Building scheme for IWV

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1. Periodic Building Unit:

IWV can be built using building units composed of 19 T atoms: three finite zigzag chains (5 T atoms each and parallel to *b*) and two T2-dimers (Fig.1(left)), or two 5-1 units and a 5-2 unit (Fig.1(right); compare this building unit with those in **BIK**, **CAS** and **NSI**; see also: **Alternative description**). The two-dimensional Periodic Building Unit (PerBU) is obtained when T19-units, related along *c* by a 2-fold screw axis parallel to *c* and related along *a* by a 2-fold screw axis parallel to *a*, are linked into into the *ac* layer shown in Figure 2. [Compare this PerBU with those in **EUO**, **NES** and **NON**]. When the D4Rs in **IWV** are replaced by single 4-rings the framework of **NES** is obtained.
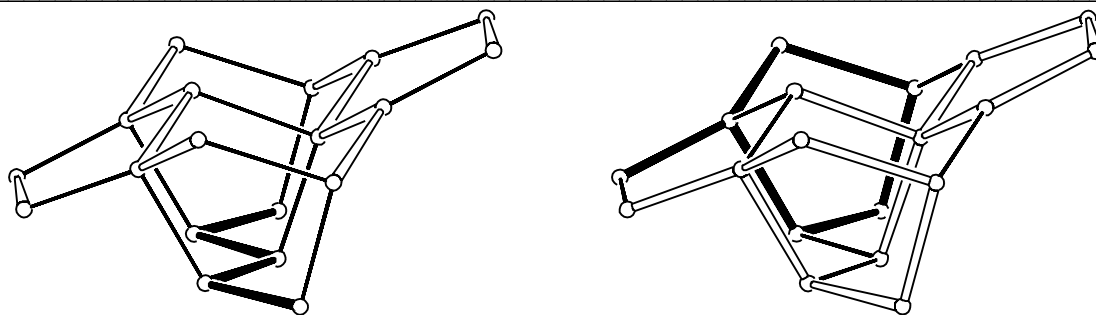

Figure 1. Finite building unit built from three (finite) zigzag chains (one in bold) and two T2-dimers (left) and finite building unit built from two 5-1 units (one in bold) and a 5-ring (right).
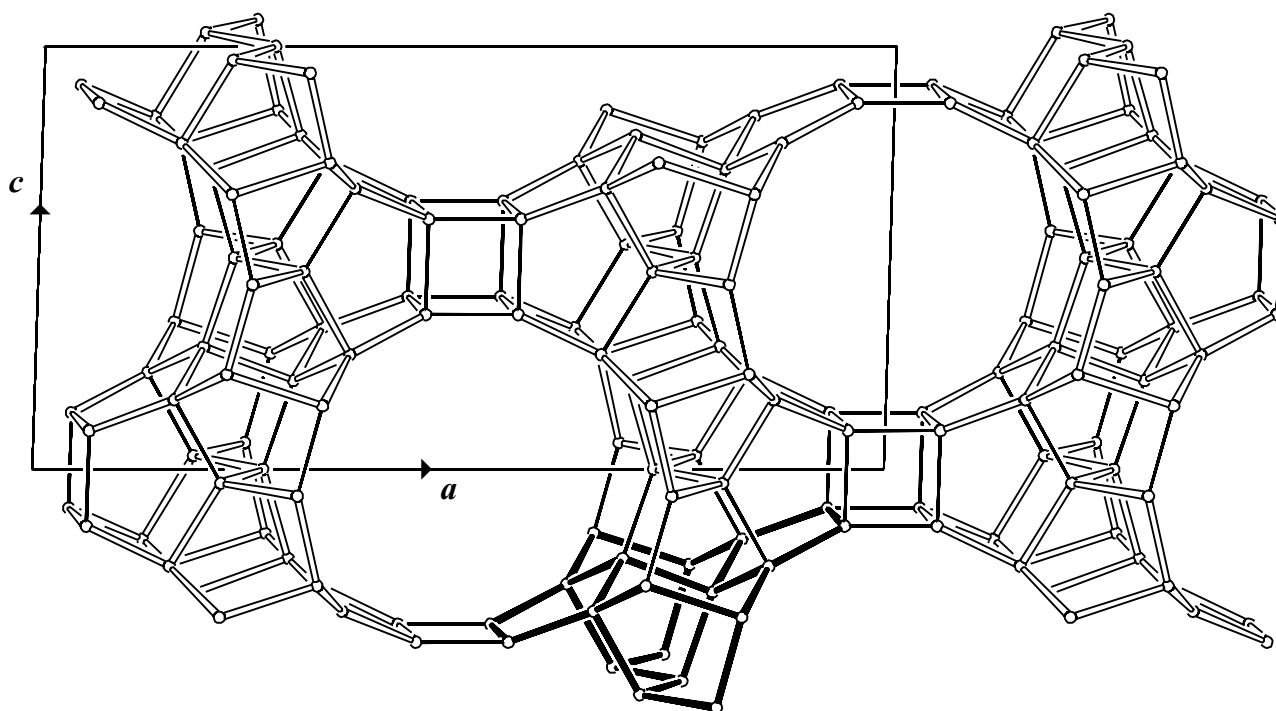

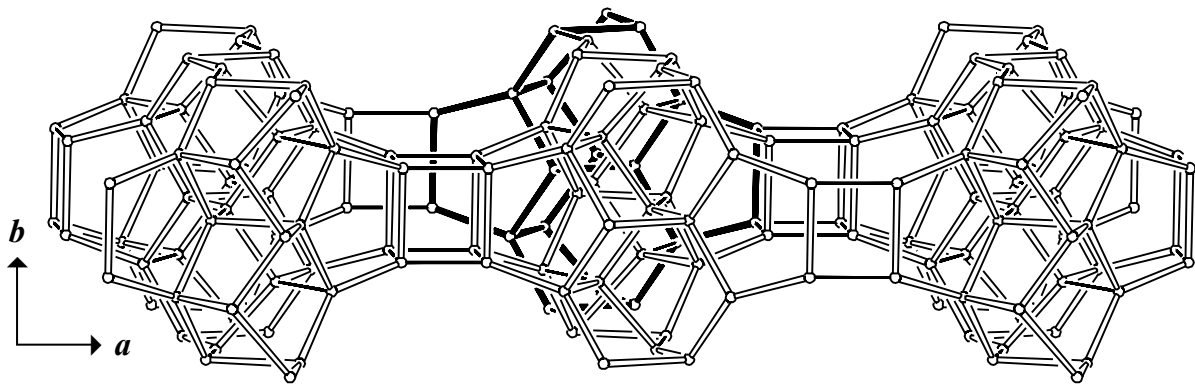Figure 2. PerBU in **IWV** viewed along *b* (one T19-unit in bold). [Fig. 2 is continued on next page]

Figure 2 [Cont'd]. PerBU viewed along *c*.   ▲

2. Connection mode:

Neighboring PerBUs, related by a shift of ½*a* (or ½*c*), are connected along *b* as shown in Figure 3.
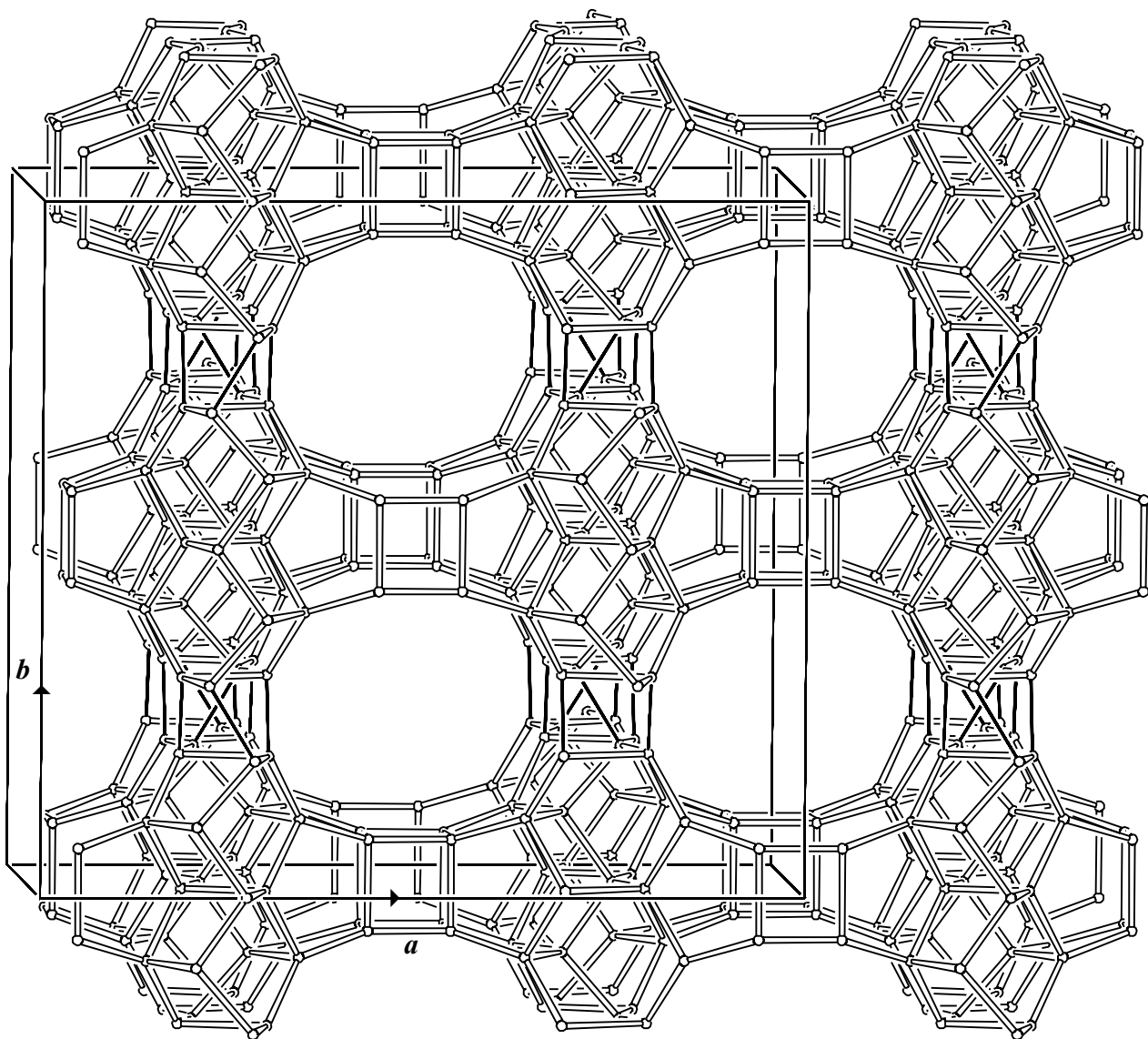

Figure 3. Connection mode (and unit cell content) in **IWV** viewed along *c*.
[Figure 3 is continued on next page]   ▲

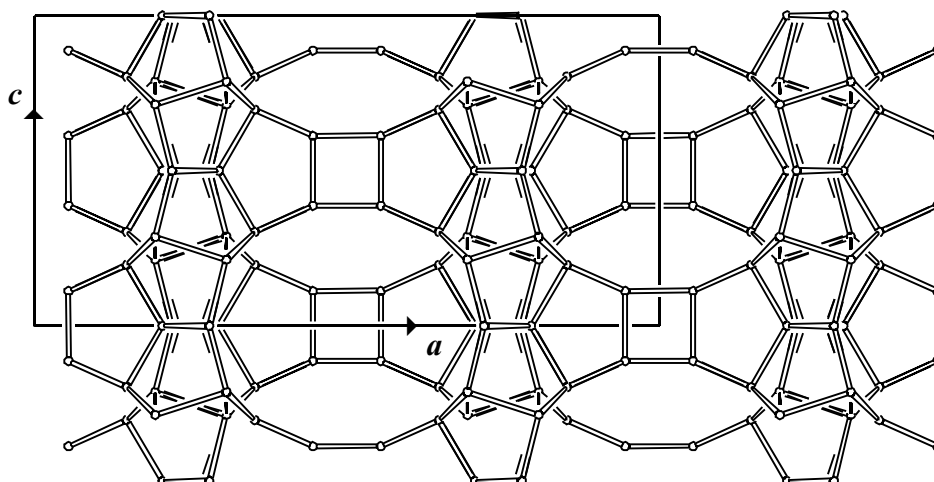## 3. Projections of the unit cell content:

Figure 3 [Cont'd]. Unit cell content projected along **b**.

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4. Channels and/or cages:

The double-cavity is depicted in Figure 4. The **pore descriptor** is added. The two sets of 12-ring windows within the double cavity are interconnected through 14-rings in the double-cavity. Double-cavities are connected along **c** through common 12-rings into 12-ring channels parallel to **c** as illustrated in Figure 5 on next page.

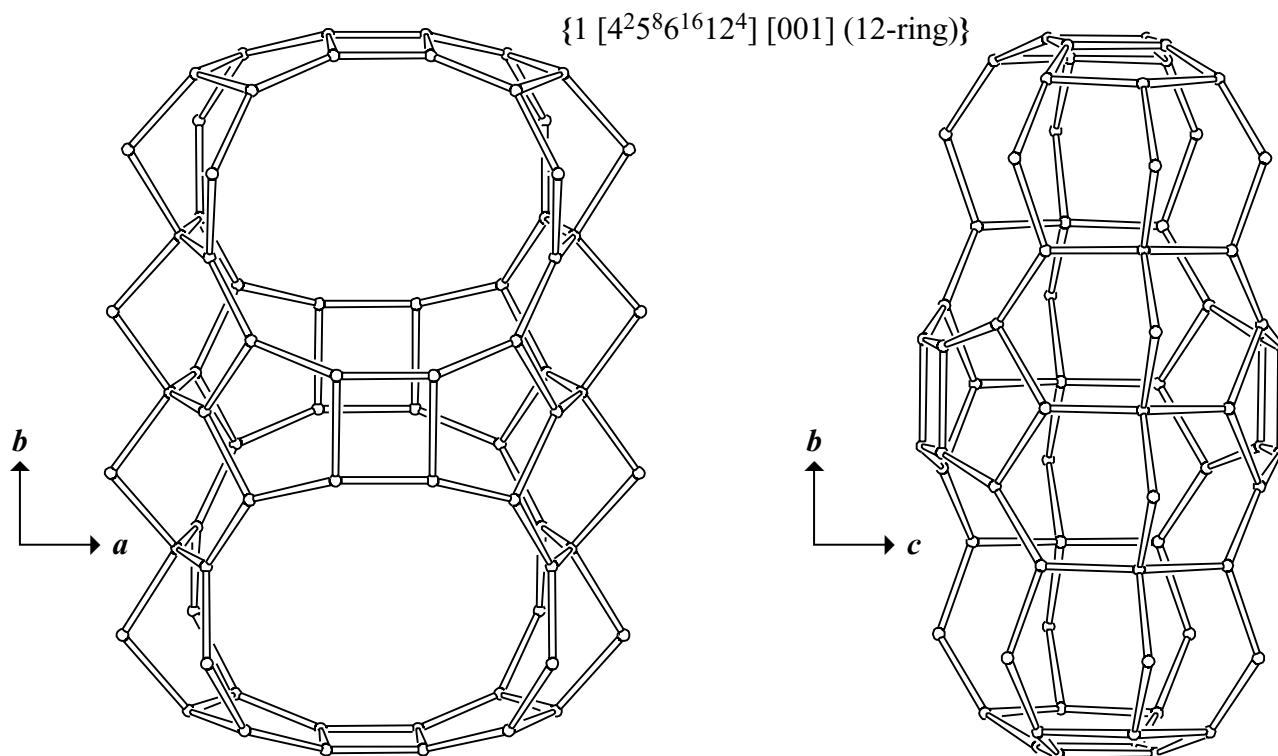$$\{1\ [4^2 5^8 6^{16} 12^4]\ [001]\ (12\text{-ring})\}$$

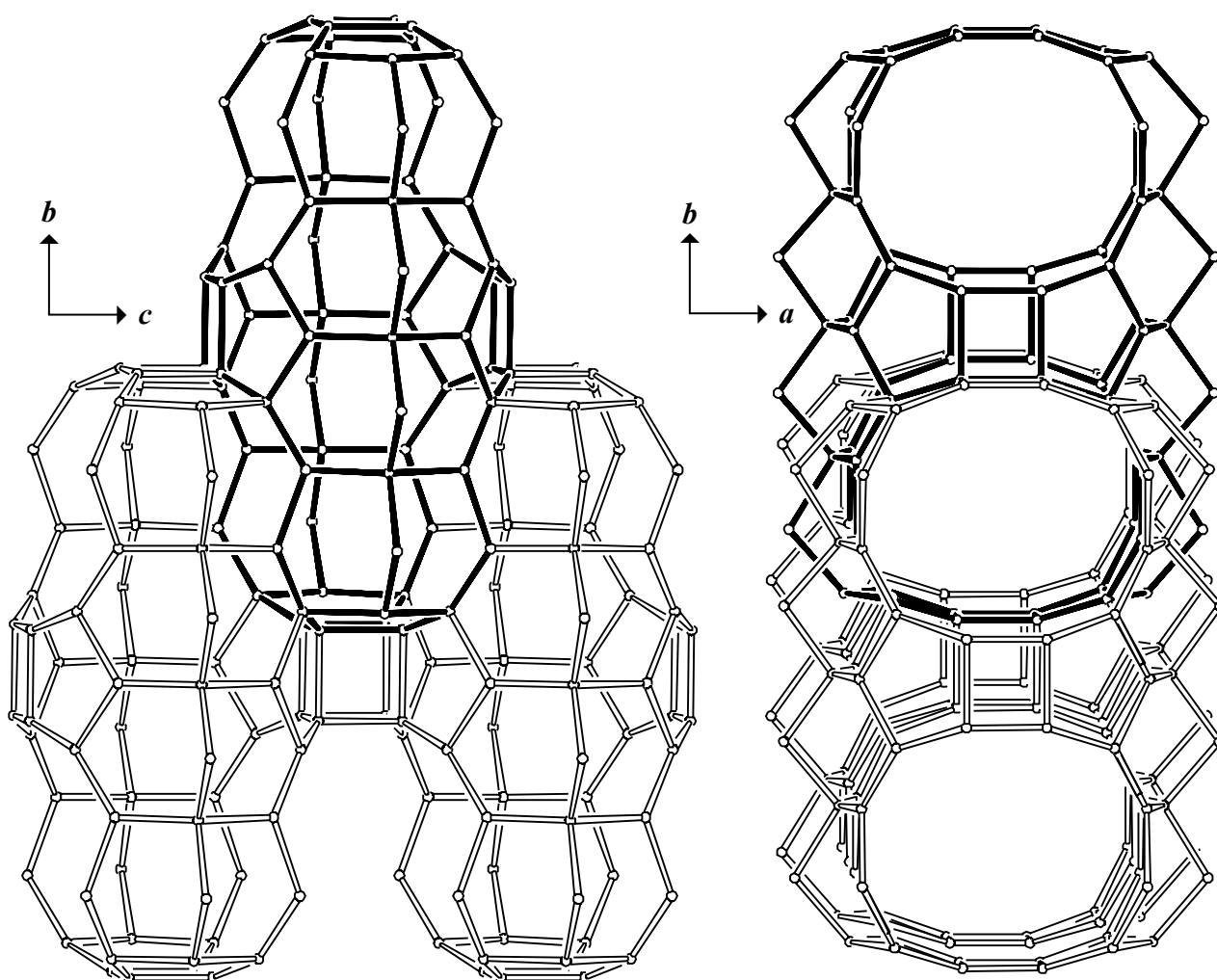Figure 4. Double-cavity viewed along **c** (left) and along **a** (right).

Figure 5. Cavities are linked into interconnecting 12-ring channels parallel *c*. Pairs of 12-ring channels are interconnecting along *b* through 14-rings in the cavity. View along *a* (left) and along *c* (right).

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5. Supplementary information:

Other framework types containing zigzag chains

In several framework types at least one of the unit cell dimensions is about n*5.2 Å (where n = 1, 2, 3, etc.). In many cases this indicates the presence of zigzag chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Zigzag chains**). 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 1**).

Alternative description using (modified) 5-rings

Several framework types, like **NES**, can be constructed using (modified) 5-rings.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **5-Rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).

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