The ABC-6 Family

1. The periodic building unit (PerBU) equals the layer shown in Figure 1:

![Diagram of PerBU](image)

Figure 1: The PerBU is an arrangement of single T6-rings in the \(ab\)-plane of a hexagonal unit cell. In (a) a single layer, and in (b) a projection of a 3-layer stacking sequence ABC is shown.

The PerBU in the ABC-6 family of framework types consists of a hexagonal array of non-connected planar T6-rings (depicted in Fig. 1a in bold), which are related by pure translations along \(a\) and \(b\). The T6-rings are centered at \((0,0)\) in the \(ab\) layer. This position is usually called the A position (Fig. 1b).

2. Type of faulting: 1-dimensional stacking disorder of the PerBU’s along [001].

3. The plane space group of the PerBU is P (6) m m.
4. Connectivity pattern of the PerBU:

Neighbouring PerBU’s can be connected through tilted 4-rings along +[001] in three different ways:

(a): the second layer is shifted by \((2/3a + 1/3b)\) before connecting it to the first layer; so the T6-rings in the second layer are centered at \((2/3, 1/3)\). This position is usually denoted as the B position (Fig. 1b). The same connection mode can be repeated to generate a third PerBU shifted with respect to the second layer by (again) \((2/3a + 1/3b)\). The T6-rings are now centered at \((4/3, 2/3)\) [or, equivalently, at \((1/3, 2/3)\)]. This position is called the C position (See Fig. 1b). 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 again]. The resulting stacking sequences, exhibiting the same connection mode, are denoted as AB, BC and CA, respectively. The connection mode is illustrated in Fig. 2a viewed down [001] (left), nearly along [010] (top right), and along [010] (bottom right).

(b): the second and third layers are shifted by \(-(2/3a + 1/3b)\) before connecting them along +[001] to the previous layer to give stacking sequences AC, CB and BA. The connection modes are the same and illustrated in Fig. 2b.

(c): the second layer 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 layer is connected to a layer with T6-rings in the A, B or C position, respectively. The connection mode is shown in Fig. 2c.
Once the stacking sequence along [001] is known, the 3-dimensional framework is defined.

Examples of faulted frameworks in the ABC-6 family of zeolites:

5. The simplest ordered end-members in the ABC-6 family:

<table>
<thead>
<tr>
<th>Name</th>
<th>Code</th>
<th>#Repeat layers</th>
<th>Stacking sequence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancrinite (1)</td>
<td>CAN</td>
<td>2</td>
<td>AB(A)........</td>
</tr>
<tr>
<td>Sodalite (2)</td>
<td>SOD</td>
<td>3</td>
<td>ABC(A)......</td>
</tr>
<tr>
<td>Losod (3)</td>
<td>LOS</td>
<td>4</td>
<td>ABAC(A).........</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>cont’d on next page</td>
</tr>
</tbody>
</table>
Examples of ordered end-members in the ABC-6 family are presented in Figure 4 in the same sequence as in the Table above.

<table>
<thead>
<tr>
<th>Name</th>
<th>Code</th>
<th>#Repeat layers</th>
<th>Stacking sequence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liottite (4)</td>
<td>LIO</td>
<td>6</td>
<td>ABACAC(A)........</td>
</tr>
<tr>
<td>Afganite(5)</td>
<td>AFG</td>
<td>8</td>
<td>ABABACAC(A)........</td>
</tr>
<tr>
<td>Franzinite (6)</td>
<td>FRA</td>
<td>11</td>
<td>ABCABACABC(A)........</td>
</tr>
<tr>
<td>Offretite (7)</td>
<td>OFF</td>
<td>3</td>
<td>AAB(A)........</td>
</tr>
<tr>
<td>Erionite (8)</td>
<td>ERI</td>
<td>6</td>
<td>AABAAC(A)........</td>
</tr>
<tr>
<td>TMA-E(AB)(9)</td>
<td>EAB</td>
<td>6</td>
<td>AABCCB(A)........</td>
</tr>
<tr>
<td>Levyne (10)</td>
<td>LEV</td>
<td>9</td>
<td>AABCCABBC(A)........</td>
</tr>
<tr>
<td>STA-2 (11)</td>
<td>SAT</td>
<td>12</td>
<td>AABABBCBCCAC(A).......</td>
</tr>
<tr>
<td>Gmelinite (12)</td>
<td>GME</td>
<td>4</td>
<td>AABB(A)........</td>
</tr>
<tr>
<td>Chabazite (13)</td>
<td>CHA</td>
<td>6</td>
<td>AABBC(A)........</td>
</tr>
<tr>
<td>SAPO-56 (14)</td>
<td>AFX</td>
<td>8</td>
<td>AABBCCBB(A)........</td>
</tr>
<tr>
<td>AlPO-52 (15)</td>
<td>AFT</td>
<td>12</td>
<td>AABBCBBAACC(A).......</td>
</tr>
</tbody>
</table>

Figure 4: Perspective drawing (left) and parallel projection along [010] of the unit cell content (right) of periodic end-members in the ABC-6 family. The hexagonal c axis points towards the top of the page and the horizontal axis is equal to acos30 as indicated for CAN. (Fig.4 is cont’d on next page)
Figure 4 (Continued): For legend: See previous page. (Fig. 4 is continued on next page)
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6. Disordered materials synthesized and characterized to date:
Linde T (ERI/OFF) (16); Babelite (random stacking) (17); Linde D (disordered CHA) (18); Phi (disordered CHA) (19); ZK-14 (disordered CHA) (20); LZ-276 (disordered CHA) (21); LZ-277 (disordered CHA) (21).

7. Supplementary material
Since the ABC-6 family contains 15 ordered end-members simulations of powder patterns for stacking disorder of only the most common framework types are given.

Figure 5: Simulated powder pattern of the Gmelinite/Chabazite series. In this example, the stacking of the PerBU’s in AABB- and AABBCCC-sequences is disordered.
Figure 6: Intensity ($I$, a.u.) of simulated powder patterns versus diffraction angle ($2\theta$) of the ERI-OFF series in steps of 10% intergrowth. The stacking sequences of ERI and OFF are disordered. The 0% ERI pattern corresponds to the 100% OFF pattern.
8. References


(2) a) L. Pauling, Z. Kristallogr. 74, 213 (1930).


