The ABC-6 Family

1. The periodic building unit (PerBU) equals the layer shown in Figure1:

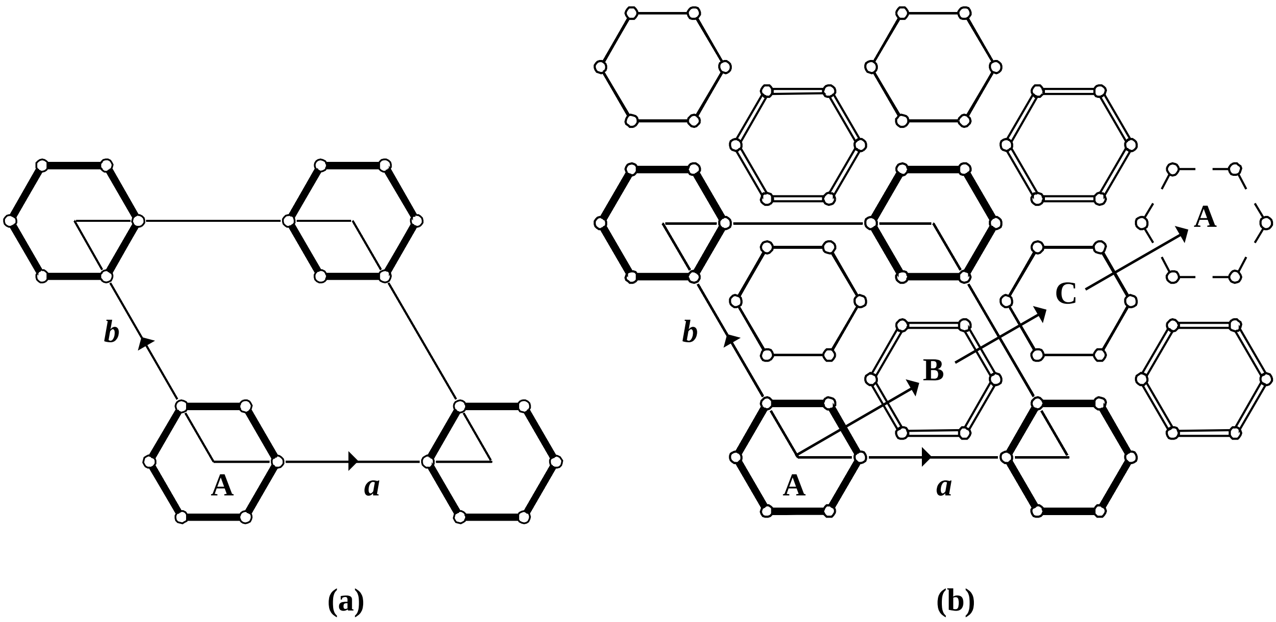


Figure 1: The PerBU is an arrangement of single T6-rings in the ***ab***-plane of a hexagonal unit cell. In (a) a single layer, and in (b) a projection of a 3-layer stacking sequence ABC is shown

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.

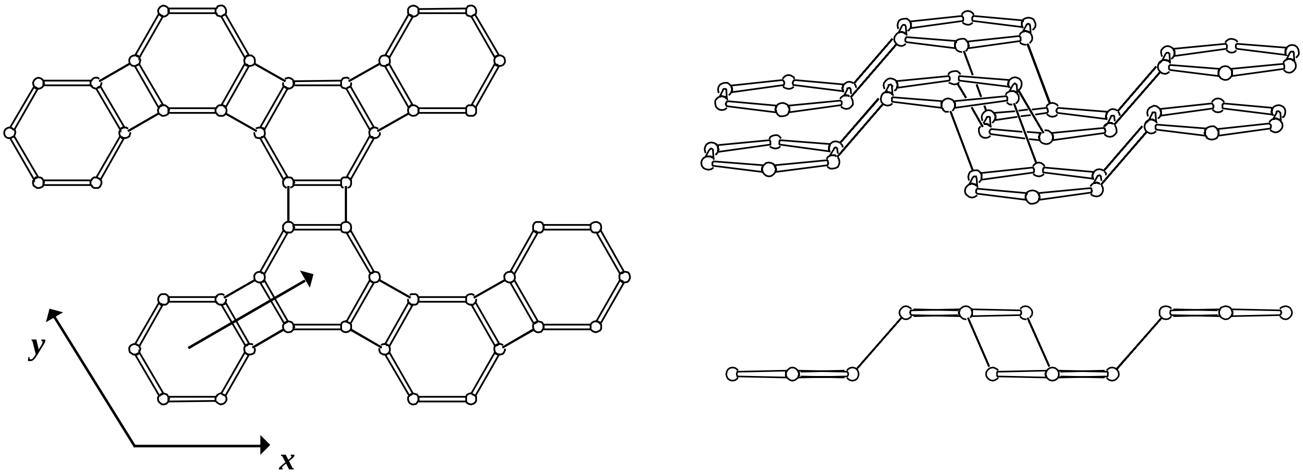
4. Connectivity pattern of the PerBU:

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

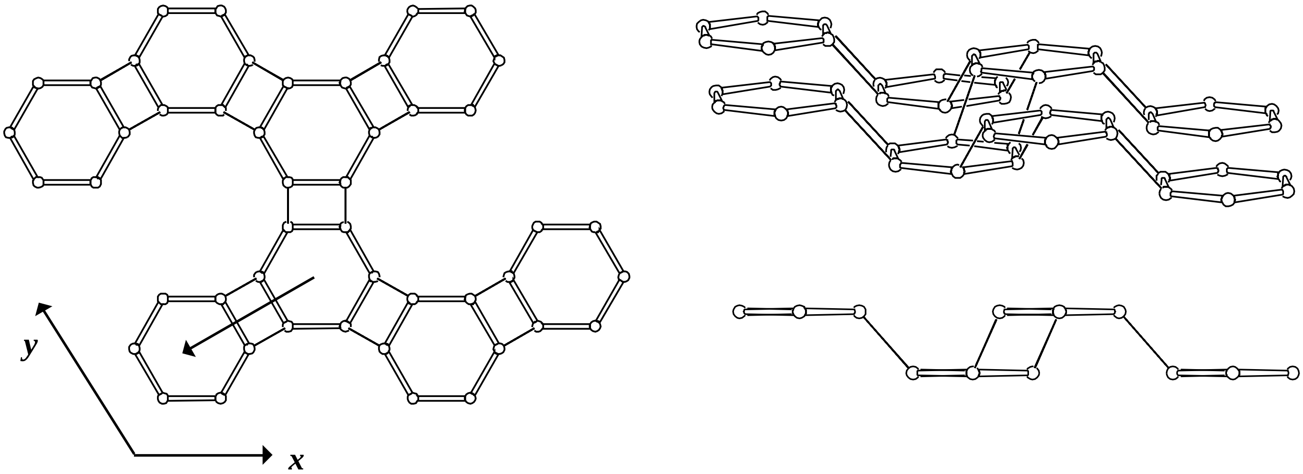
(a): the second layer is shifted by +(2/3***a*** + 1/3***b***) before connecting it to the first layer; so the T6-rings in the second layer are centered at (2/3, 1/3). This position is usually denoted as the B position (Fig.1b). The same connection mode can be repeated to generate a third PerBU shifted with respect to the second layer by (again) +(2/3***a*** + 1/3***b***). 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 (2***a*** + ***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 -(2/3***a*** + 1/3***b***) 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.

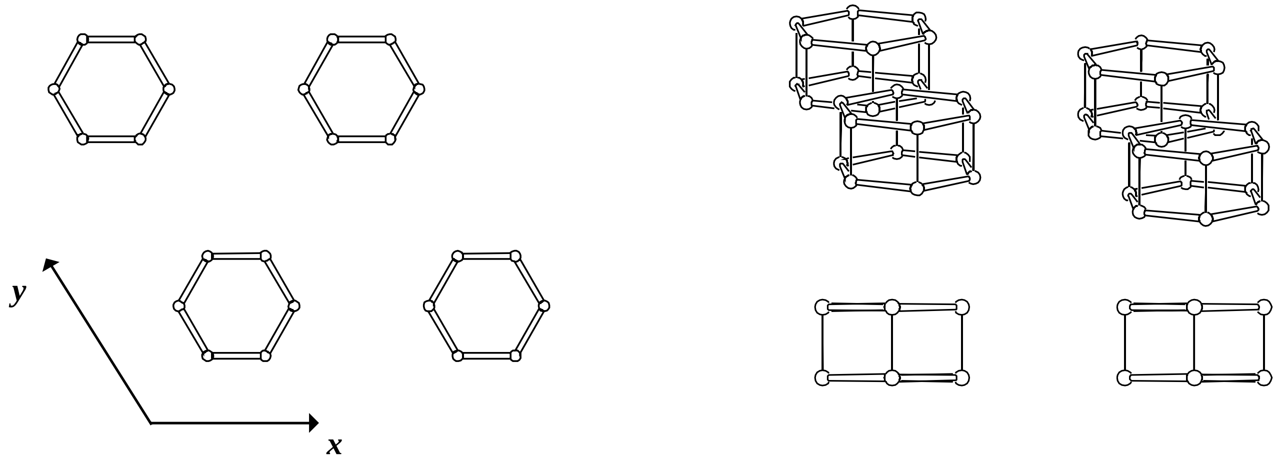
(c): the second layer has a zero lateral shift along ***a*** and ***b***. This connection mode leads to an AA, BB or CC stacking sequence depending on whether the added layer is connected to a layer with T6-rings in the A, B or C position, respectively. The connection mode is shown in Fig. 2c.



(a)



(b)

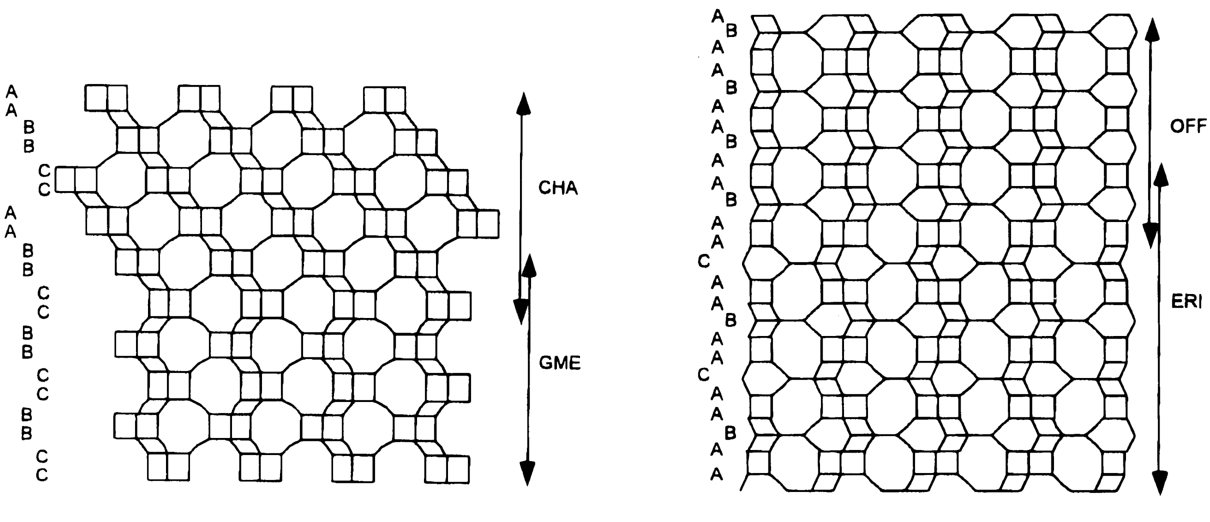


(c)

Figure 2: Connectivity modes in the ABC-6 family of zeolites

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:



(a) **(b)**

Figure 3: Examples of stacking disorder with **CHA**/**GME** (a) and **OFF**/**ERI** (b) sequences

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

Name	*Code*	*#Repeat layers*	*Stacking sequence*
Cancrinite (1)	CAN	2	AB(A).........
Sodalite (2)	SOD	3	ABC(A)......
Losod (3)	LOS	4	ABAC(A)...

cont’d on next page

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

Examples of ordered end-members in the ABC-6 family are presented in Figure 4 in the same sequence as in the Table above.

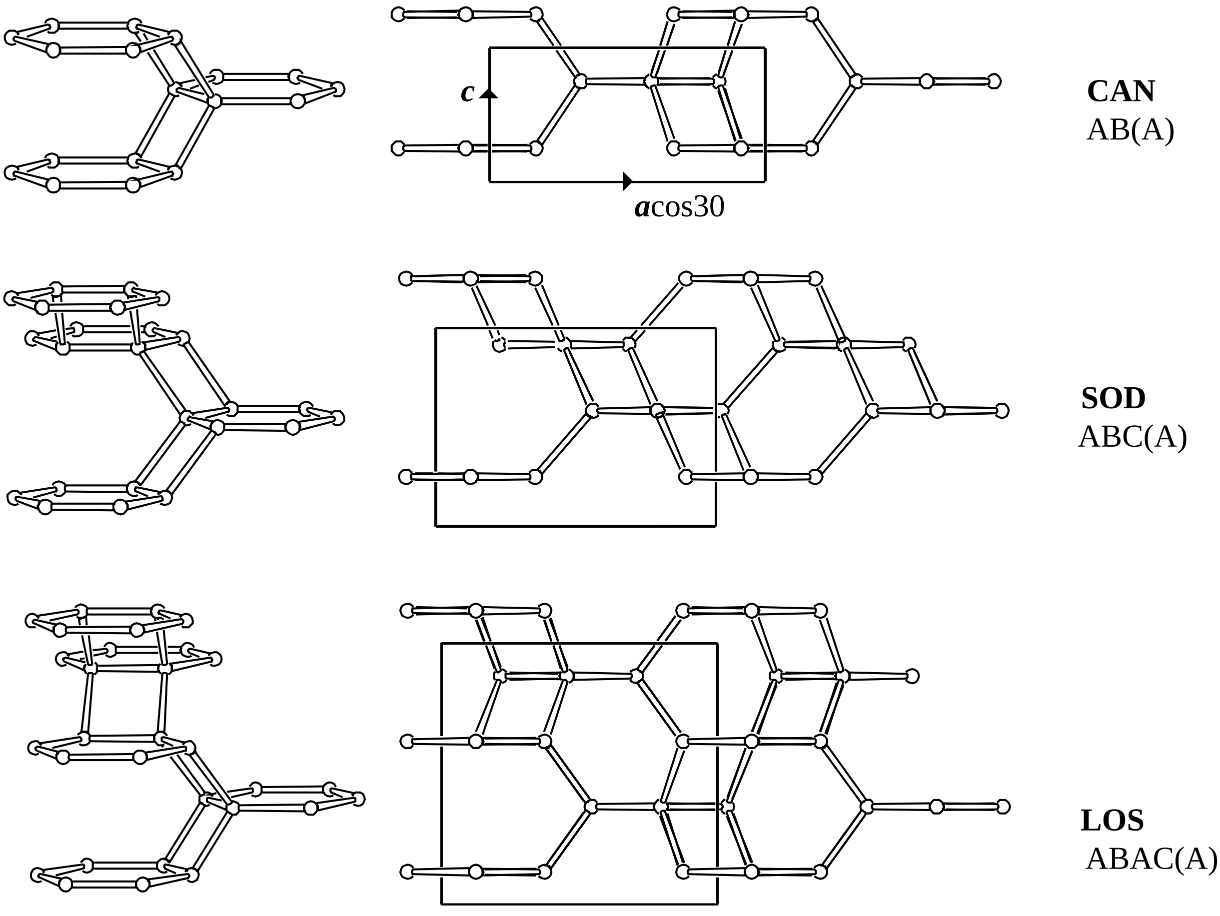
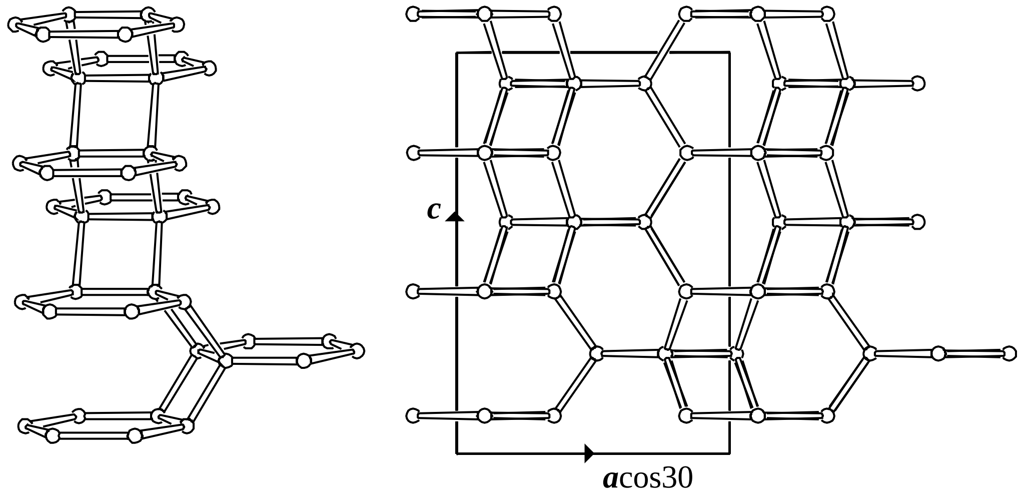
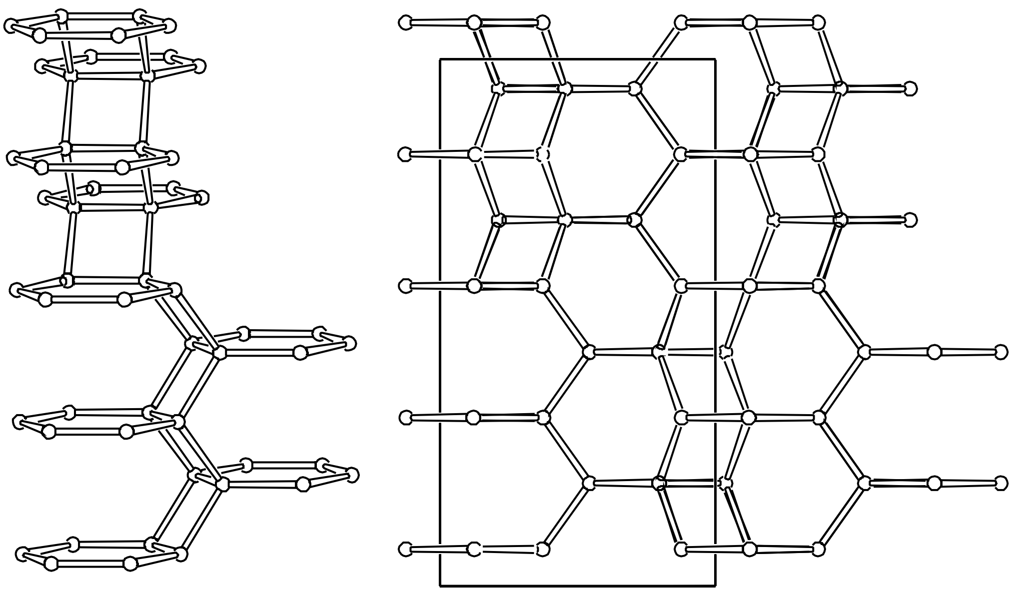


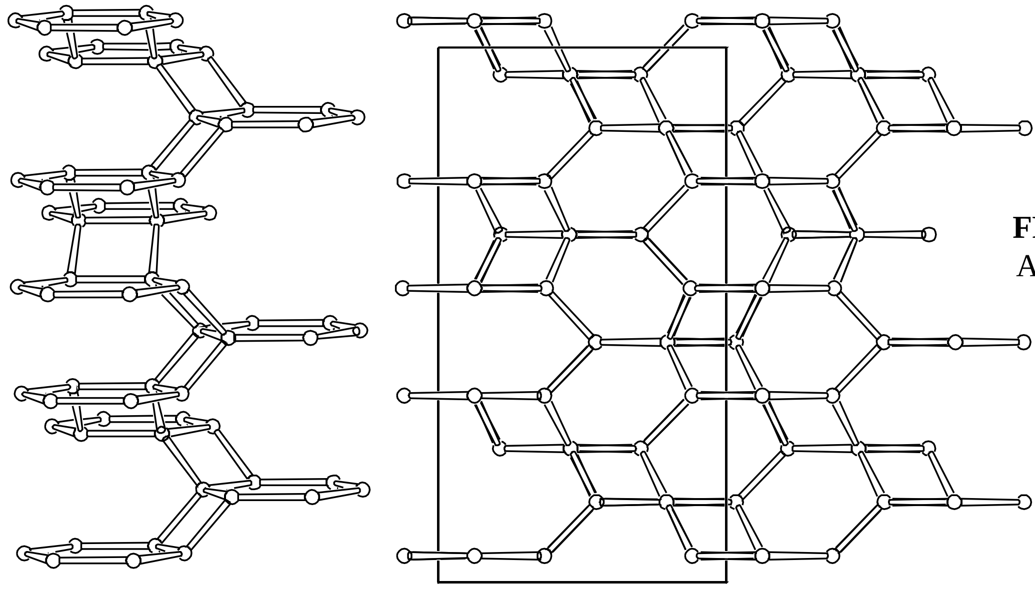
Figure 4: Perspective drawing (left) and parallel projection along [010] of the unit cell content (right) of periodic end-members in the ABC-6 family. The hexagonal ***c*** axis points towards the top of the page and the horizontal axis is equal to ***a***cos30 as indicated for CAN. (Fig.4 is cont’d on next page)



LIO
ABACAC(A)

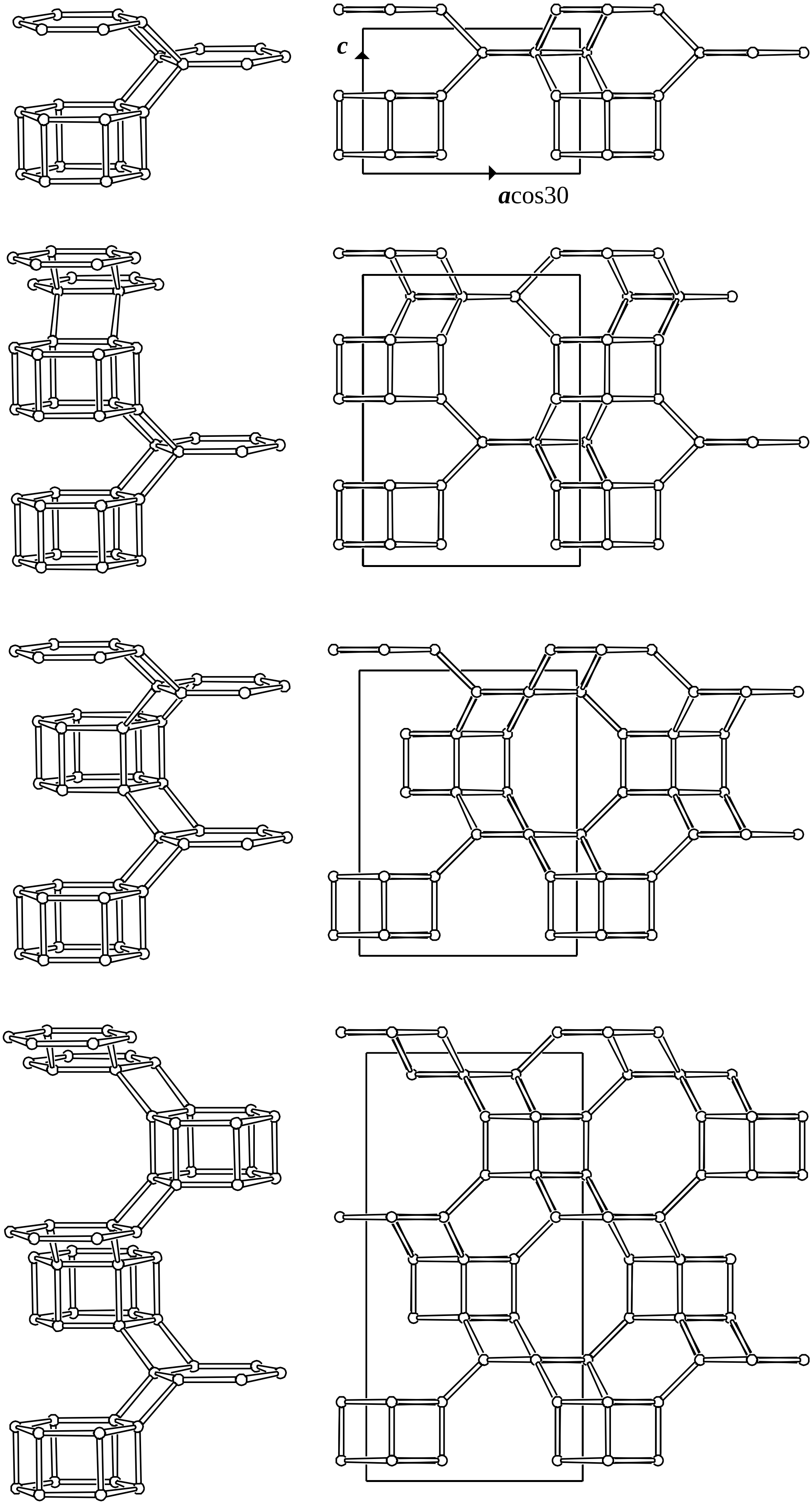


AFG
ABABACAC(A)



FRA
ABCABACABC(A)

Figure 4 (Continued): For legend: See previous page. (Fig.4 is continued on next page)



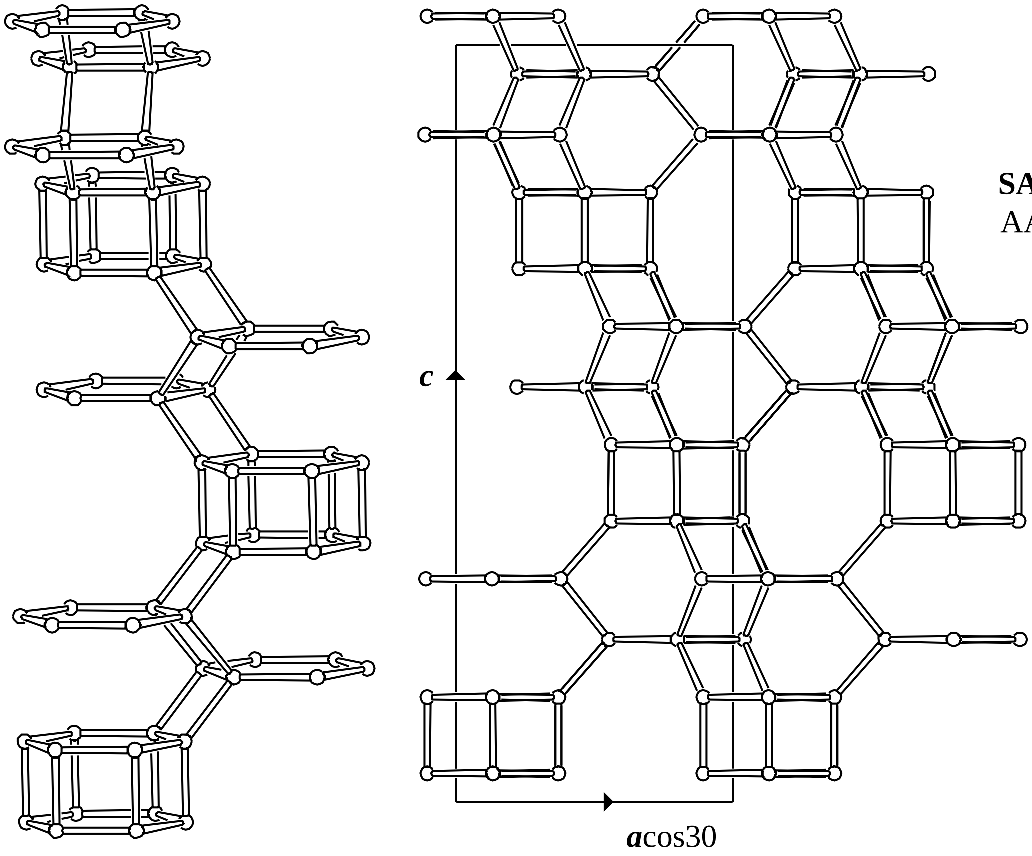
OFF
AAB(A)

ERI
AABAAC(A)

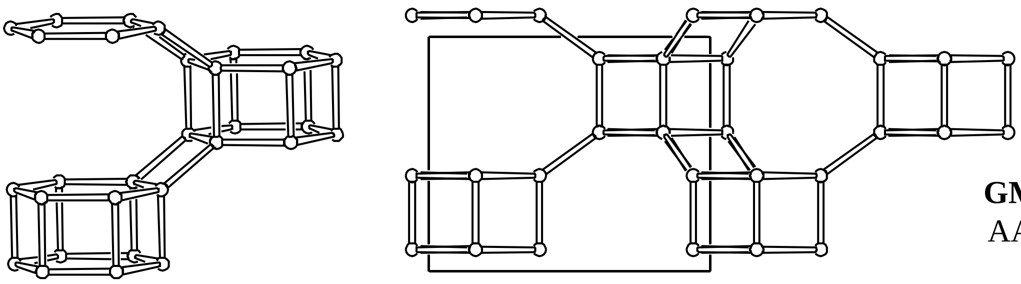
EAB
AABCCB(A)

LEV
AABCCABBC(A)

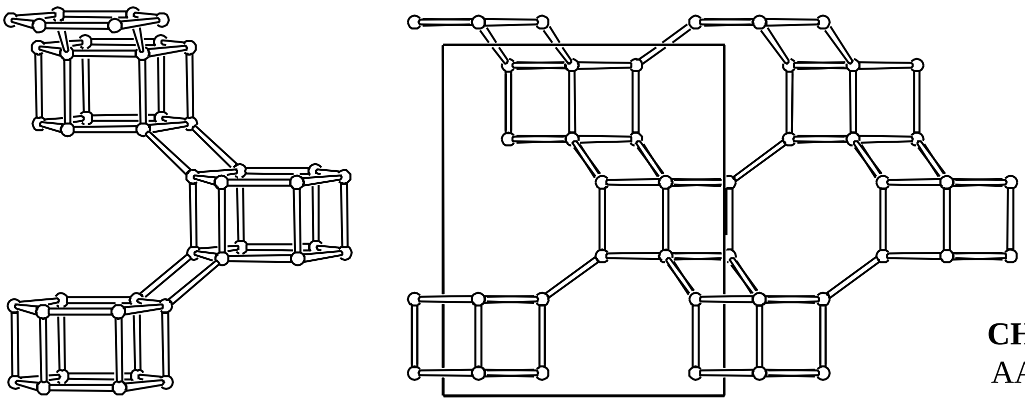
Figure 4 (Continued): For legend: See next page. (Fig.4 is continued on next page)



SAT
AABABBCBCCAC(A)

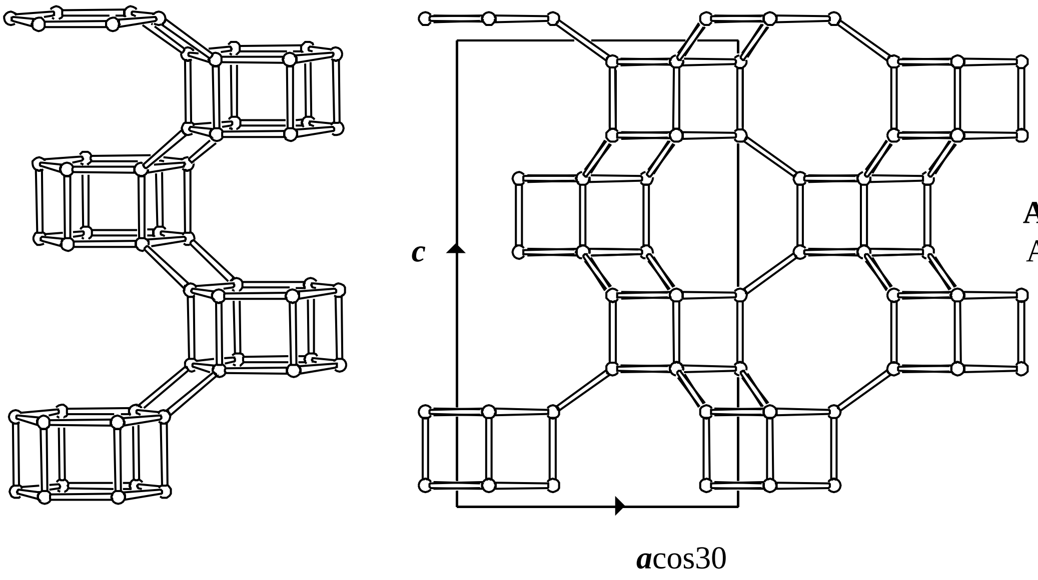


GME
AABB(A)

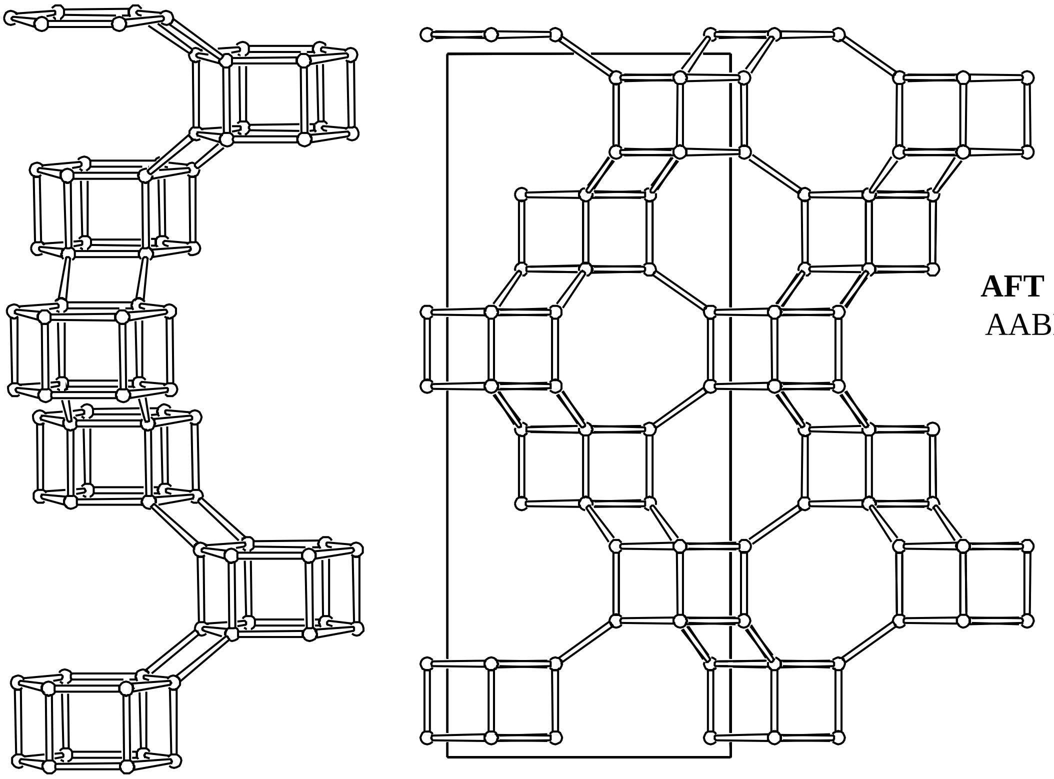


CHA
AABBCC(A)

Figure 4 (Continued): 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; the horizontal axis is equal to ***a***cos30. (Fig.4 is continued on next page)



AFX
AABBCCBB(A)



AFT
AABBCCBBAACC(A)

Figure 4 (Continued): 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; the horizontal axis is equal to ***a***cos30. (Final page of Figure 4)

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.

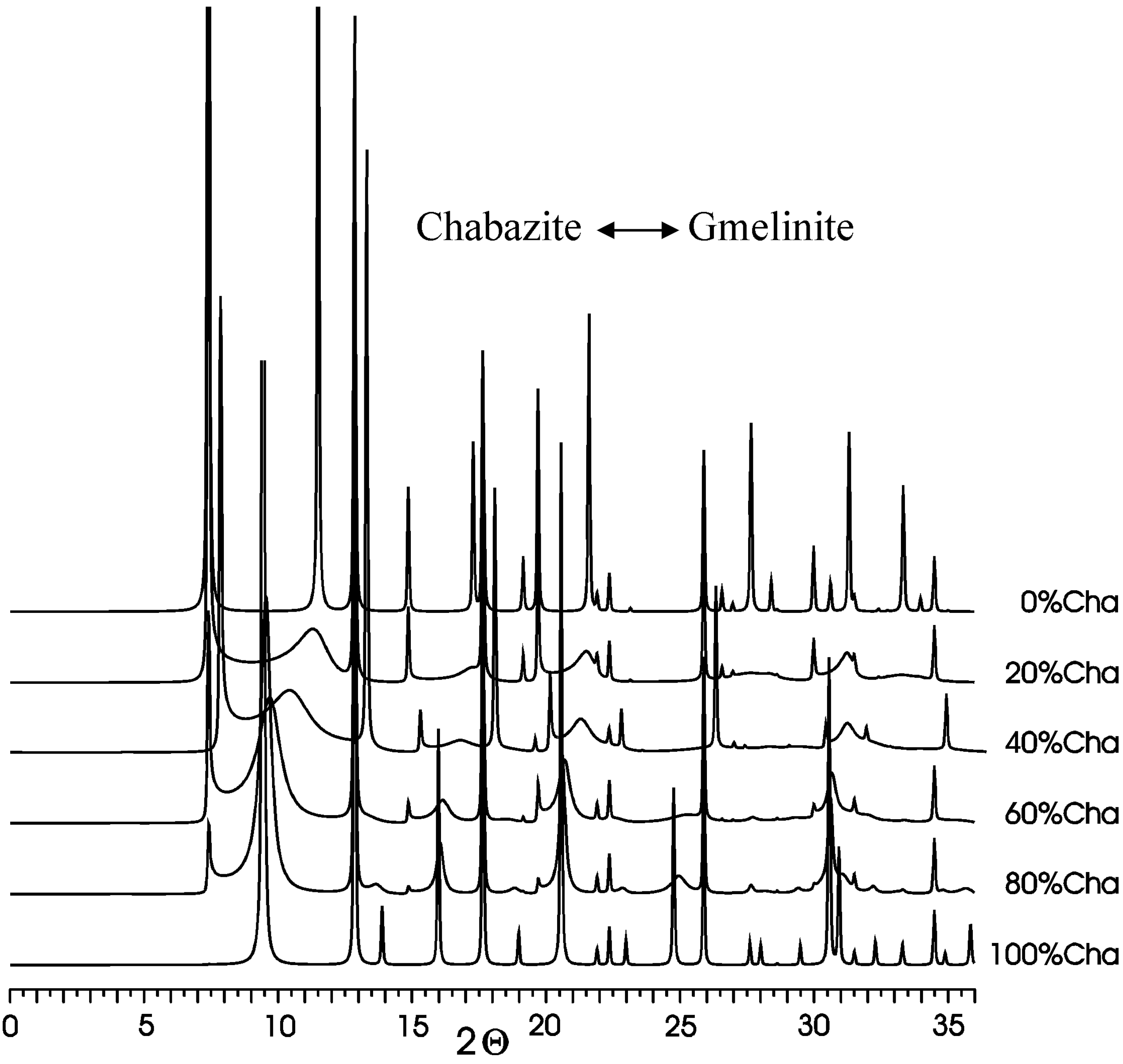


Figure 5: Simulated powder pattern of the Gmelinite/Chabazite series. In this example, the stacking of the PerBU's in AABB- and AABBCC-sequences is disordered

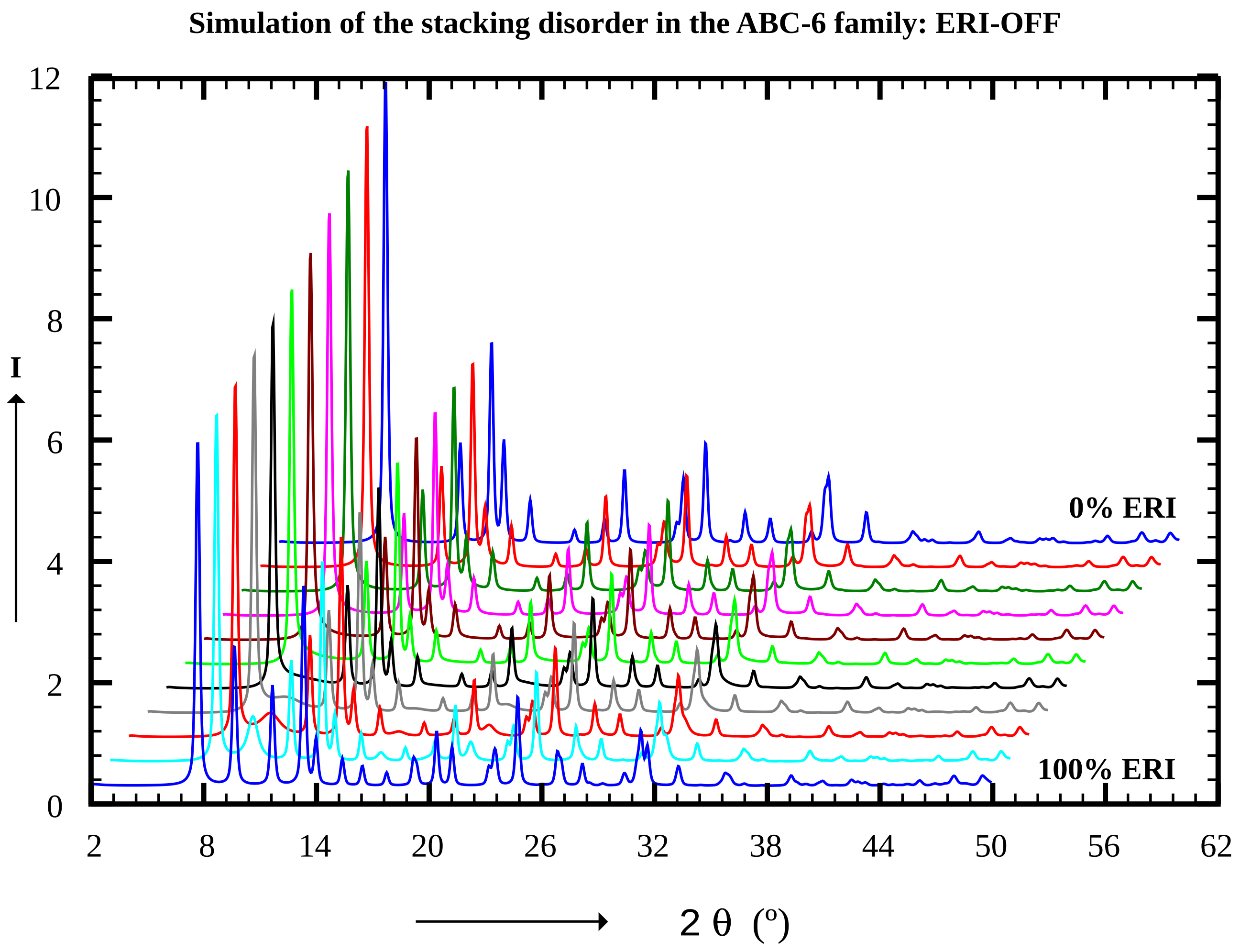


Figure 6: Intensity (**I**, a.u.) of simulated powder patterns versus diffraction angle (**2 θ**) of the ERI-OFF series in steps of 10% intergrowth. The stacking sequences of ERI and OFF are disordered. The 0% ERI pattern corresponds to the 100% OFF pattern

8. References

(1) a) L. Pauling, Proc. Natl. Acad. Sci. **16**, 453 (1930).
b) O. Jarchow, Z. Kristallogr. **122**, 407 (1965).

(2) a) L. Pauling, Z. Kristallogr. **74**, 213 (1930).
b) J. Loens and H. Schulz, Acta Cryst. **23**, 434 (1967).

(3) W. Sieber and W.M. Meier, Helv. Chim. Acta **57**, 1533 (1974).

(4) S. Merlino and P. Orlandi, Am. Mineral. **62**, 321 (1977).

(5) P. Bariand, F. Cesbron and R. Giraud, Bull. Soc. Fr. Mineral. Cristallogr. **91**, 34 (1968).

(6) P. Ballirano, E. Bonaccorsi, A. Maras and S. Merlino, Can. Mineral. **38**, 657 (2000).

(7) J.M. Bennett and J.A. Gard, Nature **214**, 1005 (1967).

(8) L.W. Staples and J.A. Gard, Mineral. Mag. **32**, 261 (1959).

(9) R. Aiello and R.M. Barrer, J. Chem. Soc. A **1970**, 1470 (1970).

(10) R.M. Barrer and I.S. Kerr, Trans. Farad. Soc. **55**, 1915 (1959).

(11) G.W. Noble, P.A. Wright and Å. Kvick, J. Chem. Soc. Dalton Trans. **23**, 4485 (1997).

(12) K. Fischer, N. Jb. Miner. Mh. **1966**, 1 (1966).

(13) a) L.S. Dent and J.V. Smith, Nature **181**, 1794 (1958).
b) J.V. Smith, R. Rinaldi and L.S. Dent, Acta Cryst. **16**, 45 (1963).

(14) a) S.T. Wilson, N.K. McGuire, C.S. Blackwell, C.A. Bateman, and R.M. Kirchner. In: *Zeolite Science 1994: Recent Progress and Discussions*. Studies in Surface Science and Catalysis, Vol. 98. Elsevier Science B.V., 1995, p 9.
b) R.F. Lobo, S.I. Zones and R.C. Medrud, Chem. Mater. **8**, 2409 (1996).

(15) a) J.M. Bennett, R.M. Kirchner and S.T. Wilson. In: Proc. 8th IZC, *Zeolites: Facts, Figures, Future*. P.A. Jacobs and R.A. van Santen (eds.). Elsevier Science Publishers B.V., Amsterdam, 1989, p 731.
b) N.K. Mcguire, C.A. Bateman, C.S. Blackwell, S.T. Wilson and R.M. Kirchner, Zeolites **15**, 460 (1995).

(16) D.W. Breck, Zeolite Molecular Sieves. Wiley, 1974, p 173.

(17) R. Szostak and K.P. Lillerrud, J. Chem. Soc. Chem. Commun. **1994**(20), 2357 (1994).

(18) K.P. Lillerud, R. Szostak and A. Long, J. Chem. Soc. Faraday Trans. **90**, 1547 (1994).

(19) K.P. Lillerud, R. Szostak and A. Long, J. Chem. Soc. Faraday Trans. **90**, 1547 (1994).

(20) G.H. Kuehl. In: Molecular Sieves. S.C.I., London, 1967, p 85.

(21) G.W. Skeels, M. Sears, C.A. Bateman, N.K. McGuire, E.M. Flanigen, M. Kumar and R.M. Kirchner, Micropor. Mesopor. Mater. **30**, 335 (1999).