

The SSZ-33 Family

1. The Periodic Building Unit (PerBU) - 2. Type of Faulting - 3. The Layer Symmetry
4. Connectivity Pattern - 5. Ordered End-Members - 6. Disordered materials synthesized to date
7. Supplementary Information - 8. References

1. The Periodic Building Unit (PerBU) is composed of parallel chains formed by connecting T14 units along c (as shown in Figure 1) and equals the bc layer depicted in Figure 2.

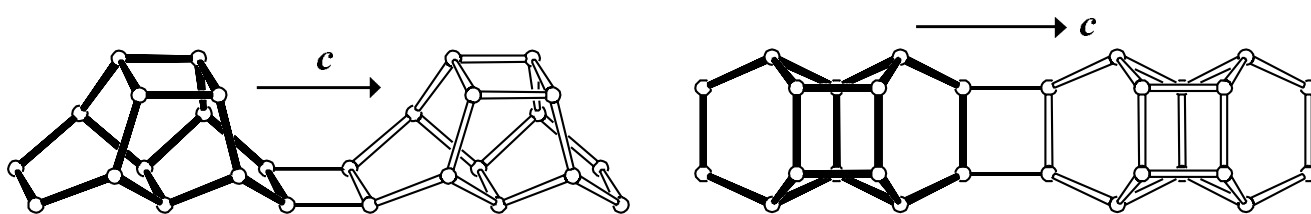


Figure 1: T14 units (in bold), related by pure translations along c , are connected into chains. The chains at left and right differ by a rotation of 90° about the chain axis c

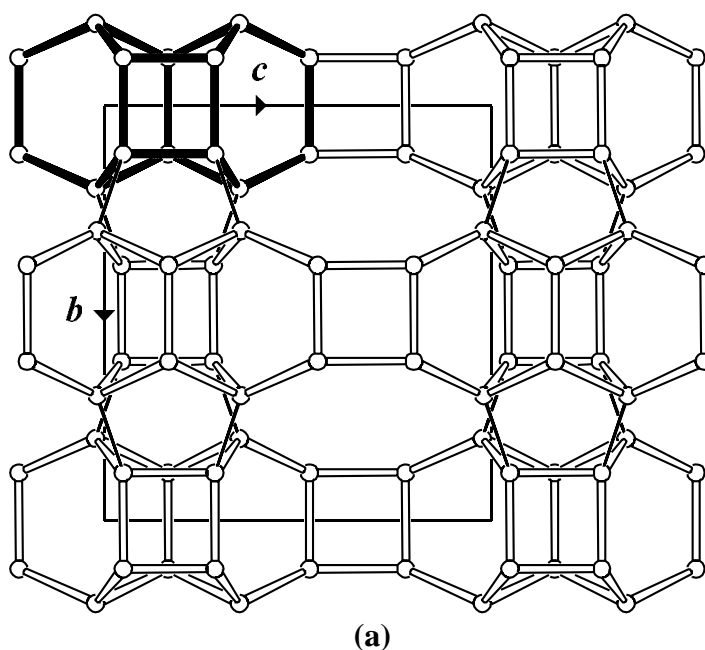


Figure 2: PerBU of the SSZ-33 family viewed along a (a). Figure 2 is continued on next page

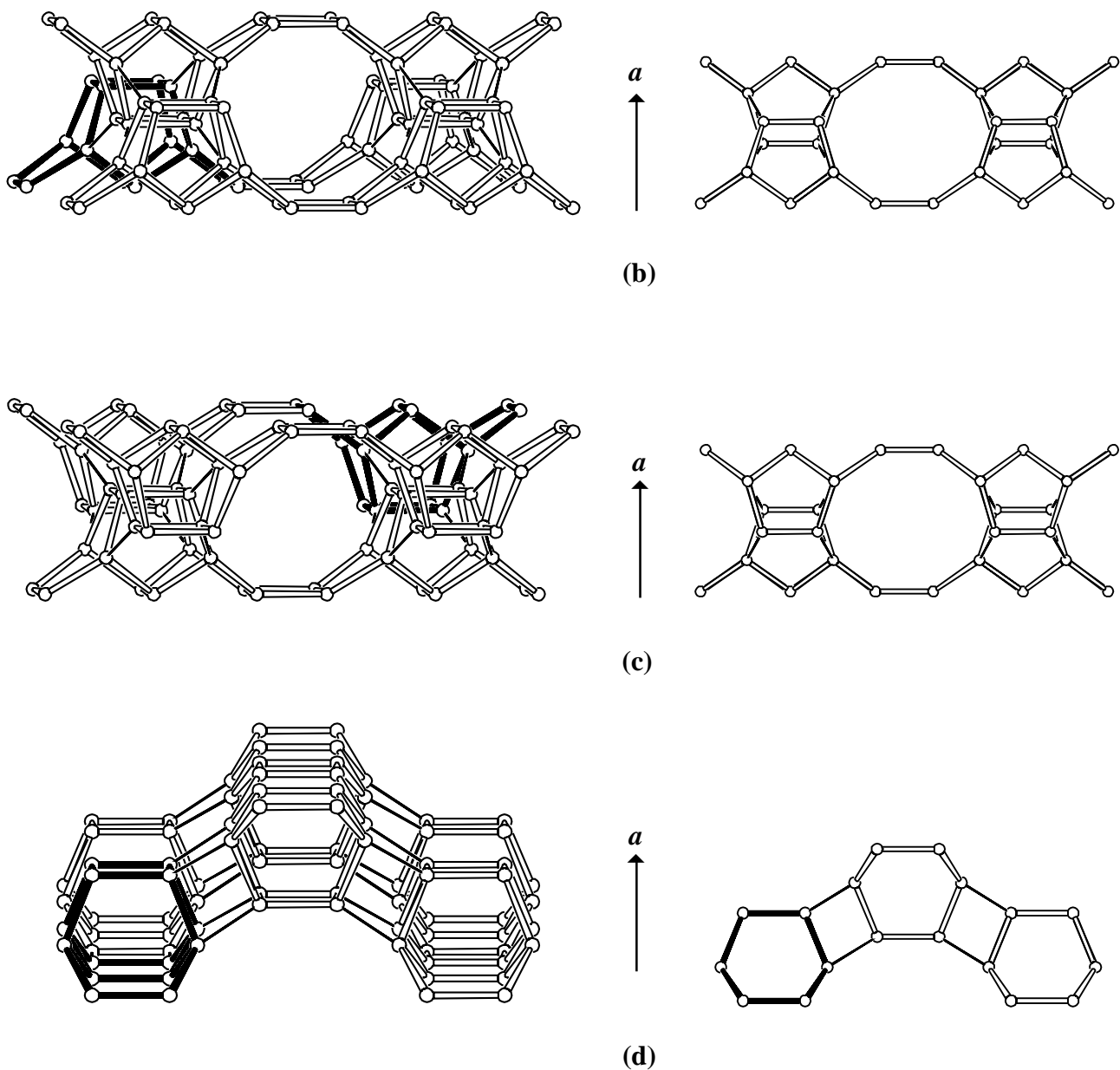


Figure 2 (Continued): PerBU of the SSZ-33 family. Perspective views (left) and parallel projections (right) along \mathbf{b} (b and c), and along \mathbf{c} (d) are shown

In the PerBU, direct neighbouring chains are related by a rotation of 180° about \mathbf{b} (or \mathbf{c}). Chains are connected along \mathbf{b} to form a puckered PerBU (Fig. 1d). The PerBU's, depicted in (Fig. 1b and c) in perspective view (left) and in parallel projection (right), are identical and related by a lateral shift of $\frac{1}{2}\mathbf{b}$, by a rotation of 180° about \mathbf{b} or by a mirror operation perpendicular to \mathbf{c} . ▲

2. Type of faulting: 1-dimensional stacking disorder of the PerBU's along \mathbf{a} .

3. The plane space group of the PerBU is $P(2)mm$. ▲

4. Connectivity pattern of the PBU:

Neighbouring PerBU's, related by a mirror operation, are connected along a in three different ways: (a) the lateral shift of the top layer along c is zero; denoted as (0) (this connectivity, which shows mirror symmetry ($\mathbf{m}; \parallel$) between successive layers, has not been observed yet).

(b) the lateral shift of the top layer is $+1/3c$; denoted as $(+1/3)$. The connectivity exhibits inversion symmetry ($\mathbf{i}; \circ$) between successive layers.

(c) the lateral shift of the top layer is $-1/3c$, denoted as $(-1/3)$. This connectivity also shows inversion symmetry ($\mathbf{i}; \circ$) between the layers.

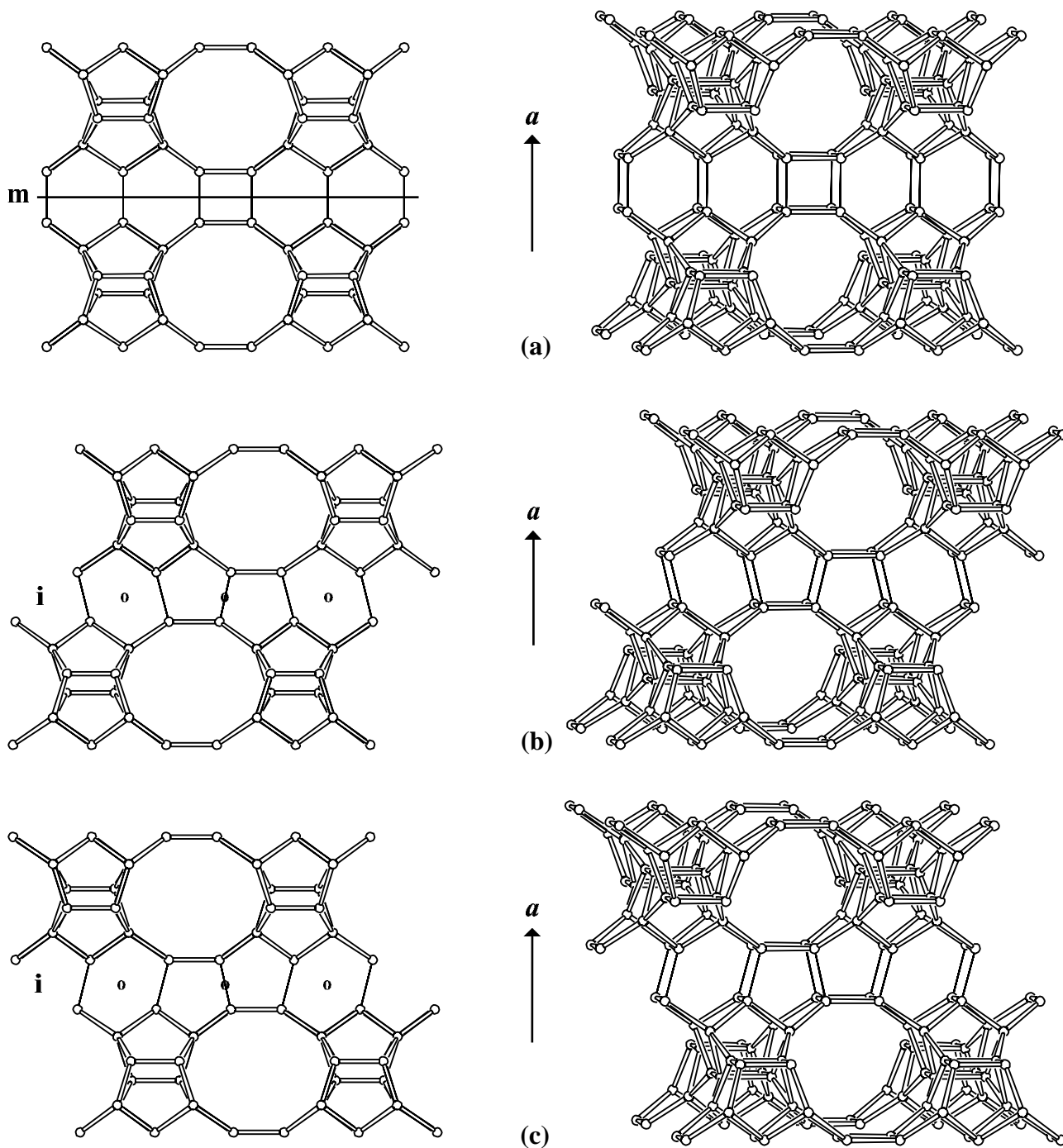


Figure 3: Perspective view (right) and parallel projection (left) of the connection modes (a),(b) and (c) in the SSZ-33 family of framework types seen along b . In connection mode (a) the neighbouring PerBU's are connected through (fused) T6-T6-T4 ring sequences and in connection modes (b) and (c) through (fused) T6-T5-T5 ring sequences ▲

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

5. The simplest ordered end-members in the SSZ-33 family are given below. Only end-member 2 has been observed as pure single crystal material and represents the structure with framework type code CON. There is no difference in the projection of the framework of the end-members along c .

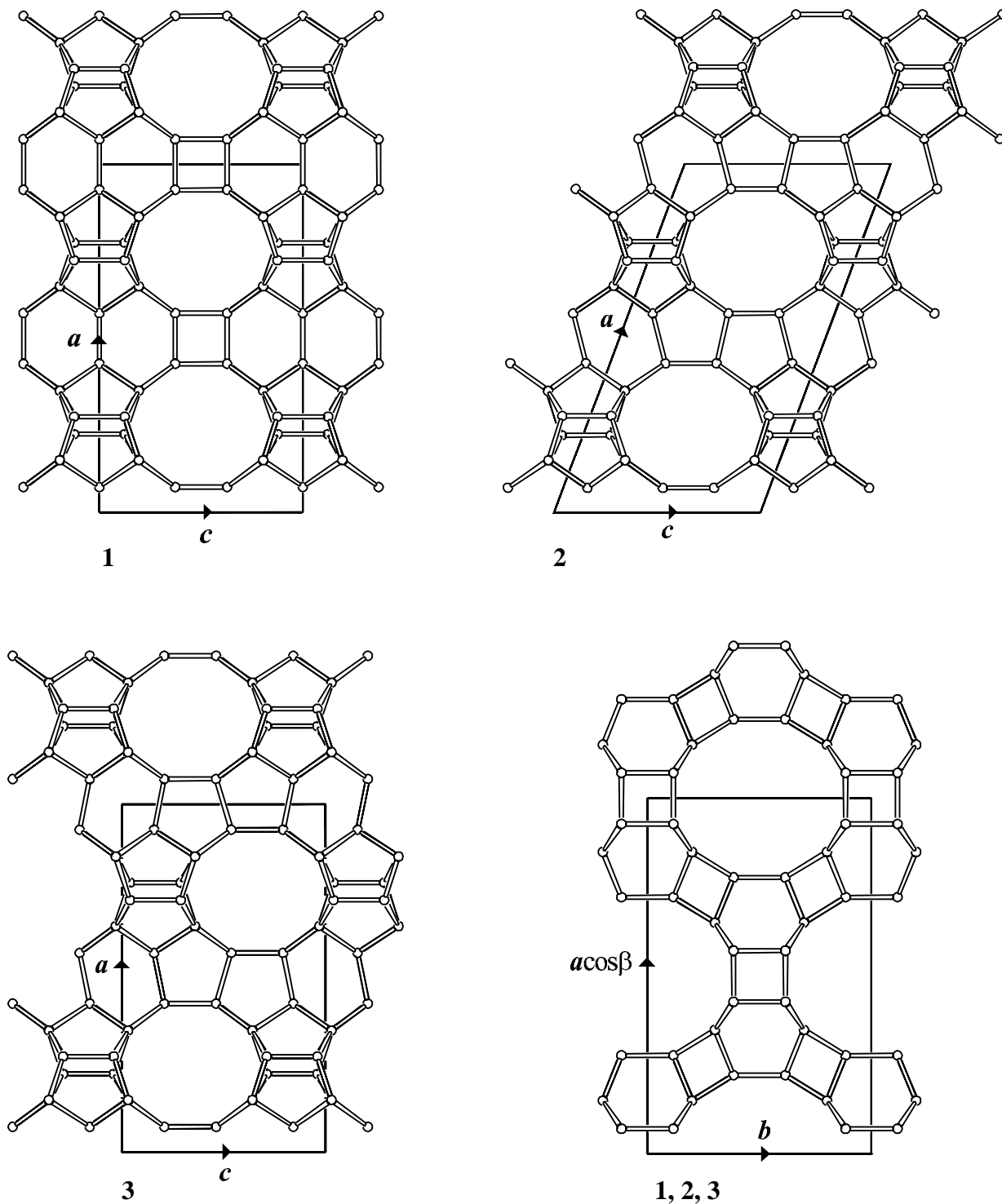


Figure 4: Projections of the simplest ordered end-members in the SSZ-33 family (cf. Table 1 on next page). The projection along c (last figure) is the same for all three end-members ▲

Table 1: Stacking sequences of PerBU's for the simplest ordered end-members in the SSZ-33 family. The end-member number refers to the framework plots **1-3** on the previous page.

<i>End-Member</i>	<i>Lateral shifts between subsequent PerBU's stacked along a; shifts are in fractions of c</i>			<i>space group</i>
1	(0);	(0);	(0);.....	Pmmm
2	(+1/3);	(+1/3);	(+1/3);.....	C2/m ^{1,2}
3	(+1/3);	(-1/3);	(+1/3);.....	Pncm ^{2,3}

¹ This is the end-member with framework type code CON.

² Space group is centrosymmetric; the same structure is obtained by reversing the signs of all lateral shifts.

³ The standard space group Pmna (with *a*, *b* and *c*) has been transformed to the non-standard space group Pncm (with *b*, *c*, and *a*) for comparison reasons.

6. Disordered materials synthesized and characterized to date:

SSZ-26(1,2), SSZ-33(2,3). ▲

7. Supplementary material

to be added

8. References

- (1) S. I. Zones, D. S. Santilli, J. N. Holtermann, T. A. Pecoraro and R. A. Innes, US Patent 4,910,006(1990).
- (2) R. F. Lobo, M. Pan, I. Chan, R. C. Medrud, S. I. Zones, P. A. Crozier and M. E. Davis, J. Phys. Chem. **98**, 12040 (1994).
- (3) S. I. Zones, US Patent 4,963,337(1990). ▲