# **Building scheme for NES**



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:**

**NES** can be built using building units composed of 17 T atoms: three finite zigzag chains (5 T atoms each and parallel to *a*) and a T2-dimer (Figure 1(left)), or two 5-1 units and a 5-ring (Figure 1(right)) [See: Alternative description; Compare this building unit with those in **BIK**, **CAS** and **NSI**]. The two-dimensional Periodic Building Unit (PerBU) is obtained when T17-units, related along *b* by a 2-fold screw axis parallel to *b* and related along *c* by a 2-fold axis parallel to *a*, are connected into the *bc* layer shown in Figure 2. [Compare this PerBU with those in **EUO** and **NON**]

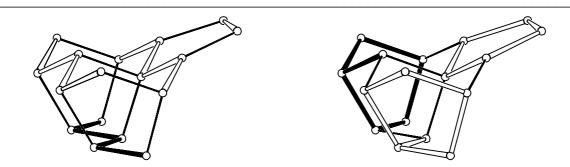


Figure 1. Finite building unit, viewed along *a*, built from three (finite) zigzag chains (one in bold) and a T2 dimer (left) and finite building unit built from two 5-1 units (one in bold) and a 5-ring (right).

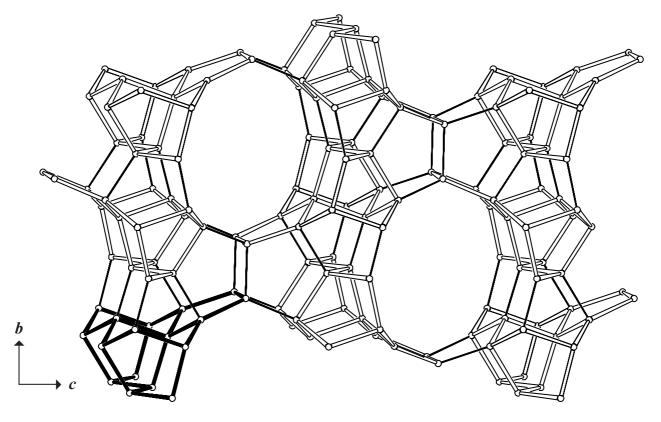
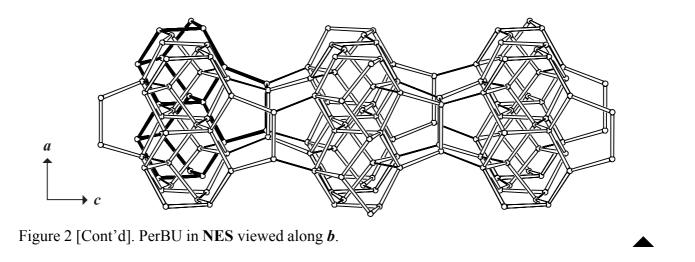


Figure 2. PerBU in NES viewed along *a* (one T17-unit in bold. [Figure 2 is continued on next page]



# 2. Connection mode:

Neighboring PerBUs, related by a shift of  $\frac{1}{2}c$  (or  $\frac{1}{2}b$ ), are connected along *a* as shown in Figure 3.

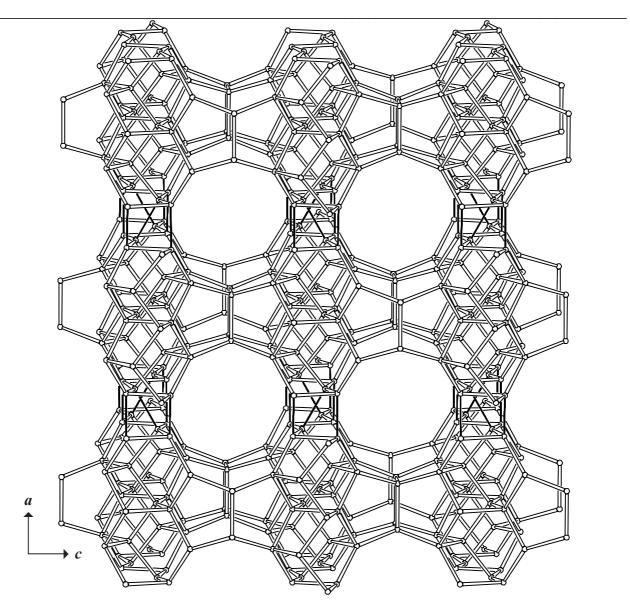


Figure 3. Connection mode in **NES** viewed along *b*.

# 3. Projections of the unit cell content:

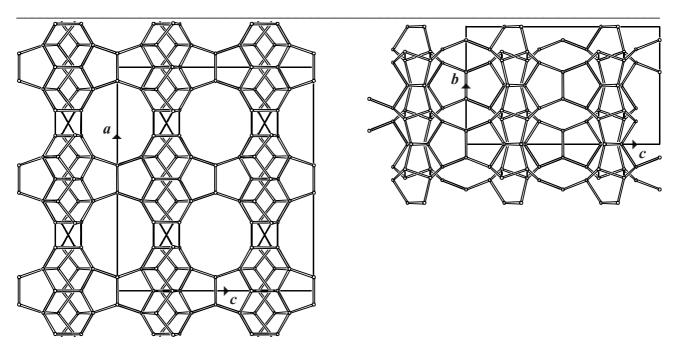


Figure 4. Unit cell content in NES projected along *b* (left) and along *a* (right).

## 4. Channels and/or cages:

The double-cavity in **NES** is depicted in Figure 5. The **pore descriptor** is added. Fused double-cavities form 10-ring channels parallel to **b** as illustrated in Figure 6. The 10-ring channels are interconnected through 12-rings in the double-cavity.

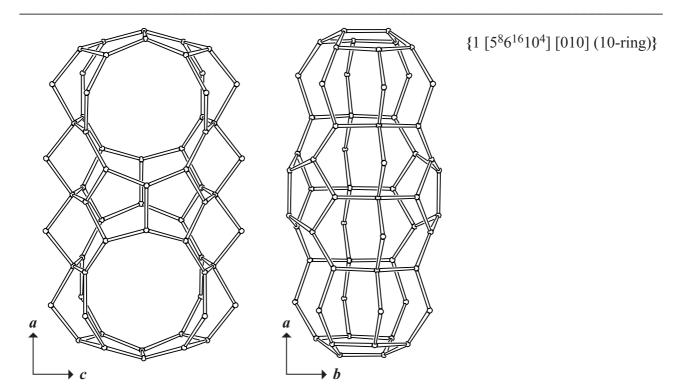


Figure 5. Double-cavity viewed along b (left) and along c (right). The two sets of 10-ring windows are interconnected through 12-rings in the double-cavity.

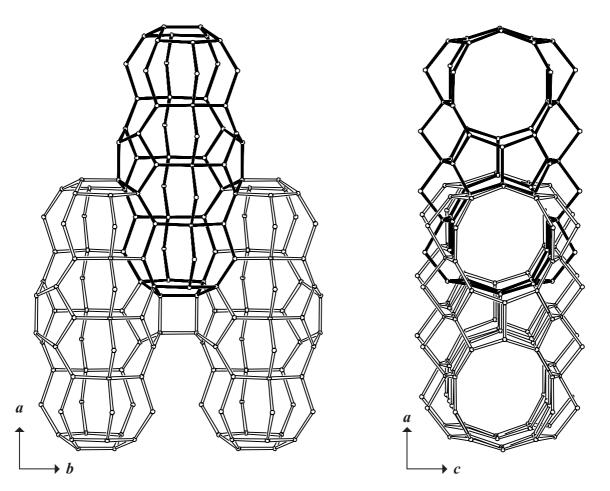


Figure 6. Fused double-cavities, viewed along c (left) and along b (right), form interconnected 10-ring channels along b.

## 5. Supplementary information:

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**).