1. **The Periodic Building Unit (PerBU)** is the layer shown in Figure 1 (a - c):

![Figure 1: Top view (a), and side views (b) and (c) of the PerBU of the lovdarite family of framework types](image)

The PerBU in the lovdarite family of structures is composed of T9 units (two 4-rings connected through a single T atom; depicted in bold in Fig. 1a) related by pure translations along \( \mathbf{a} \) and \( \mathbf{b} \). Projections along \([001]\) (a), along \([100]\) (b) and along \([010]\) (c) are shown. The PerBU’s, depicted in Fig. 1b and 1c, in perspective view (left) and in parallel projection (right), are identical and related by a 90° rotation about the plane normal or by a mirror operation perpendicular to the plane normal.

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

3. **The plane space group** of the PerBU is \( P(\bar{4})m2 \)
4. Connectivity pattern of the PerBU:

Neighbouring PBU’s, related by a mirror operation (or by a 90° rotation about the plane normal), can be connected along [001] via O-bridges in two different ways:
(a): the lateral shift of the top layer along \( a \) or \( b \) is zero; denoted as (0, 0).
(b): the lateral shift of the top layer is \( \frac{1}{2}a \) or \( \frac{1}{2}b \); denoted as \( \frac{1}{2}, 0 \) or \( 0, \frac{1}{2} \), respectively.

![Figure 2: Connection modes in the lovdarite family. (a): connection mode (0, 0); The PerBU’s are connected through T4-T6-ring sequences; (b): connection mode \( \frac{1}{2}, 0 \) or \( 0, \frac{1}{2} \); The PerBU’s are connected through T5-ring sequences](image)

Once the distribution of the lateral shifts between the layers stacked along [001] is known, the 3-dimensional framework is defined.

5. The simplest ordered end-members in the lovdarite family are defined in Table 1 and shown in Figure 3. All three end-members have been observed as pure single crystal material (1,2,3).

Table 1: Stacking sequences of the PerBU’s for the simplest ordered end-members in the lovdarite family. The end-member number refers to the framework plots 1-3 on the next page.

<table>
<thead>
<tr>
<th>End-member</th>
<th>Lateral shifts between subsequent mirrored PerBU’s along [001]; shifts are in fractions of ((a, b))</th>
<th>Space Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>1(^1)</td>
<td>((0,0); (0,0); (0,0); \ldots)</td>
<td>(P_4_{2}/mmc)</td>
</tr>
<tr>
<td>2(^2)</td>
<td>((0,\frac{1}{2}); (\frac{1}{2},0); (0,\frac{1}{2}); (\frac{1}{2},0); (0,\frac{1}{2}); \ldots)</td>
<td>(I4_{1}/amd)</td>
</tr>
<tr>
<td>3(^3)</td>
<td>((0,0); (0,\frac{1}{2}); (0,0); (0,\frac{1}{2}); (0,0); \ldots)</td>
<td>(A2/m^4)</td>
</tr>
</tbody>
</table>

\(^1\) This is the end-member with framework type code LOV (1).
\(^2\) This is the end-member with framework type code VSV (2).
\(^3\) This is the end-member with framework type code RSN (3).
\(^4\) For comparison reasons the maximum topological symmetry of end-member number 3 has been transformed from \(C2/m\) to \(A2/m\).
Figure 3: Skeletal drawings of the three ordered end-members of the lovdarite family of structures. The $ac$ projections in LOV and VSV are equivalent to the their $bc$ projections, respectively. The lateral shifts between subsequent (mirror related) PerBU’s along [001] is given in the drawings in fractions of $(a, b)$. In LOV there are only T4-T6-ring sequences along $a$ and $b$. In VSV there are only T5-ring sequences along $a$ and $b$ and in RSN T5-ring sequences alternate with T4-T6-ring sequences.
6. Disordered materials synthesized and characterized to date:

No disordered materials known to date.

7. Supplementary material

Figure 4: Simulated powder pattern of the lovdarite materials containing T5- and T4-T6-ring sequences between neighbouring PerBU’s. The number indicates the fraction of T5-ring sequences in the material

8. References

