Building scheme for MWW

1. Periodic Building Unit:

MWW can be built using units of 36 T atoms. The T36-unit resembles a "half-cage" (or 12-ring cup) consisting of cylindrical 6-ring band closed at one side by a 6-ring to which two T2-dimers and two T atoms are bonded (or built from four 6-1 units and one 1-6-1 unit). The one-dimensional Periodic Building Unit (PerBU) is obtained when T36-units, related by a mirror plane perpendicular to *c*, are connected into columns along *c* through double 6-rings and single T-T bonds (Figure 1(a)).

(b)

(a)   **(c)**

(d)
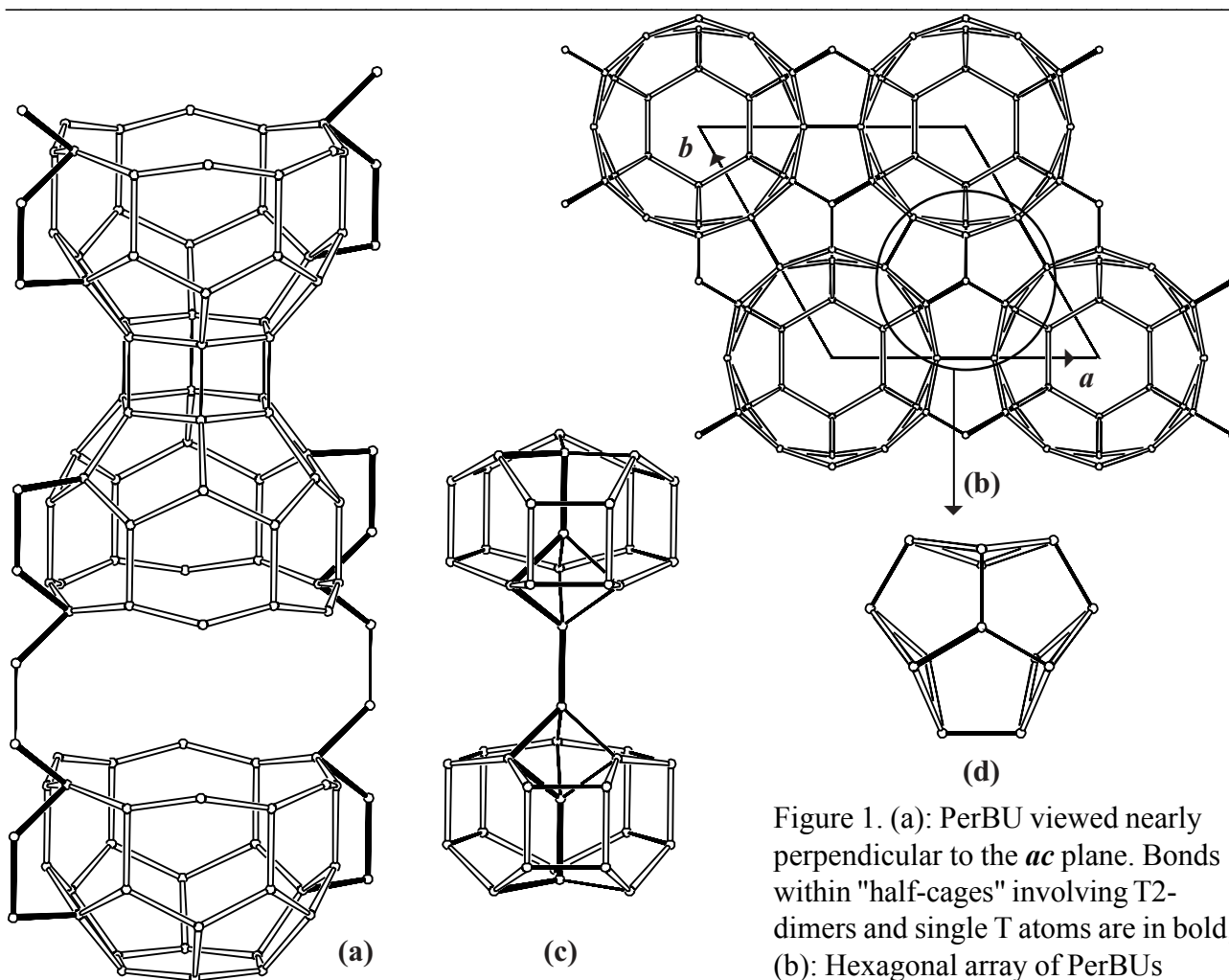
Figure 1. (a): PerBU viewed nearly perpendicular to the *ac* plane. Bonds within "half-cages" involving T2-dimers and single T atoms are in bold; (b): Hexagonal array of PerBUs viewed along *c*. The newly formed cage **1** is indicated; (c): Cage **1** is formed by the connection modes between "half-cages" within the hexagonal layer; (d): Parallel projection of cage **1** along *c*.

2. Connection mode:

The **MWW** framework is obtained when PerBUs, related by pure translations along the hexagonal *a* and *b* axes, are linked into the hexagonal packing shown in Figure 1(b). The hexagonal packing of the PerBUs generates a double layer which contains a new cage (cage **1**): each 6-ring of a 6-ring band in a "half-cage" is connected (around a 3-fold axis) through a T2-dimer and a single T atom to two 6-rings from two neighboring "half-cages" (Figure 1(c) and 1(d)).

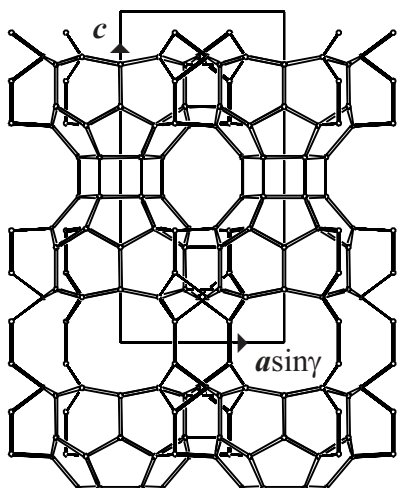**3. Projections of the unit cell content:** See Figure 1(b) and Figure 2.

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Figure 2. Cell content viewed along **b**. A projection of the cell content along **c** is shown in Figure 1(b).

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4. Channels and/or cages:

In hexagonal **MWW** two non-intersecting types of 10-ring channels are parallel to <100>. The channel intersection within the double layer is equal to cavity **1** and the channel intersection between the double layers is equal to the cavity **2**. Both cavities are depicted in Figure 3. The **pore descriptors** are added. The new cage **1**, formed upon connecting "half-cages" into the hexagonal layer, is shown in Figure 1(c) and Figure 1(d). The linkage of the cavities and cage is illustrated in Figure 4.
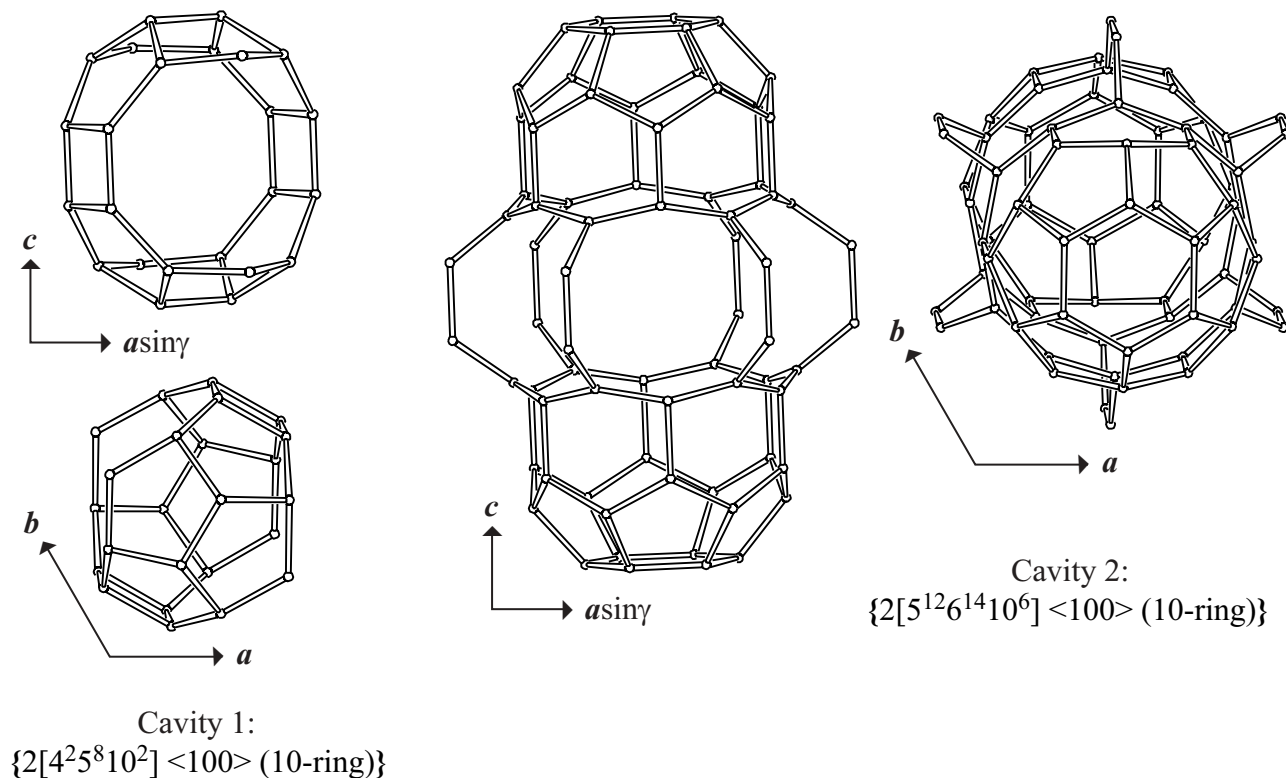
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Cavity 1:
{2[$4^2 5^8 10^2$] <100> (10-ring)}

Cavity 2:
{2[$5^{12} 6^{14} 10^6$] <100> (10-ring)}

Figure 3. Cavity **1** within the double layer viewed along <010> (top left), and along [001] (bottom left), and cavity **2** between double layers viewed along <010> (middle), and along [001] (right).
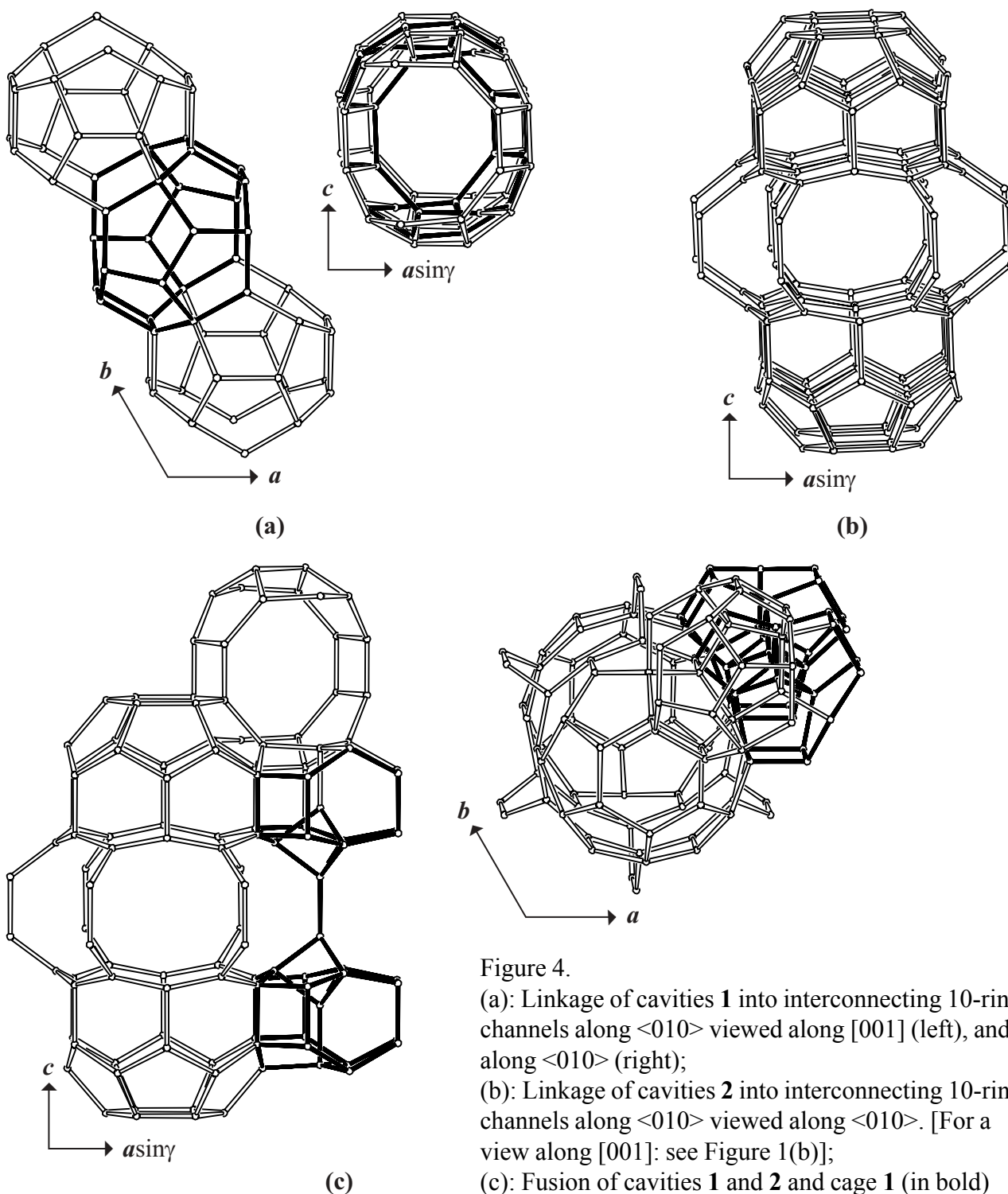
(a)

(b)

(c)

Figure 4.
(a): Linkage of cavities **1** into interconnecting 10-ring channels along <010> viewed along [001] (left), and along <010> (right);
(b): Linkage of cavities **2** into interconnecting 10-ring channels along <010> viewed along <010>. [For a view along [001]: see Figure 1(b)];
(c): Fusion of cavities **1** and **2** and cage **1** (in bold) viewed along <010> (left), and along [001] (right).

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5. Supplementary information:

Other miscellaneous framework types

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Miscellaneous**). 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 12**).

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