

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 ac layer shown in Figure 1:

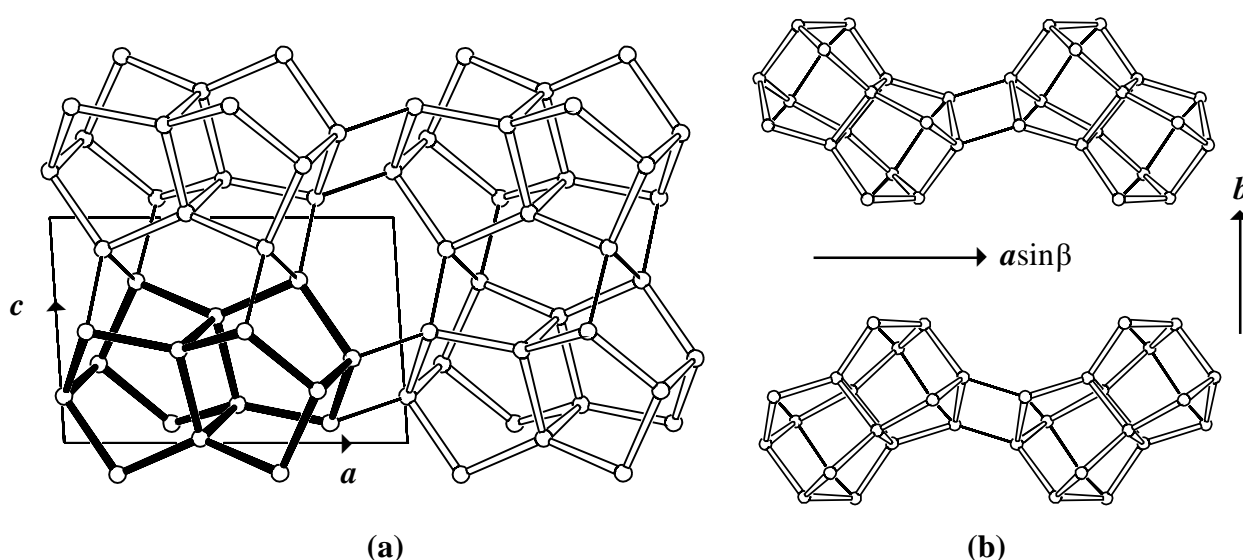


Figure 1: PerBU in the SFF/STF family of zeolite frameworks. (a): perspective view along b ; (b): two parallel projections along c

The PerBU in the SFF/STF family is composed of T16 units (bold in Fig.1), related by pure translations along a and c . The T16 unit consists of a T4-ring capped on both sides by “roofs” of six T aoms. The PerBU’s depicted in Figure 1b are identical and related by a rotation of 180° about b or by a mirror plane perpendicular to b . [Compare the T16 unit with the T16 units in IFR and STT].

2. **Type of Faulting:** 1-dimensional stacking disorder of the PerBU’s along b .

3. **The Layer Symmetry:** the plane space group of the PerBU is $P \bar{1} \bar{1} (\bar{1})$.

4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's can be connected along b in two different ways:

(a): neighbouring PerBU's are related by a pure translation along b . The resulting connectivity exhibits inversion symmetry (i ; o) between successive layers.

(b): neighbouring PerBU's are related by a rotation of 180° about b . The connectivity now shows mirror symmetry (m ; l) between successive layers.

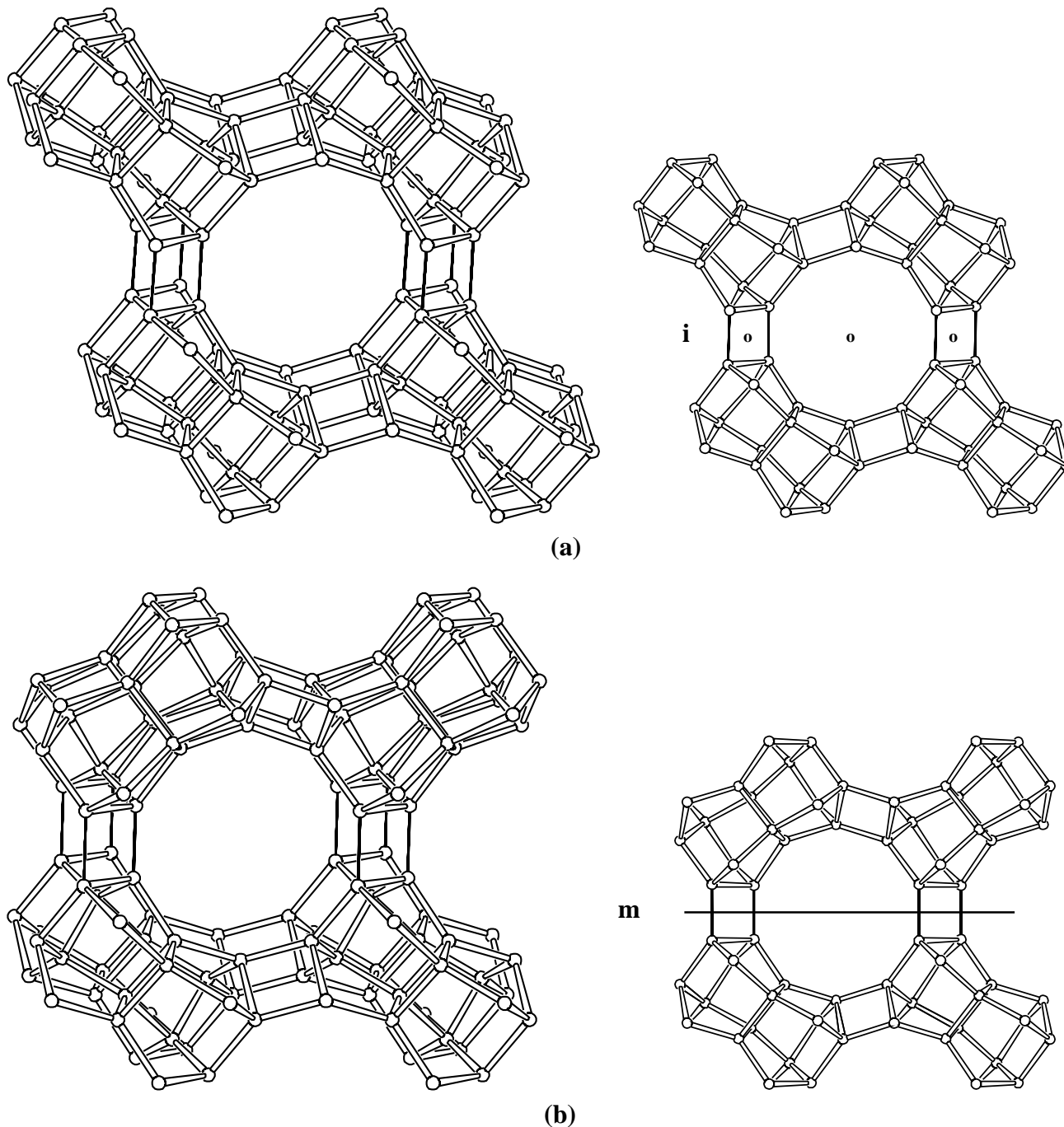


Figure 2: Perspective view (left) and parallel projection of the connection modes (a) and (b) in the SFF/STF family of zeolite frameworks seen along c

Once the distribution of the symmetry elements i and m between the PerBU's stacked along b is known, the 3-dimensional structure is defined. ▲

5. The Simplest Ordered End-Members in the SFF/STF family are presented in Figure 3:

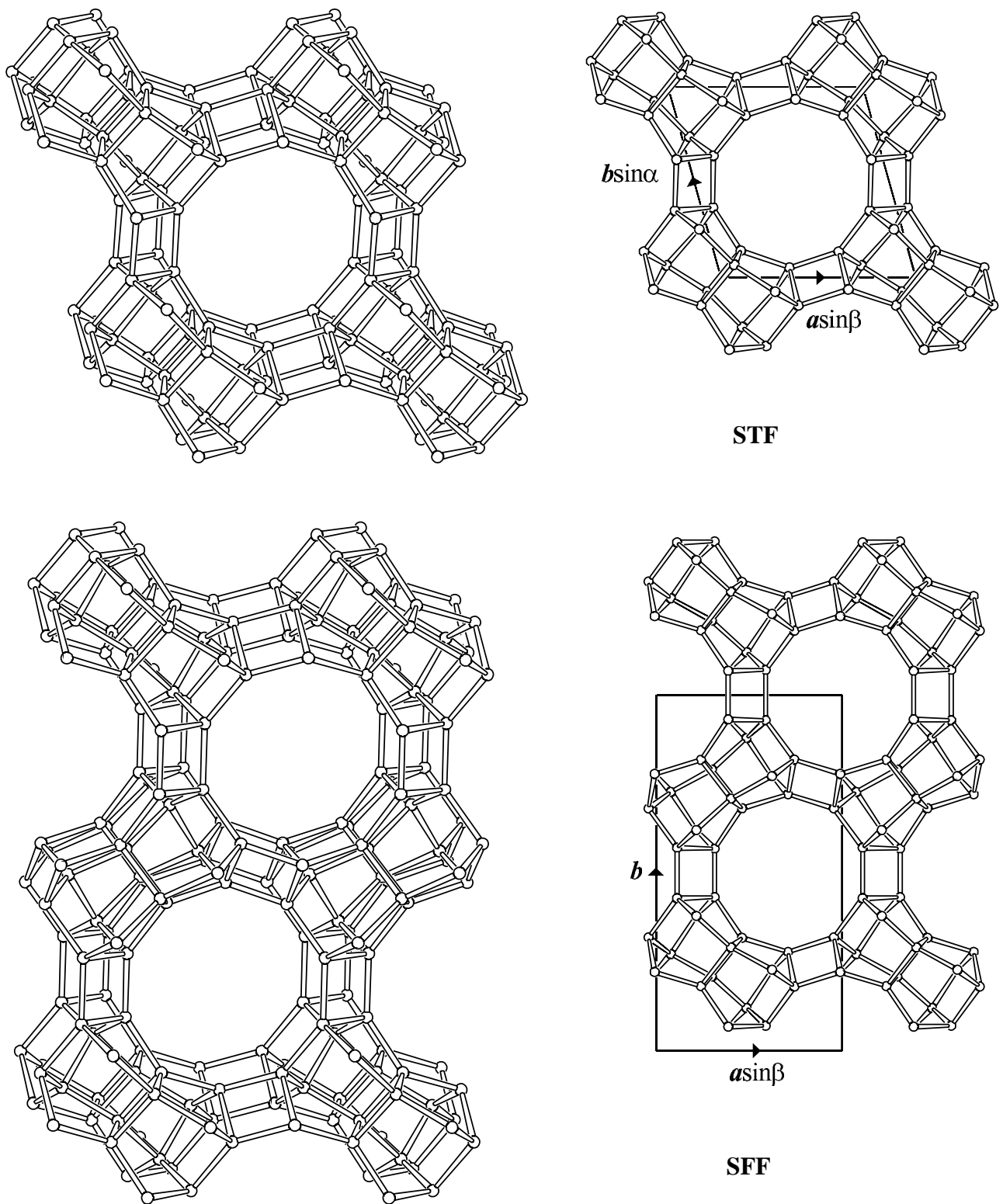


Figure 3: Perspective view and parallel projection along c of the unit cell content of the two simplest ordered end-members in the SFF/STF family: STF (top) and SFF (bottom)

Pure STF(1) and SFF(1) are obtained when neighbouring PerBU's, stacked along the plane normal of the PerBU, are exclusively related by \mathbf{i} and \mathbf{m} , respectively. ▲

6. Disordered Materials Synthesized and Characterized to Date:

to be added



7. Supplementary Information

7.1 Comparison with IFR and STT:

The PerBU's in IFR and STT are also composed of T16 units and equal the chain (in IFR) and the *ac* layer (in STT) shown in Figure 4. These T16 units very much resemble the T16 unit in SFF/STF.

[For more details: see the building schemes of IFR and STT in 'Schemes for Building Zeolite Framework Models' on <http://www.iza-structure.org/databases/>

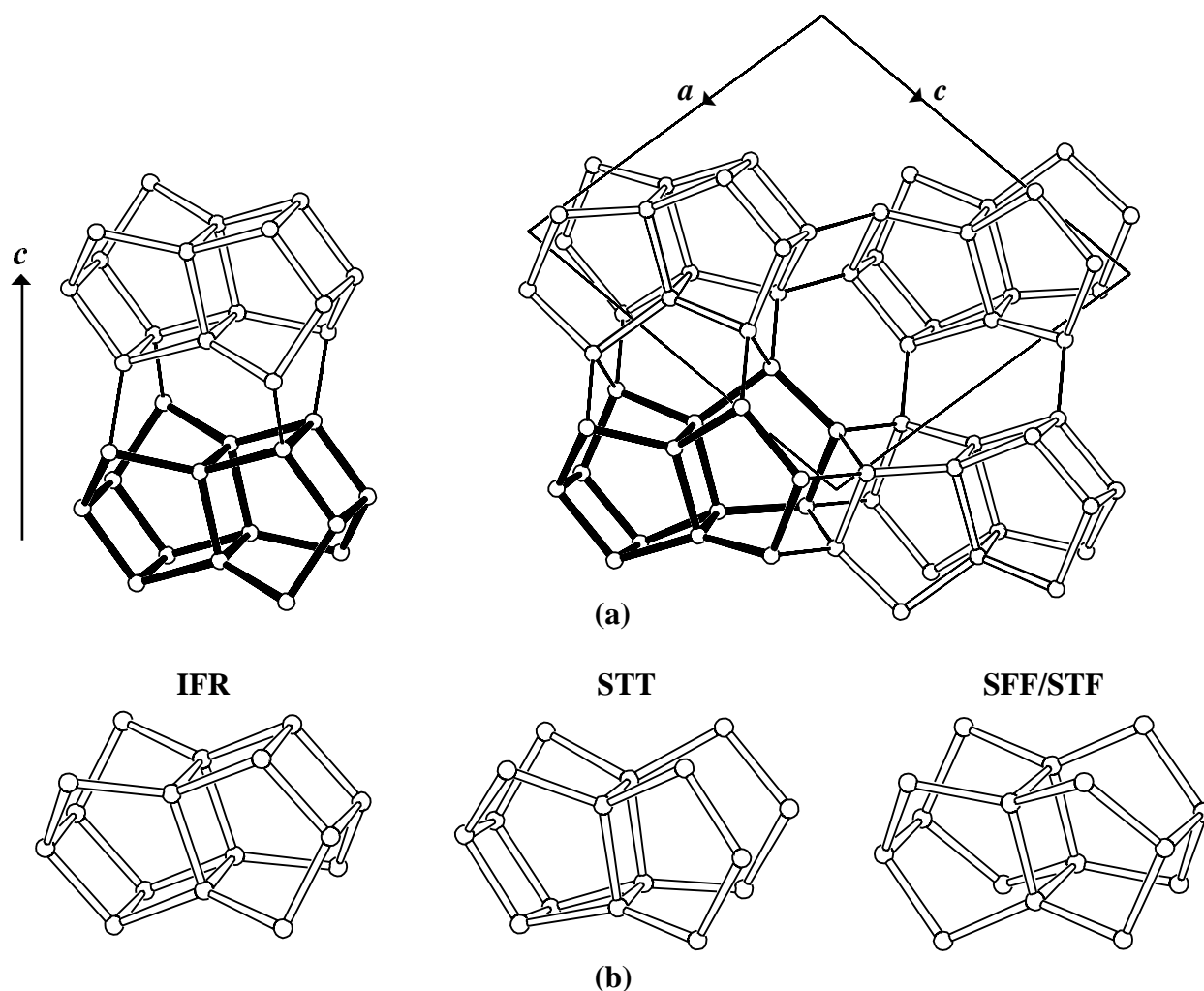


Figure 4: (a): Perspective view of the PerBU in IFR (left) and in STT (right); (b): T16 unit in IFR (left), in STT (middle) and (for comparison) in SFF/STF (right)



8. References

- (1) P. Wagner, S.I. Zones, M.E. Davis and R.C. Medrud, *Angew. Chem., Int. Ed.* **38**, 1269 (1999).

