1. Periodic Building Unit (PerBU):

Trigonal DDR belongs to the clathrasil family and can be built using the 12-ring double cups, shown in Figure 1. The 12-ring double cups consist of 30 T atoms. T30-units are connected into a hexagonal layer. The "empty" spaces between the T30-units are filled with T2-dimers. The connection of T30-units through the dimers generates [5^{12}]-cages in the layer. The layer reveals two types of nest-like recesses: site A with the 6-ring and site B (and site C) where [5^{12}]-cages share faces. This layer is equal to the PerBU in DOH and MTN. The two-dimensional PerBU in DDR is obtained when 6-rings from an additional 6-ring layer (bold in Figure 2) are stacked on top of the C sites. This stacking generates (small) [4^{5566}]-cages. [Compare this PerBU with the PerBU in MEP]

Figure 1. T30-unit in the clathrasil family viewed perpendicular to c and approximately along the (hexagonal) [110] direction (left) and along the cup-axis c (right). Two "zigzag" 12-rings are connected through a common 6-ring to form two half cages or a 12-ring double cup.

Figure 2. Hexagonal PerBU in DDR viewed along the cup-axis c (left) and along b (top right). Connections to the space filling dimers (in heavy bold) are dashed. The additional 6-ring layer is also in bold. The in-set shows the [5^{12}]- and [4^{5566}]-cages. The repeat unit of the PerBU consists of 40 T atoms: the T30-unit, a 6-ring and two dimers.
2. Connection mode:

Neighboring PerBUs can be connected through O-bridges along $+c$ in three different ways: 

1. the second PerBU is shifted by $+(2/3a + 1/3b)$ before connecting it to the first PerBU. The T30-units in the second PerBU are centered at $(2/3, 1/3)$. This position is usually denoted as the $B$ position as illustrated in Figure 2. The same connection mode can be repeated: a third PerBU is shifted with respect to the second layer by (again) $+(2/3a + 1/3b)$. The T30-units are now centered at $(4/3, 2/3)$ [or, equivalently, at $(1/3, 2/3)$]. This position is called the $C$ position. Adding a fourth layer with the same connection mode gives a shift with respect to the first layer of $(2a + b)$ [or zero, i.e. the $A$ position]. The resulting stacking sequences, exhibiting the same connection mode, are denoted as $AB$, $BC$ and $CA$, respectively, in analogy to stacking of dense packed spheres. The connection mode is illustrated in Figure 3(a).

2. the second and third PerBUs are shifted by $-(2/3a + 1/3b)$ before connecting them along $+c$ to the previous PerBU. The resulting stacking sequences $AC$, $CB$ and $BA$, with the same connection mode are obtained. The connection mode is illustrated in Figure 3(b).

3. the second PerBU has a zero lateral shift along $a$ and $b$. This connection mode leads to an $AA$, $BB$ or $CC$ stacking sequence depending on whether the added PerBU is connected to a PerBU with T30-units in the $A$, $B$ or $C$ position, respectively. The connection mode is illustrated in Figure 3(c).

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Figure 3. (a): Connection mode (1) ($AB$, $BC$ or $CA$ connection mode) viewed approximately along [110] (left). In the perspective drawing only one set of $A$, $B$ and $C$ positions in each (shifted) PerBU is given in order to illustrate the new inter-layer cages formed. The projection along $b$ (bottom right) shows the connection mode between complete PerBUs. (Parts of) the additional 6-rings are in bold. The inter-layer cages are shown at the top right. [Figure 3 is continued on next page]
Figure 3 [Cont’d]. (b): Mode (2) (AC, CB or BA connection mode) and (c): mode (3) (AA, BB or CC connection mode) viewed approximately along [110] (left). In these drawings only one set of A, B and C positions in each (shifted) PerBU is given in order to illustrate the new inter-layer cages formed. The projection along b (bottom right) shows the connection mode between complete PerBUs. (Parts of) the additional 6-rings are in bold. The inter-layer cages are shown at the top right.
In DDR only connection mode (1) is observed.

3. Projections of the unit cell content: See Figure 4.

![Figure 4. Unit cell content in DDR viewed along [110] (left), along b (middle) and along c (right). In the perspective drawing (left) each PerBU is represented by one T30-unit. (Parts of) the additional 6-rings are in bold. The stacking sequence is given in italics. The italic letters give the position of the T30-unit relative to the A position in the first PerBU.](image)

4. Channels and/or cages:

The [5^{12}]-cage and [4^{15}\times6^{1}]-cage in the PerBU are shown in Figure 1. The two new types of inter-layer cages in DDR are depicted in Figure 3(a). The pore descriptor is added. DDR can be considered as link between zeolites and clathrasils because it possesses zeolitic properties through a two-dimensional pore system along <100> with 8-ring windows.

5. Supplementary information:

Other framework types containing a layer of (modified) T30-units

Three other framework types can be constructed using the (modified) PerBU described in Section 1. They belong to the clathrasil family.

In the INTRO pages links are given to detailed descriptions of these framework types (choose: Clathrasils). 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 10).