

# Building scheme for NPO



1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
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## 1. Periodic Building Unit:

NPO can be built using the zigzag chain (bold in Fig.1 (left)) running parallel to  $c$ . The repeat distance along the zigzag chain is about 5.2 Å. The repeat unit consists of 2 T atoms. The one-dimensional Periodic Building Unit (PerBU) is obtained when three zigzag chains are connected into a pore with side-pockets and a 3-ring window. The repeat unit of the PerBU is composed of 6 T atoms (bold in Fig.1 (right)). The pore wall consists of fused 6-rings. Alternatively, another building unit can be constructed from two single connected 3-rings (see Fig. 2 and [Alternative description](#))

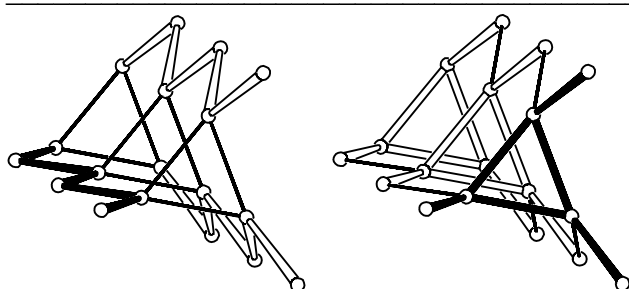


Figure 1. Perspective view of the PerBU in NPO along the chain axis  $c$ . PerBU constructed from three zigzag chains (left) and PerBU constructed from (T6) repeat units consisting of a 3-ring with three additional single T atoms (right).



## 2. Connection mode:

Neighboring PerBUs, related by pure translations along  $a$ , and along  $(a + b)$ , are connected into the three-dimensional framework type as illustrated in Figure 2.

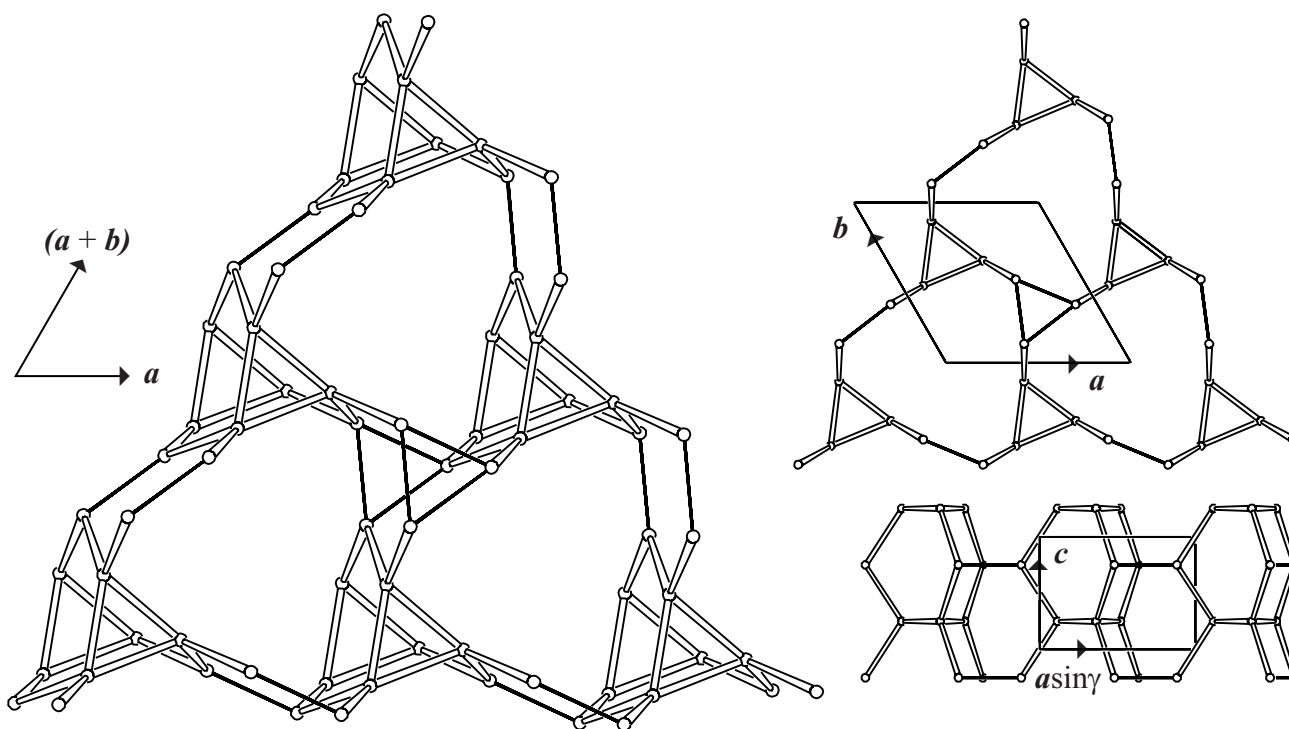


Figure 2. Connection mode viewed along  $c$  (left) and projection of the unit-cell content along  $c$  and along  $b$  (right). Only two repeat units of the PerBUs are drawn for clarity.



3. Projections of the unit cell content: See Figure 2. ▲

#### 4. Channels and/or cages:

The one-dimensional channel, shown in Figure 3 together with its **pore descriptor**, has a 12-ring window and is parallel to *c*. The channel is topologically equivalent to the PerBU in **ATO** and **CAN**. The pore wall consists of fused 6-rings only. The framework consists of fused 12-ring channels.

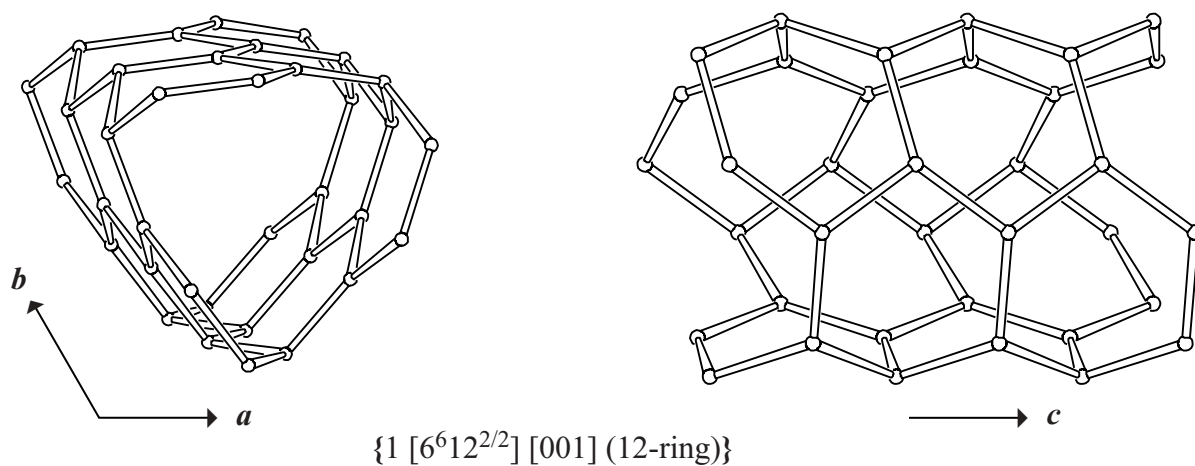


Figure 3. Channel in **NPO** in perspective view along *c* (left) and perpendicular to *c* (right). ▲

#### 5. Supplementary information:

##### ***Other framework types containing zigzag chains***

In several framework types at least one of the unit cell dimensions is about  $n \cdot 5.2 \text{ \AA}$  (where  $n = 1, 2, 3, \text{ etc.}$ ). 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 of NPO using (modified) single 3- and/or 4-rings***

Several framework types, like **NPO**, can be built using (modified) single 3- and/or 4-rings.

In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) single 3- and/or 4-rings (choose: **Single 3- and/or 4-rings**). 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 4**). ▲