tsch-cavity
{3 [$4^{24}6^8 8^{18}$] <100> (8-ring), <110> (8-ring)}



rho-cavity
{3 [$4^{12}6^8 8^6$] <100> (8-ring)}



sod-cage
{0 [$4^6 6^8$]}

Figure 1. The ***tsch*** cavity (left), ***rho***- or α-cavity (middle), and ***sod***- or β-cage (right). For each type of cavity the **pore descriptor** is added.

Figure 2: See next page.

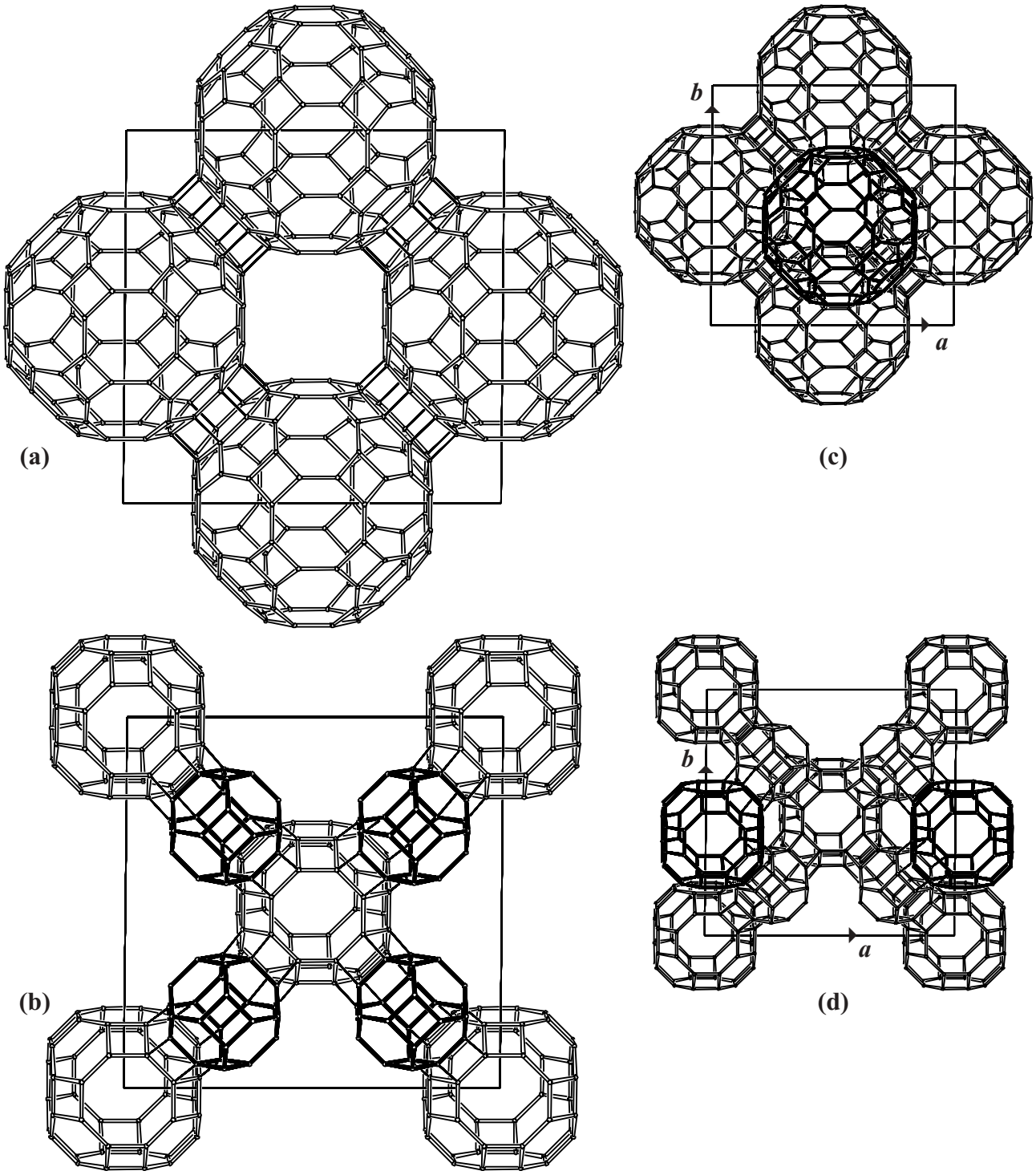


Figure 2. The PerBUs equal the content in one cubic layer. (a): PerBU1 is obtained when ***tsch*** cavities are linked through D8Rs ; (b): PerBU2 is obtained when ***rho***- or α-cavities and ***sod***- or β-cages (in bold) are linked through D6Rs.

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2. Connection mode:

Neighboring PerBU1s, related by 1/2(***a*** + ***b***), are connected along [001] through double 8-rings. Neighboring PerBU2s, related by 1/2(***a*** + ***b***), are connected along [001] through double 6-rings. The connection modes are illustrated in Figure 2(c) and (d), respectively. Only part of the neighboring PerBU (in bold) is drawn for clarity reason.

3. Projections of the unit cell content:

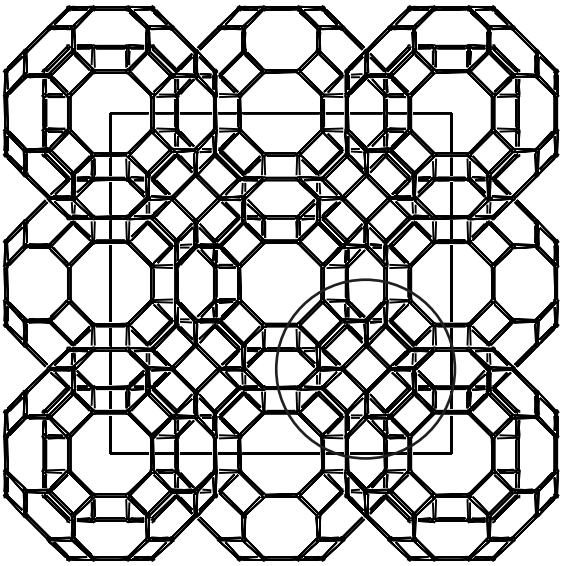

Figure 3. Unit cell content in **TSC** viewed along a cubic axis. **TSC** can also be built using units consisting of four double 6-rings (48 T atoms) that are tetrahedral coordinated around the center of the β-cage (circled in the Figure).
[see **Alternative description**]

4. Channels and/or cages:

In cubic **TSC** 8-ring channels are parallel to <100> and to <011>. The channel intersections, or cavities, are depicted in Figure 2. The fusion of the cavities and cages is illustrated in Figure 4.

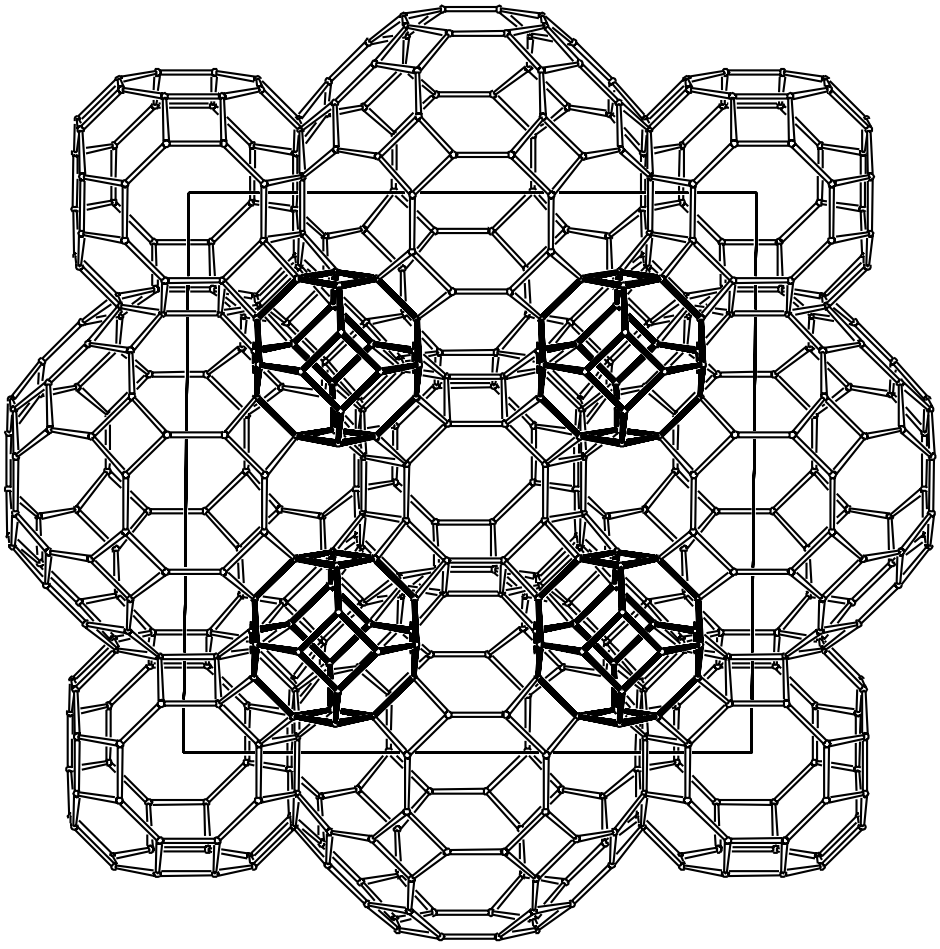

Figure 4. Fusion of the cavities and cages in **TSC** viewed along <100>. [Figure 4 is continued on next page]

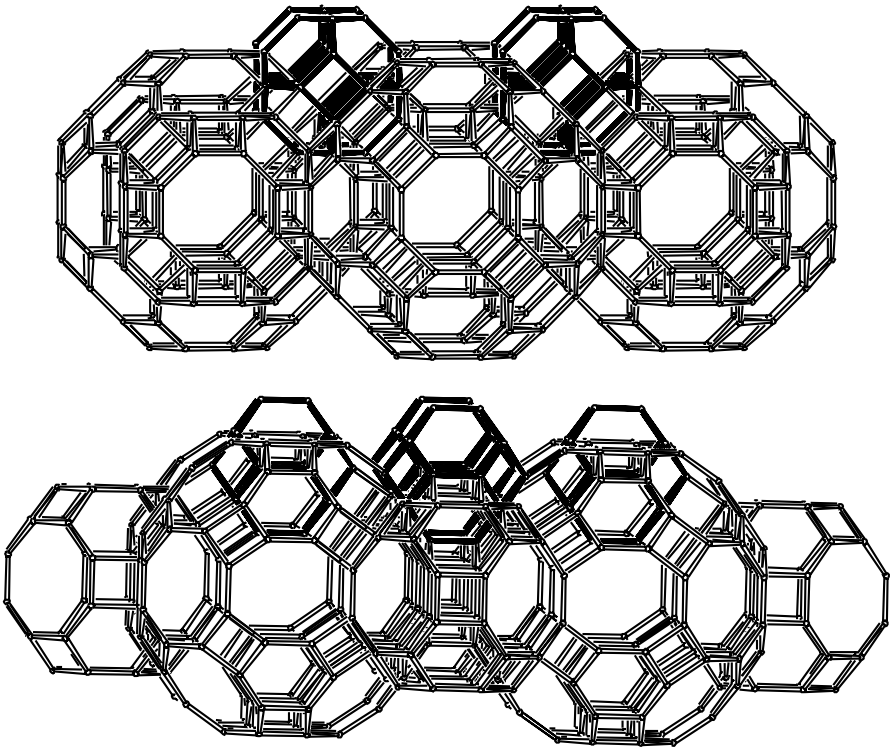

Figure 4 [Cont'd].
8-Ring channels viewed along <100> (top), and along <011> (bottom).

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5. Supplementary information:

Other framework types containing (modified) cavities
Several other framework types can be built using (modified) cavities.
In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) cavities (choose: **Cages**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 11**).

Alternative description of* TSC *using (modified) double 6-rings (D6Rs)
Several framework types, like **TSC**, can be built using (modified) D6Rs (see Figure 4).
In the **INTRO** pages links are given to a detailed description of a sub-set of framework types that contain (modified) D6Rs (choose **Double 6-rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).