

The Lovdarite Family

1. The Periodic Building Unit (PerBU) - 2. Type of Faulting - 3. The Layer Symmetry
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1. The Periodic Building Unit (PerBU) is the layer shown in Figure 1 (a - c):

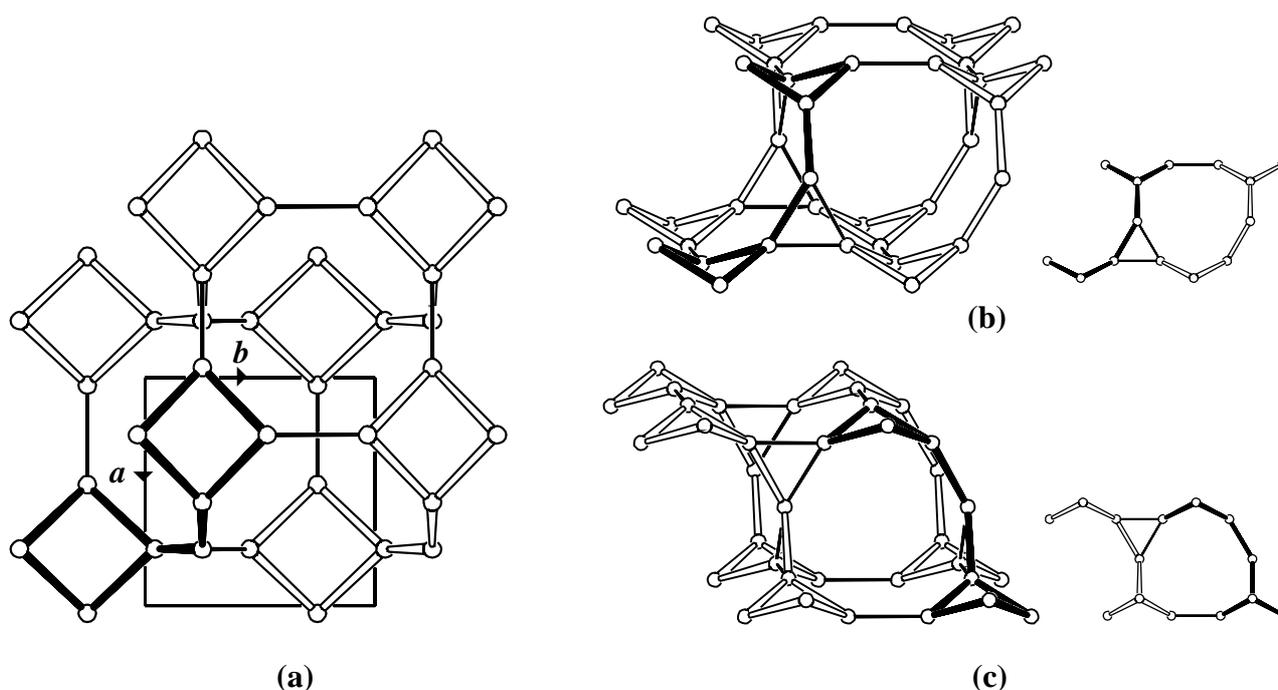


Figure 1: Top view (a), and side views (b) and (c) of the PerBU of the lovdarite family of framework types

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 a and 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.

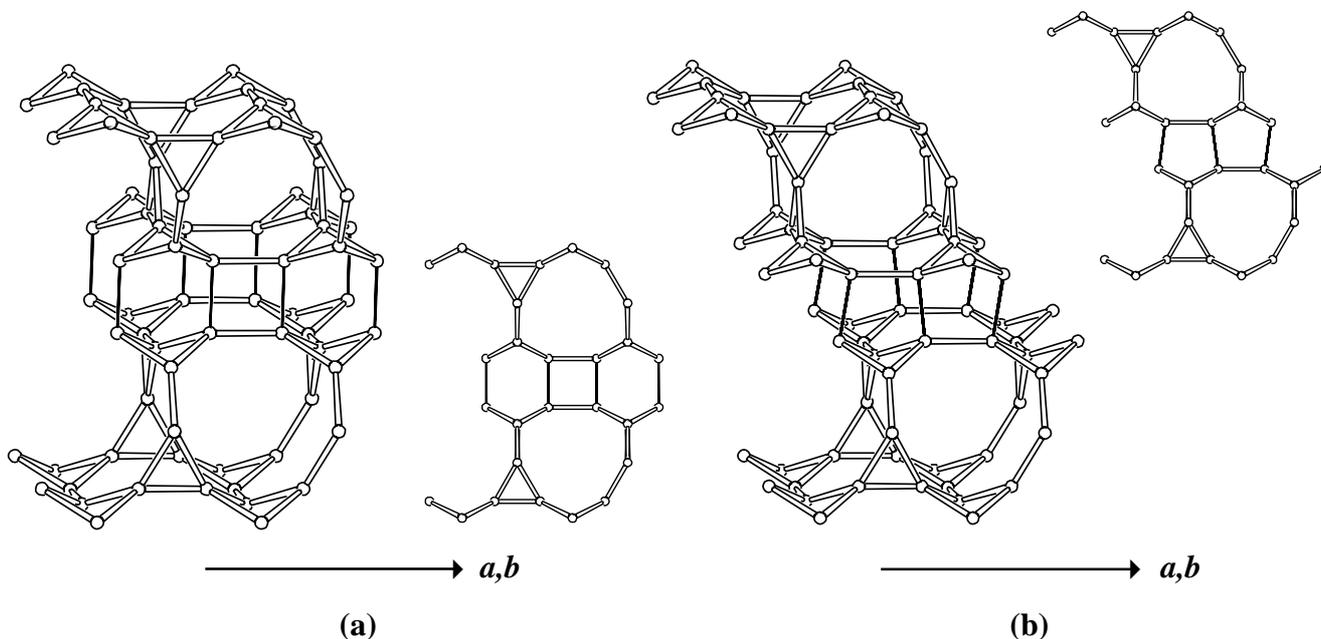


Figure 2: Connection modes in the lovdarite family. (a): connection mode $(0, 0)$; The PerBU's are connected through T4-T6-ring sequences; (b): connection mode $(\frac{1}{2}, 0)$ or $(0, \frac{1}{2})$; The PerBU's are connected through T5-ring sequences

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.

<i>End-member</i>	<i>Lateral shifts between subsequent mirrored PerBU's along [001]; shifts are in fractions of (a, and b)</i>					<i>Space Group</i>
1 ¹	$(0,0);$	$(0,0);$	$(0,0);$		$P4_2/mmc$
2 ²	$(0,\frac{1}{2});$	$(\frac{1}{2},0);$	$(0,\frac{1}{2});$	$(\frac{1}{2},0);$	$(0,\frac{1}{2});$	$I4_1/amd$
3 ³	$(0,0);$	$(0,\frac{1}{2});$	$(0,0);$	$(0,\frac{1}{2});$	$(0,0);$	$A2/m^4$

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 $A2/m$.

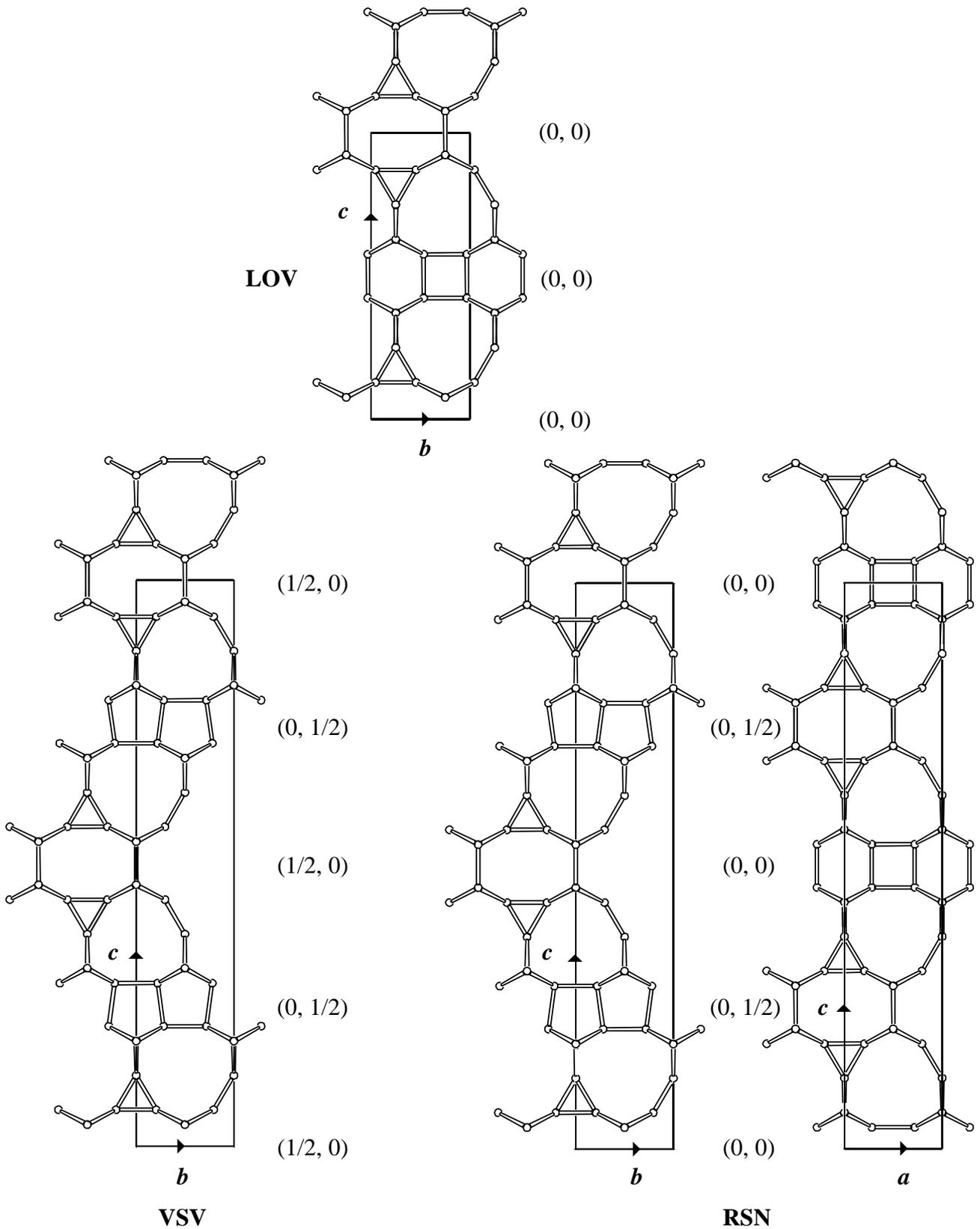


Figure 3: Skeletal drawings of the three ordered end-members of the lovdarite family of structures. The ac projections in LOV and VSV are equivalent to their bc projections, respectively. The lateral shifts between subsequent (mirror related) PerBU's along [001] is given in the drawings in fractions 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

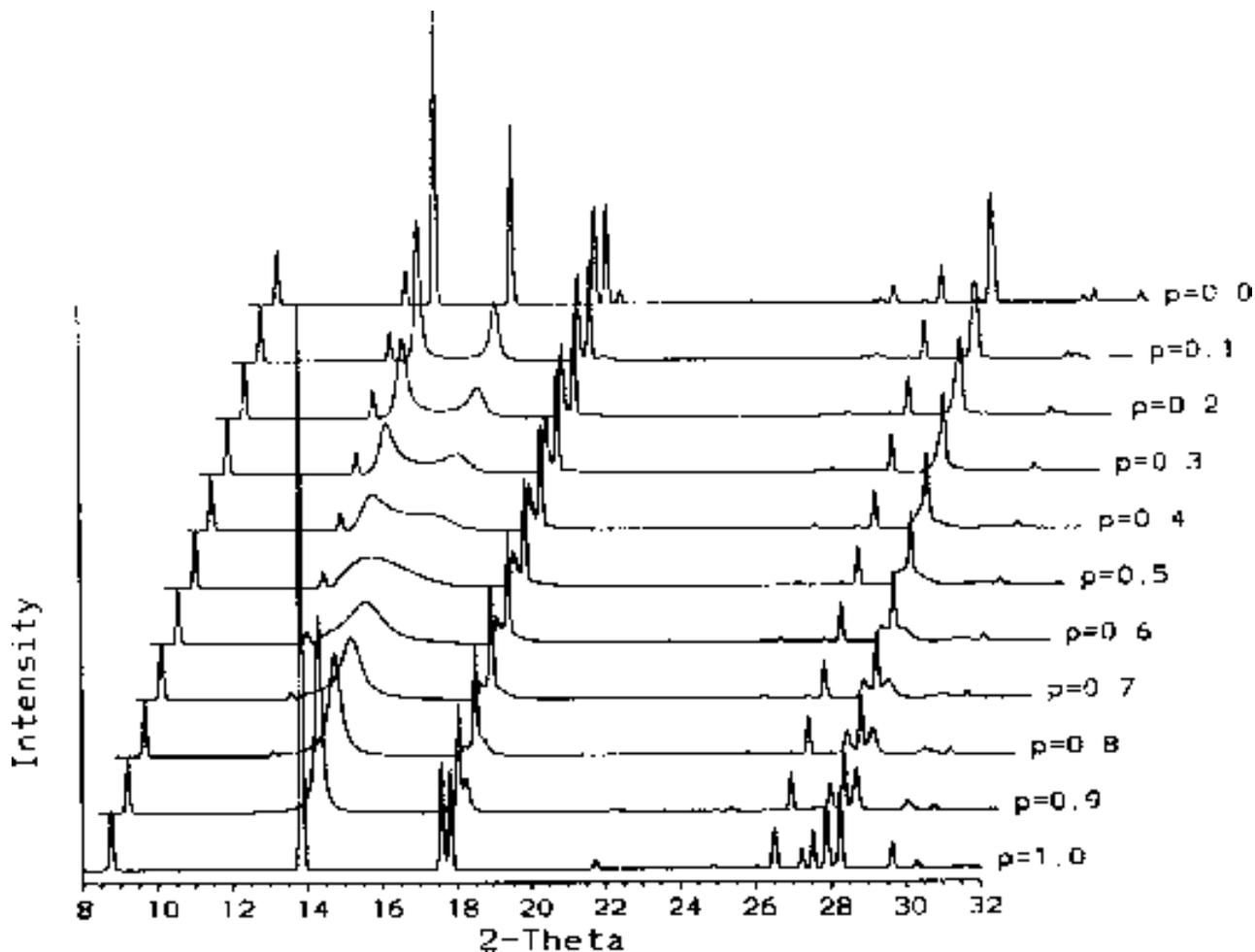


Figure 4: Simulated powder pattern of the lovdatite materials containing T5- and T4-T6-ring sequences between neighbouring PerBU's. The number indicates the fraction of T5-ring sequences in the material

8. References

- (1) S. Merlino, *Eur. J. Miner.* **2**, 809 (1990).
- (2) C. Röhrig, H. Gies and B. Marler, *Zeolites* **14**, 498 (1994).
- (3) C. Röhrig, and H. Gies, *Angew. Chem. Int. Ed. Engl.* **34**, 63 (1995). ▲