*-ITN

1. The Periodic Building Unit (PBU)

The structure of *- ITN is built from the layer shown in Figure 1 (a, b) which is built up by the building unit shown in (c and d).

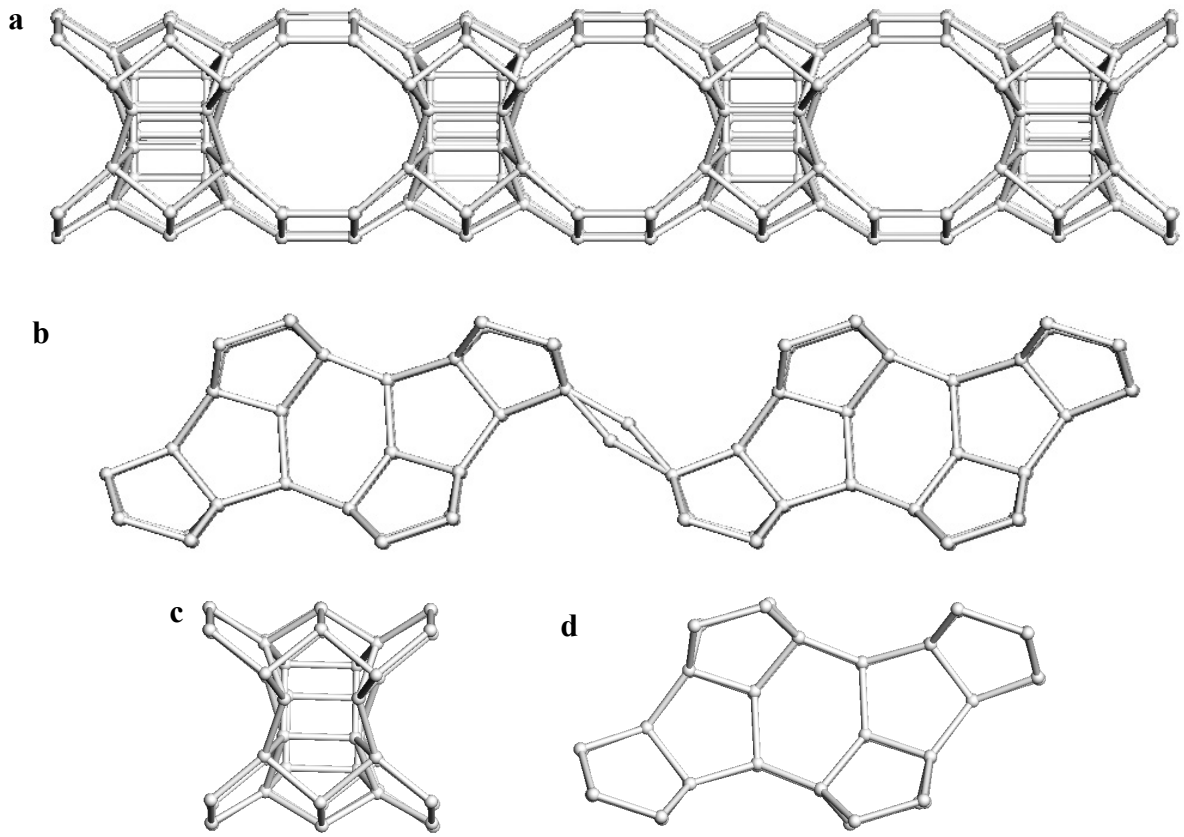

Figure 1. The periodic building unit (PBU) building up the structure of *-ITN is the layer Viewed along (a) [100] and (b) [010]. The PBU is a layer extending along the ***a*** and ***b*** directions. The layer is built from the building unit shown in (c) along [100] and (d) along [010].

2. Type of faulting:

Two basic types of disorder is present in the *-ITN structure, 1-dimensional stacking disorder of the PBU's along [001] and twinning.

3. Connectivity patterns of the PBUs

The structure of *-ITN allows two types of disorders, stacking disorder and twinning. The two can occur independent from each other.

a) Stacking disorder viewed [100]

Neighboring PBUs can be connected along [001] with three different translations along ***a***.

a) The lateral translation of the top layer is 0 ***b*** with respect to the previous layer.
b) The lateral translation of the top layer is 1/3 ***b*** with respect to the previous layer.
c) The lateral translation of the top layer is -1/3 ***b*** with respect to the previous layer.

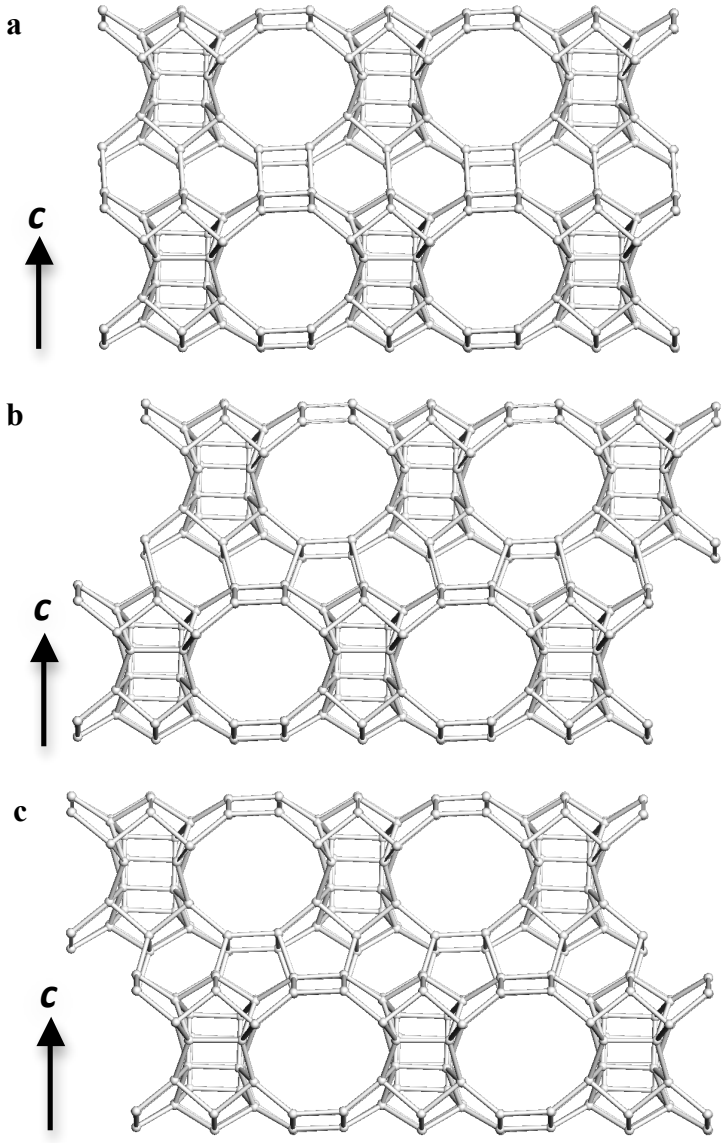

Figure 2. Connectivity of neighboring PBUs along [001] has three possibilities, via 6-6-4 – ring sequence (a) and 6-5-5 – ring sequence (b and c), respectively. View along [100]

b) Twinning in the projection along [010]

The PBU of *-ITN allows a geometrically feasible connectivity along [001] also after the PBU is mirrored perpendicular to [100]. This gives rise to twinning in the structure.

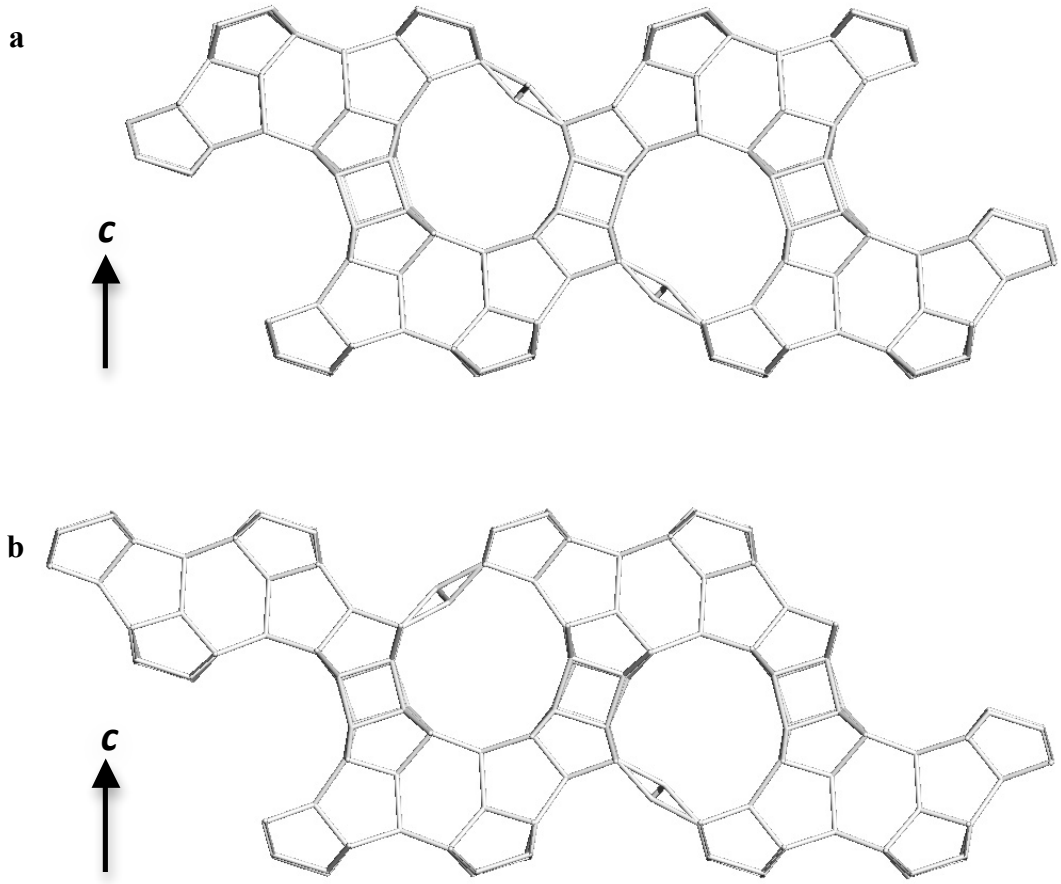

Figure 3. The bottom layer is identical in (a) and (b), the top layer in (b) is mirrored perpendicular to [100]. They PBU can still be connected along [001] with good geometry. View along [010].

4. Ordered end-members

The simplest ordered end-members in the *-ITN family are given below in Table 1 and in Figure 3. Polymorph A is built from alternating translations of +1/3***b*** and -1/3***b***. None of them has been observed yet as ordered material.

Table 1. Stacking sequences of PBU for the simplest ordered end-members in the *-ITN family.

Polymorph	Lateral shifts between subsequent PBU stacked along [001]; Shifts are given in fractions of ***b***	Space group
A	(+1/3); (-1/3); (+1/3);…	*P*2/*c*
B	(+1/3); (+1/3);… or (-1/3); (-1/3);…	*P*-1
C	(0); (0);…	*P*2/*m*

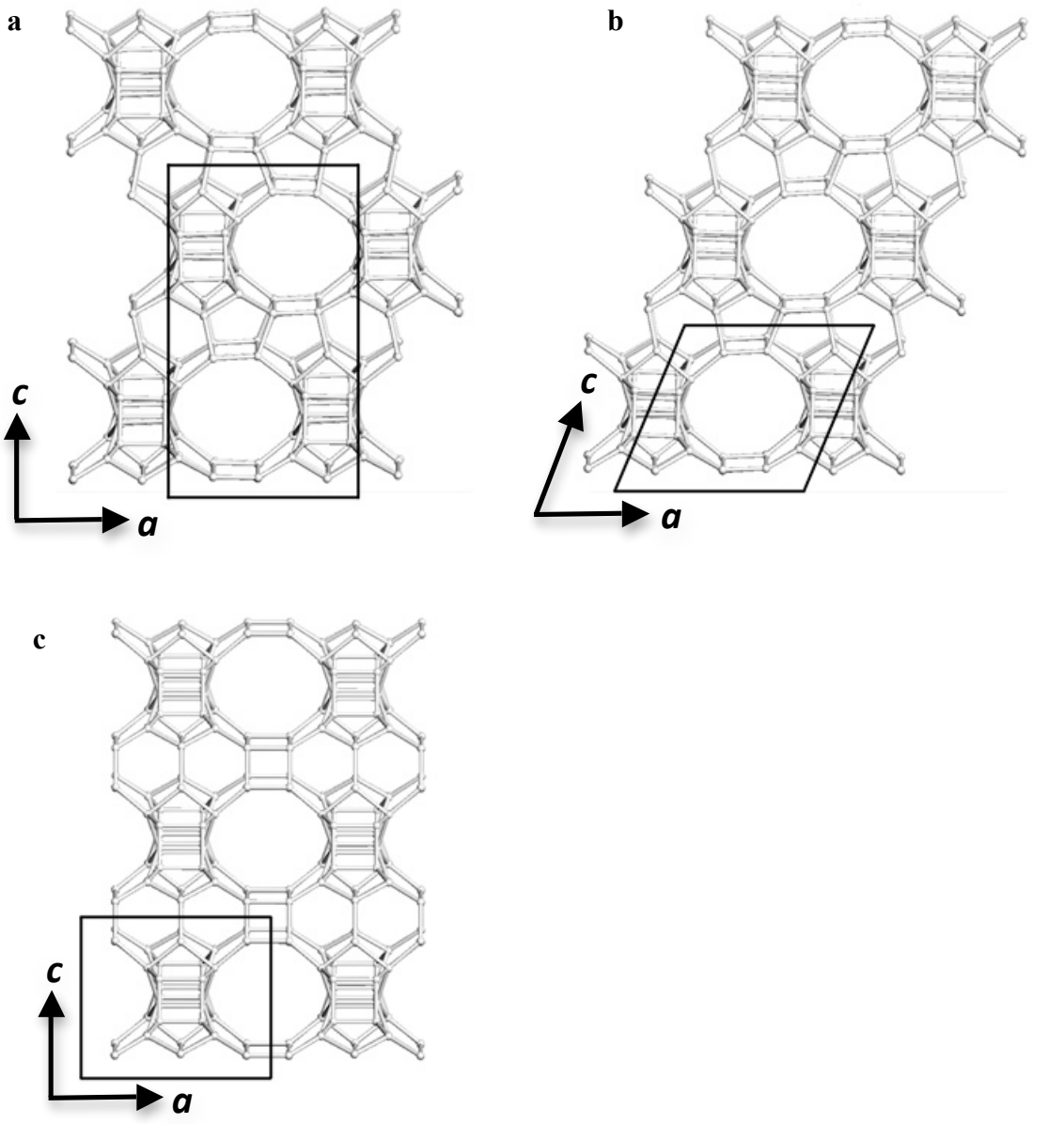

Figure 4. The structures of the three ordered polymorphs A (a), B (b) and C (c), described in the Table 1 viewed along [100].

5. Disordered materials with *-ITN structure synthesized so far:

Two materials have been synthesized so far with XRPD patterns consistent with the *-ITN structure: ITQ-39[1, 2, 3] and SSZ-83[4].

6. Supplementary Material

Simulation of XRPD patterns for *-ITN family. The simulations below shows the intergrowth between polymorph A and polymorph B as described in Table 1. The content of polymorph C as well as the effects of small twin domains are not considered in these simulations.

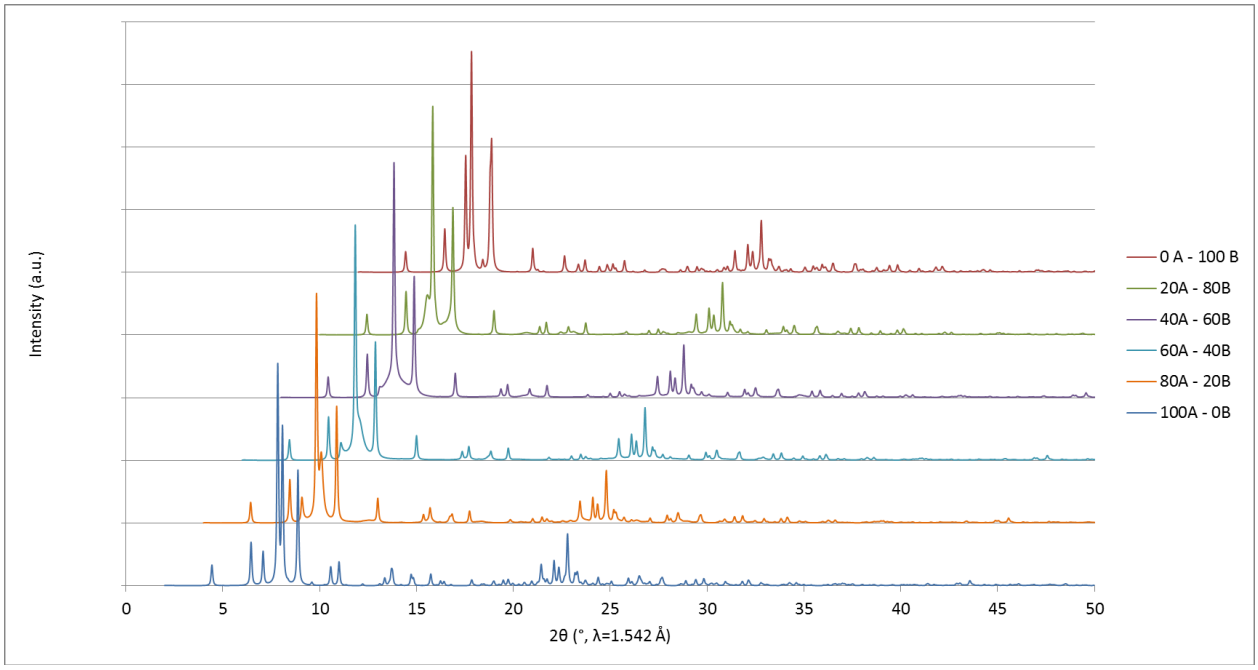

Figure 5. Simulated XRPD patterns with the intensity (a.u.) versus diffraction angle (2θ) of the intergrowth between polymorph A and polymorph B of the *-ITN family in steps of 20% intergrowth. The simulations were performed with the software DIFFaX[5].

7. References

1. Willhammar, Tom; Sun, Junliang; Wan, Wei; Oleynikov, Peter; Zhang, Daliang; Zou, Xiaodong; Moliner, Manuel; Gonzalez, Jorge; Martinez, Cristina; Rey, Fernando; Corma, Avelino Nature Chemistry 4, 188-194 2012

2. Moliner, Manuel; Gonzalez, Jorge; Portilla, M. Teresa; Willhammar, Tom; Rey, Fernando; Llopis, Francisco J.; Zou, Xiaodong; Corma, Avelino Journal of the American Chemical Society (2011), 133, 9497-9505.

3. Corma Canos, Avelino; Moliner Marin, Manuel; Rey Garcia, Fernando; Gonzalez Gonzalez, Jorge PCT Int. Appl. (2008), WO 2008092984 A1 20080807.

4. Burton, Allen W., Jr.; Zones, Stacey I. U.S. Pat. Appl. Publ. (2009), US 20090104112 A1 20090423.

5. M. M. J. Treacy, J. M. Newsam & M. W. Deem “A General Recursion Method for Calculating Diffracted Intensities From Crystals Containing Planar Faults”
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