**-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 $\mathbf{a}$.

a) The lateral translation of the top layer is $0\ \mathbf{b}$ with respect to the previous layer.

b) The lateral translation of the top layer is $1/3\ \mathbf{b}$ with respect to the previous layer.

c) The lateral translation of the top layer is $-1/3\ \mathbf{b}$ 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.

![Diagram](image.png)

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.

<table>
<thead>
<tr>
<th>Polymorph</th>
<th>Lateral shifts between subsequent PBU stacked along [001]; Shifts are given in fractions of b</th>
<th>Space group</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>(+1/3); (-1/3); (+1/3);…</td>
<td>P2/c</td>
</tr>
<tr>
<td>B</td>
<td>(+1/3); (+1/3);… or (-1/3); (-1/3);…</td>
<td>P-1</td>
</tr>
<tr>
<td>C</td>
<td>(0); (0);…</td>
<td>P2/m</td>
</tr>
</tbody>
</table>

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.

![Simulated XRPD patterns](image)

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.
