PAU

PAU.1 Zeolite framework type and topology

The framework type code is named after the mineral **PAU**lingite, $(KCa_{0.5},Na,Ba_{0.5})_{10} \cdot Al_{10}Si_{32}O_{84} \cdot 27\text{-}44\ H_2O$ [98Coo1], first found at the Rock Island Dam of the Columbia River, Washington, USA, and described in [60Kam1].

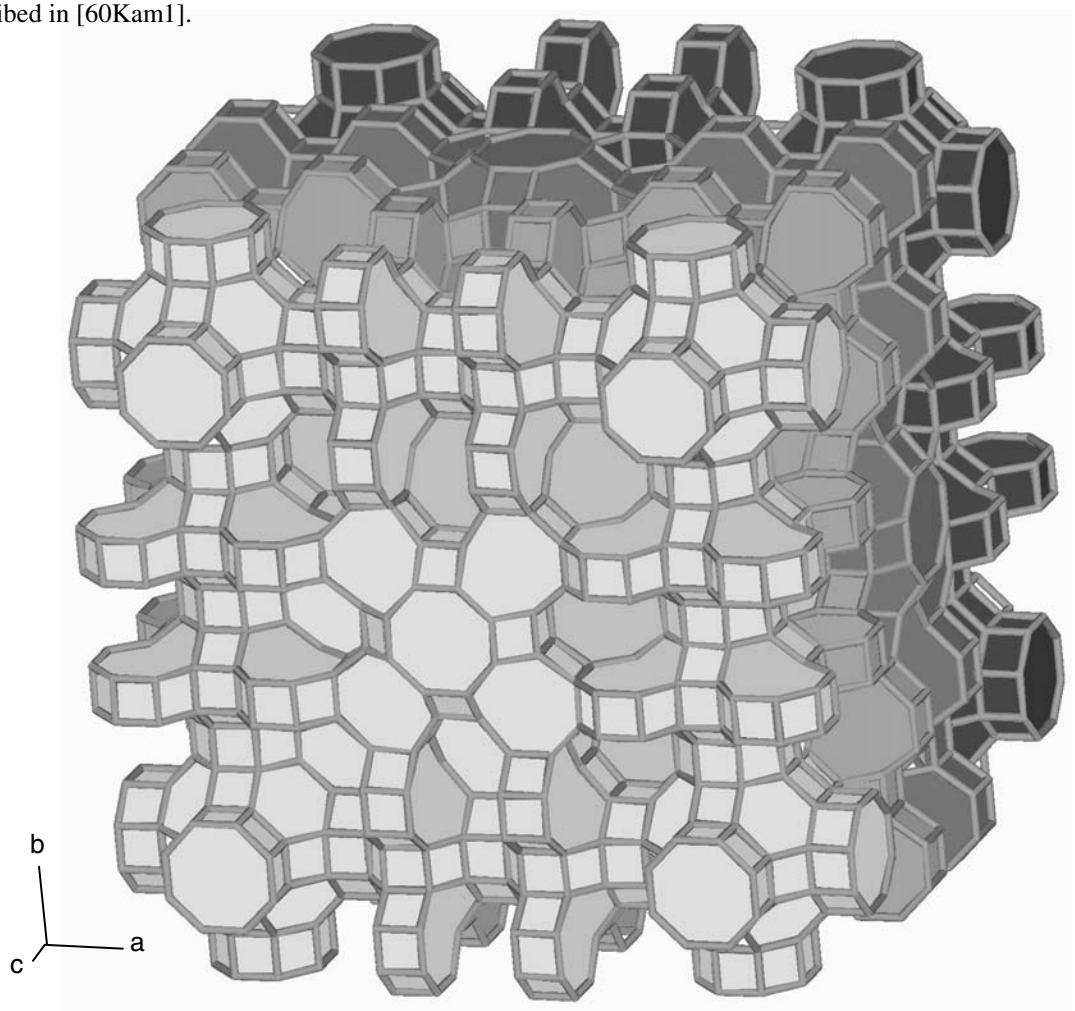
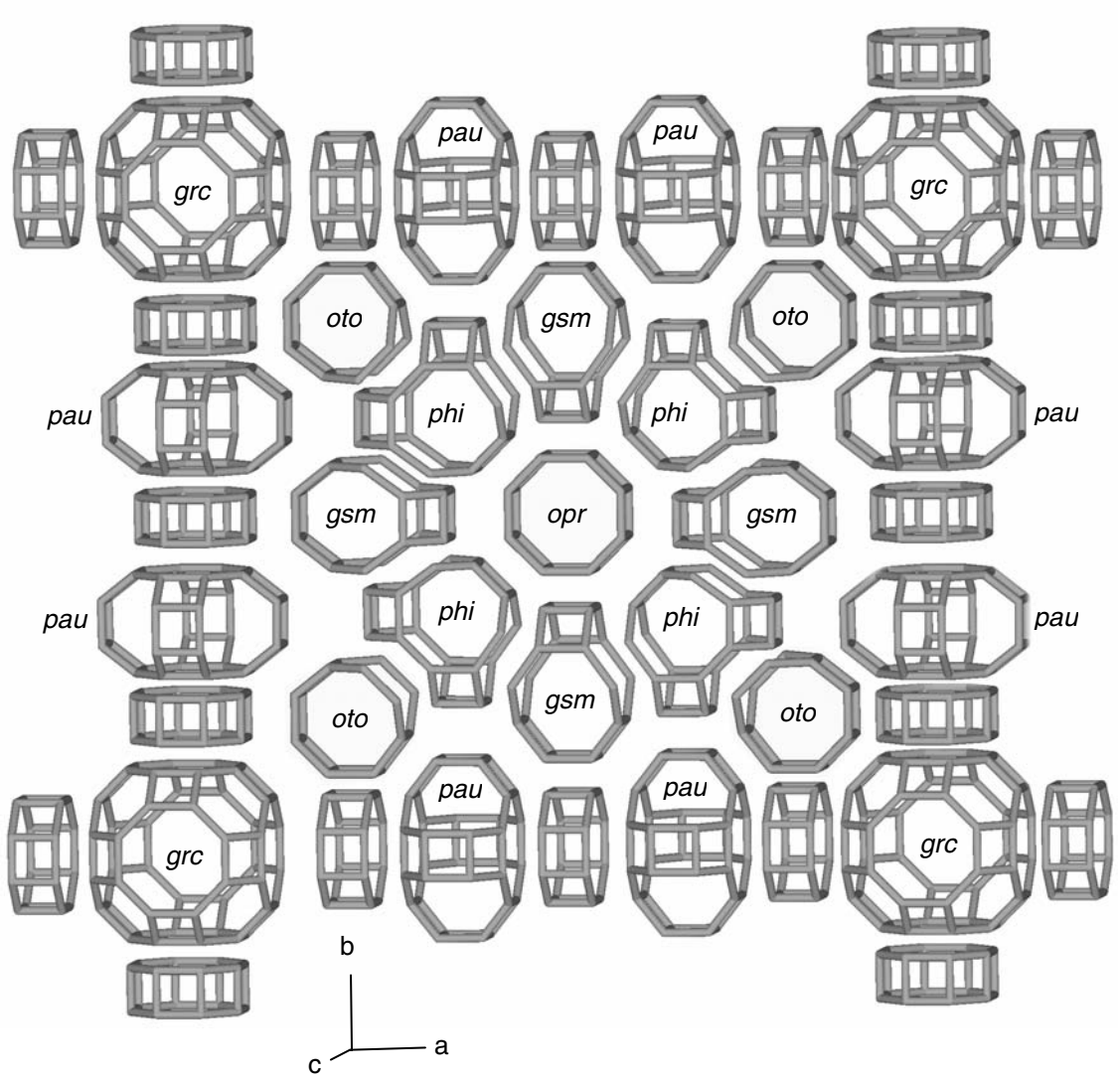


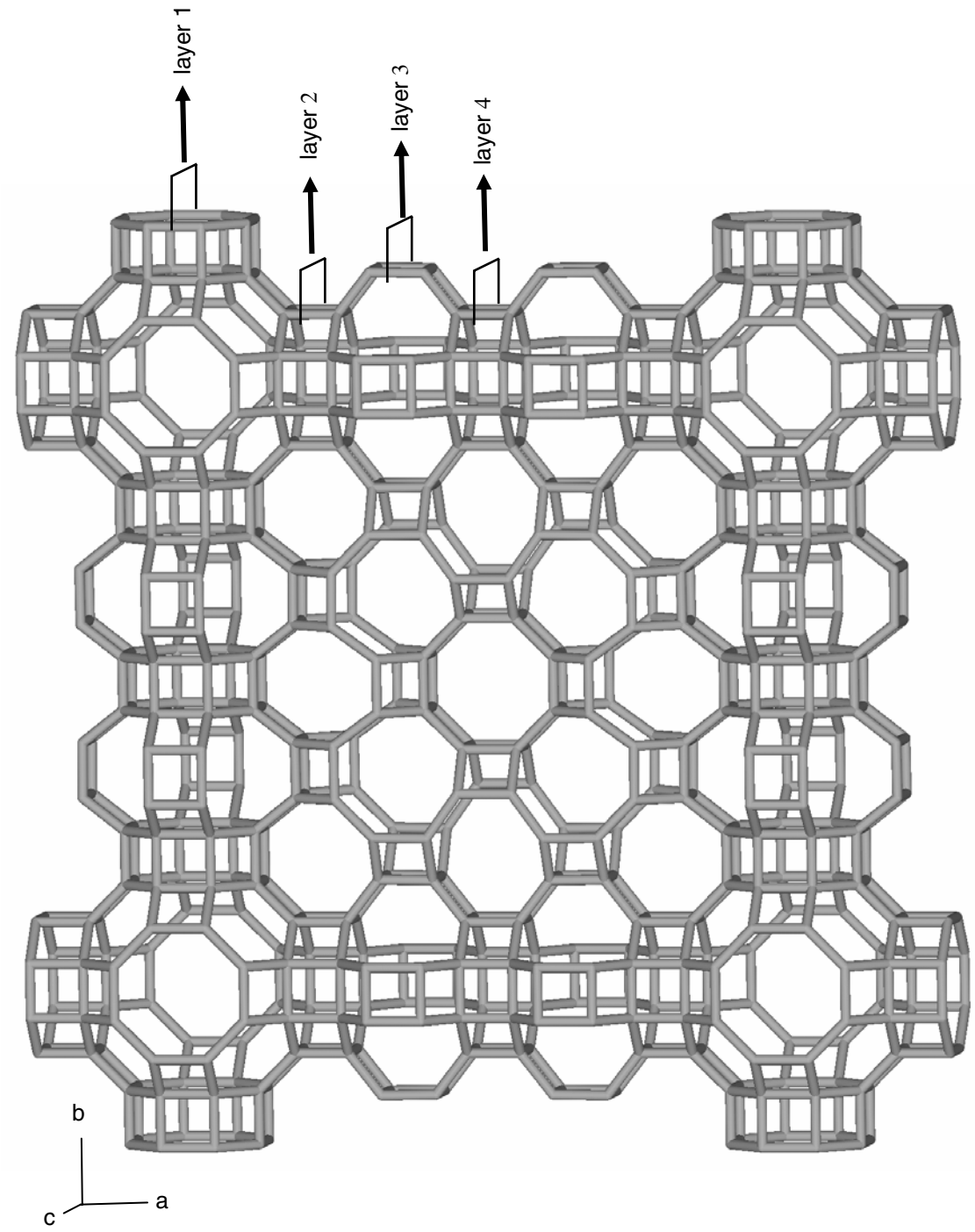
Fig. PAU.1.1. The framework structure of PAU-type compounds in the highest possible topological symmetry $I\,m\,\bar{3}\,m$. View parallel **c** rotated by 20° about **a** and **b**.

The framework structure (Fig. PAU.1.1) was solved by Gordon et al. [66Gor1] in space group $I\,m\,\bar{3}\,m$. It can be described by a close packing of *grc* ($4^{12}6^8 8^6$), *gsm* ($4^4 4^2 8^4$), *kos* ($8^4 12^2$), *opr* ($4^8 8^2$), *oto* ($4^2 4^2 4^1 8^2 8^1$), *pau* ($4^8 4^4 8^4 8^2$), *phi* ($4^4 4^2 4^1 8^2 8^2 8^1$), and *plg* ($4^6 6^2 8^6$) units as shown in Fig. PAU.1.2 forming two separate three-dimensional channel systems parallel to the basis vectors of the unit cell symmetrically related by the I-centering. The channels (**kib** units) are formed by *grc*, *pau* (also called α and γ cage, respectively, in the early zeolite literature), and *opr* units. Therefore, they represent a combination of the channels observed in LTA-type (directly linked *grc* units), RHO-type (alternating sequence of *grc* and *opr* units), and KFI-type (alternating sequence of *grc* and *pau* units) zeolites with similar channel apertures.



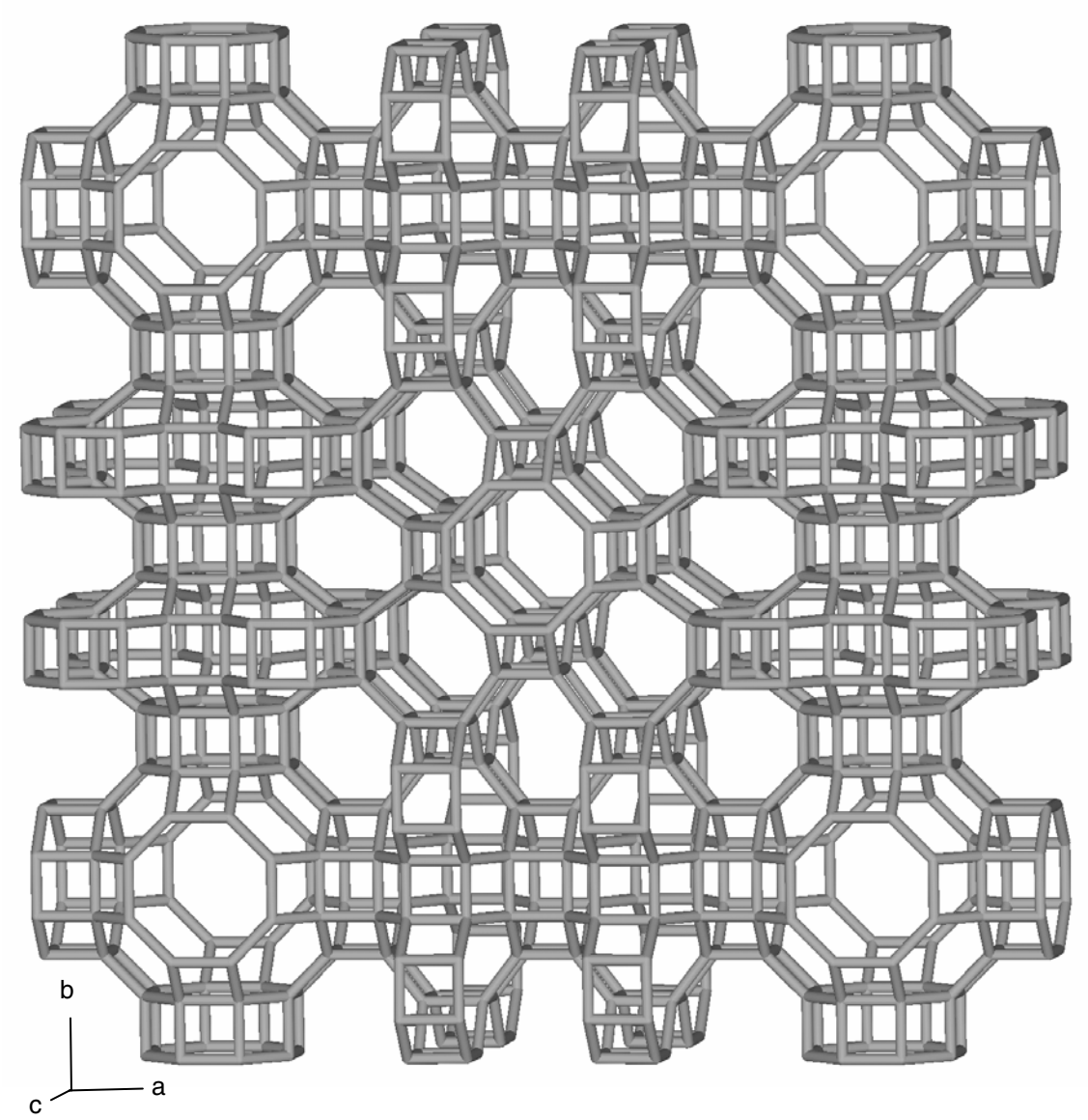
a Linkage of units in the *xy*-layer at $z = 0$. Units not labeled are *opr* units.

Fig. PAU.1.2. Building scheme of the PAU-type framework. View parallel **c** rotated 5° about **a** and 10° about **b**.

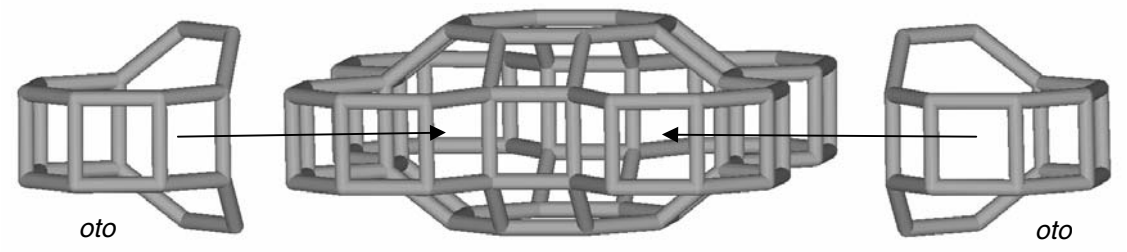


b The complete assemblage of layer 1 shown in a). Arrows indicate the planes of projections shown in the succeeding figures applied to the symmetrically equivalent **c** direction.

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.

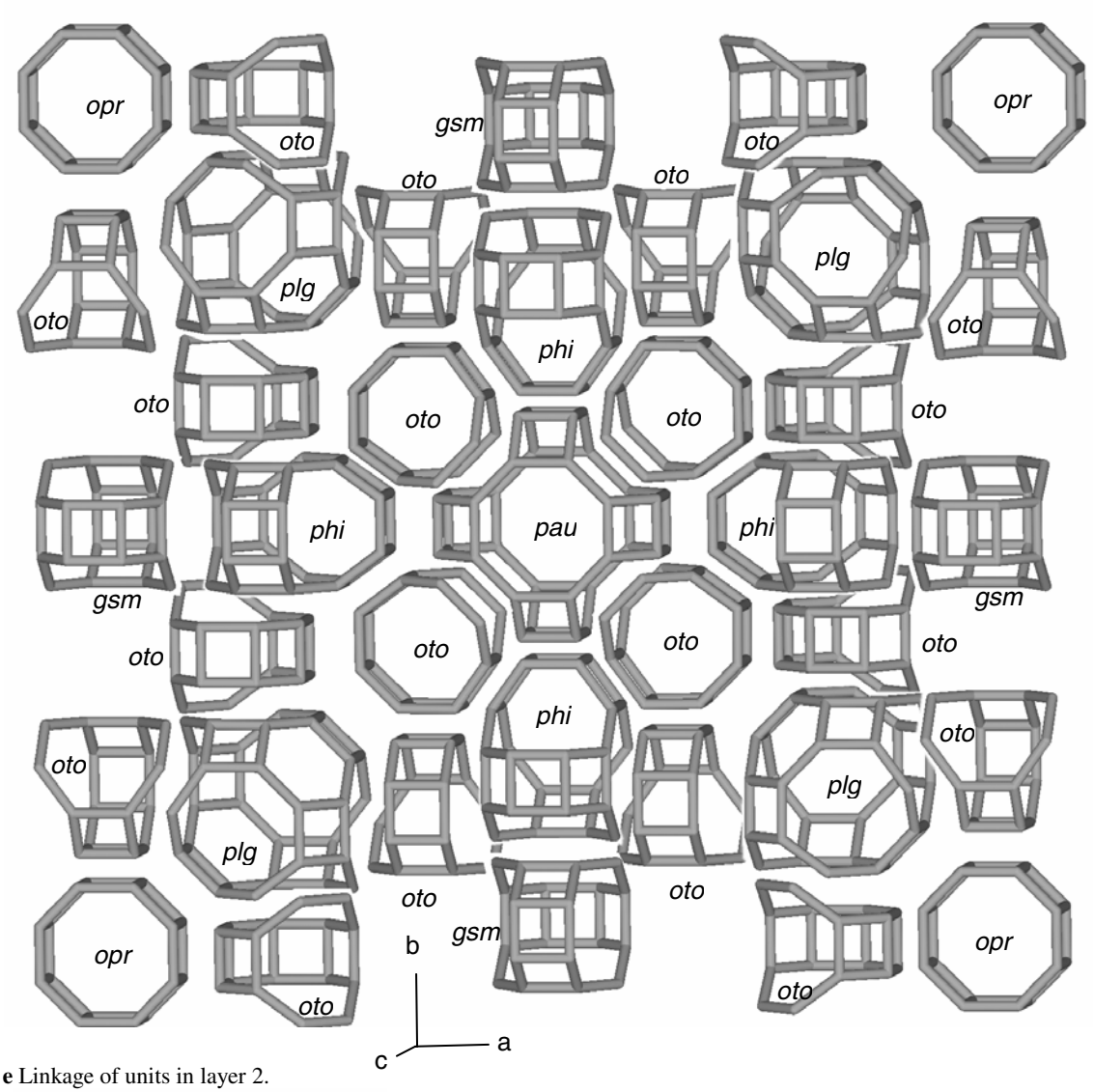


c The assemblage shown in b) extended by two *pau* units in ½, ½, *z* and by the composite units shown in d).

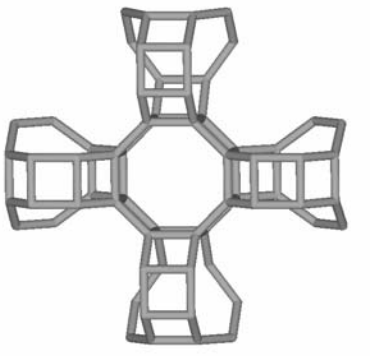


d The composite unit formed by one *pau* and four *oto* units. The two *oto* front units are shown left and right.

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.

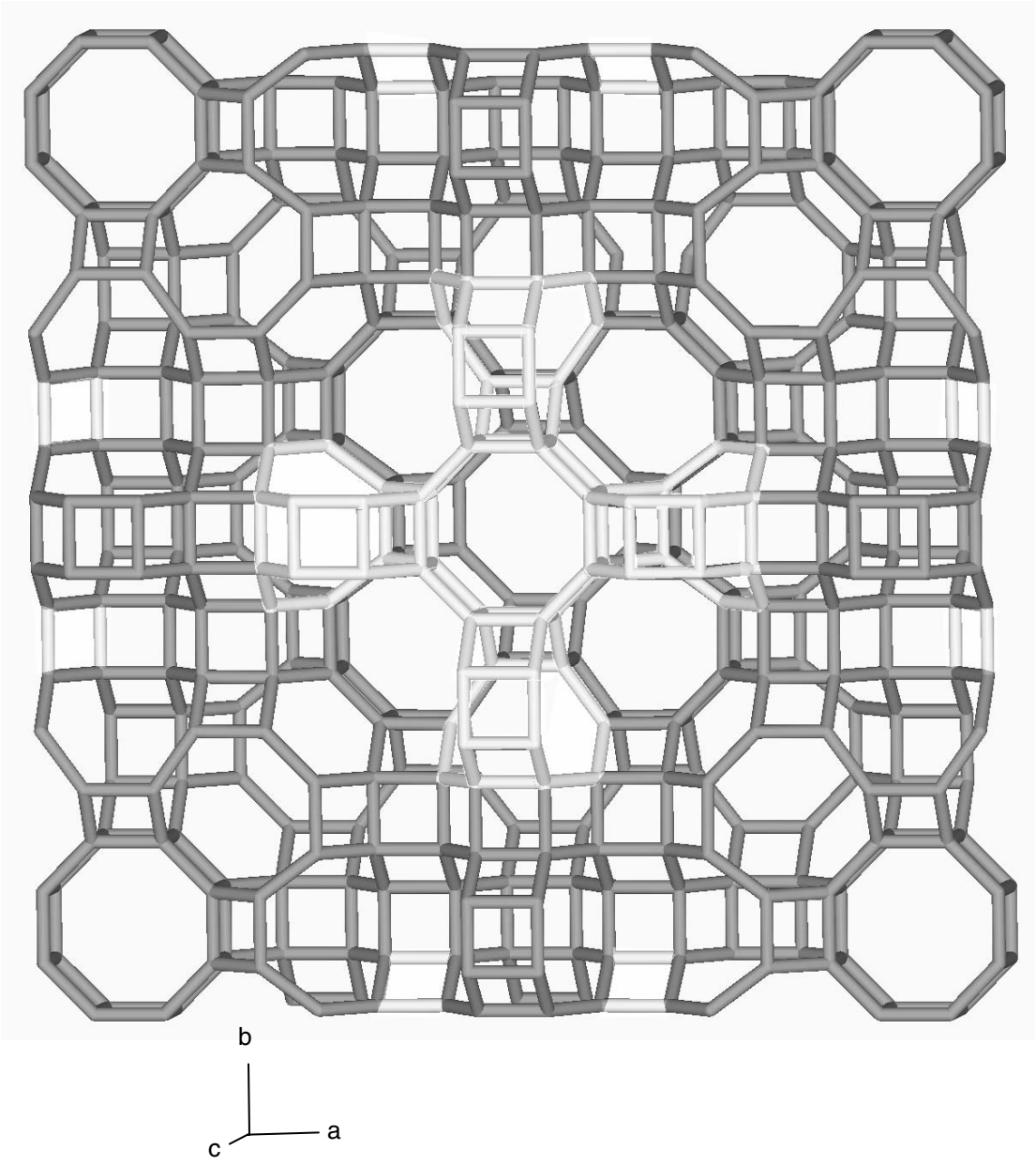


e Linkage of units in layer 2.



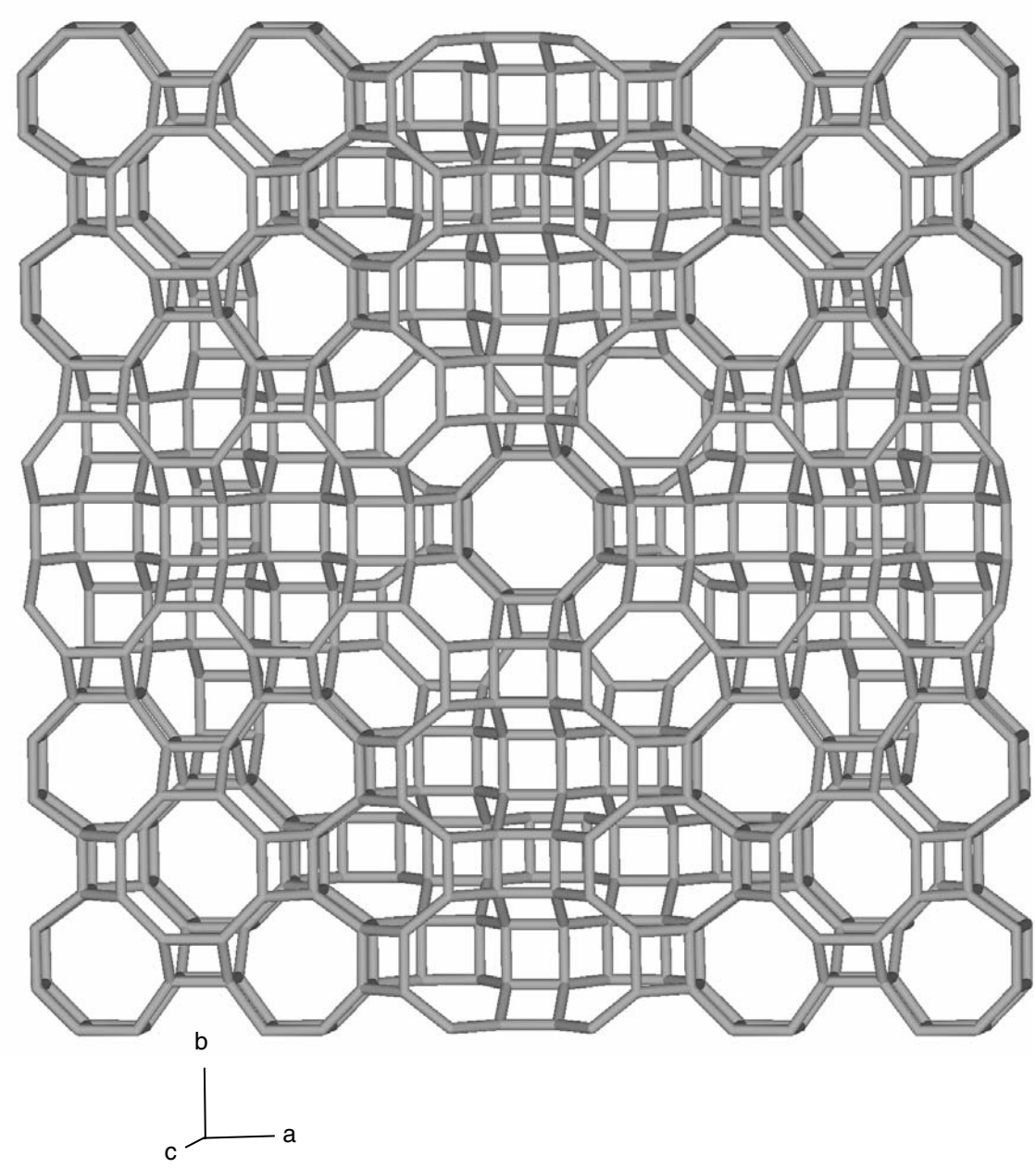
f The linkage of the *opr* unit with four *oto* units.

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.



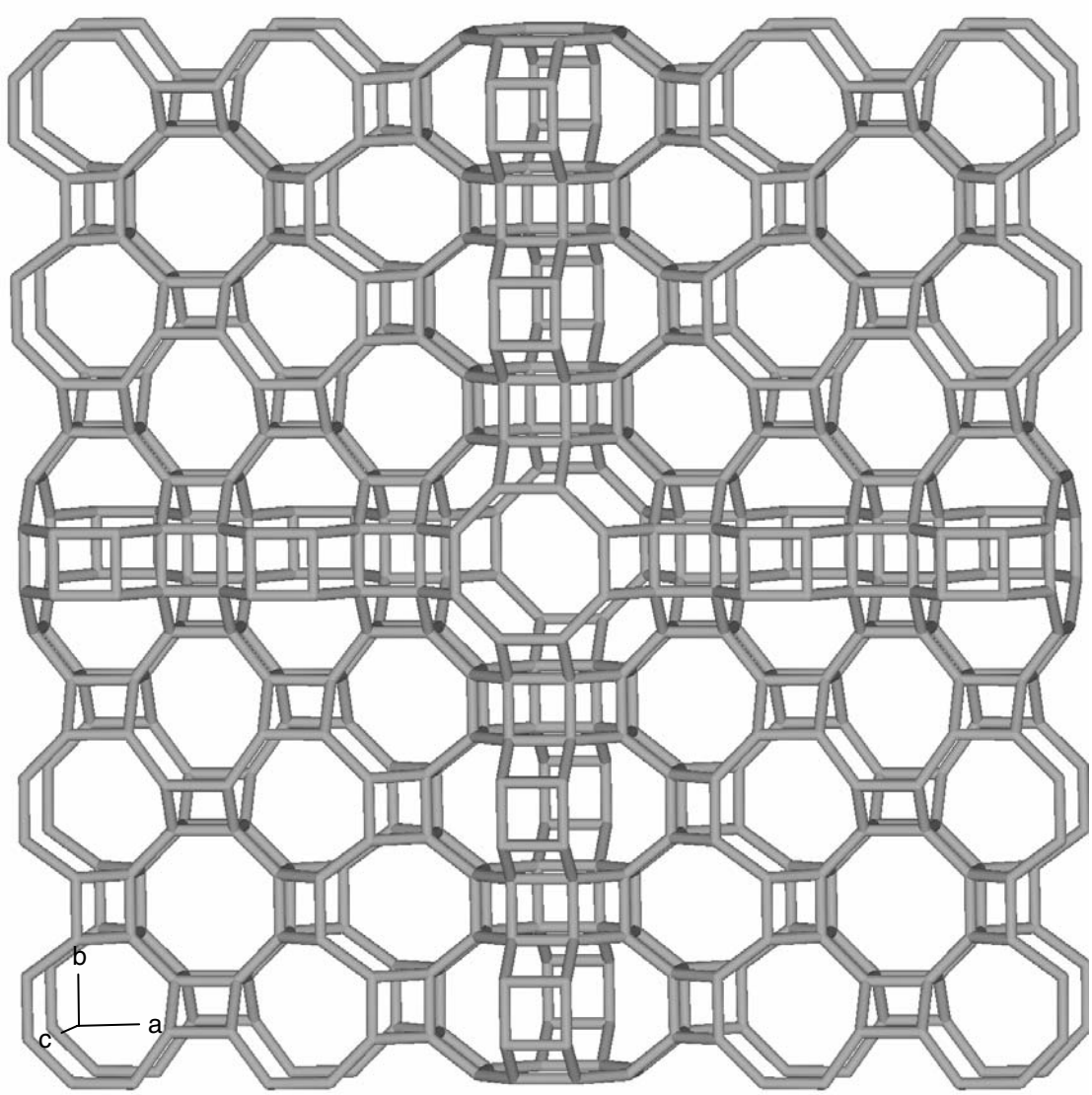
g The assemblage shown in e) extended by some additional bonds from units of the upper layer and by an *opr* and four *oto* units (light grey) separately drawn in f).

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.



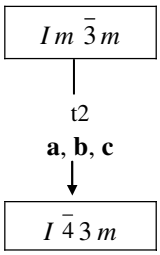
h Linkage of units in layer 3.

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.



i Linkage of units in layer 4 corresponding to layer 1 by I-centering.

Fig. PAU.1.2. (continued) Building scheme of the PAU-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.



PAU-I. Highest possible topological symmetry.

Splitting of T and O atom sites reduces space group symmetry.

PAU-II. Space group observed for partly dehydrated paulingite.

Fig. PAU.1.3 The Bärnighausen tree illustrating the symmetry relationship of the PAU types.

Table PAU.1.1 Atomic site relationships of the PAU types.

PAU-I	PAU-II	PAU-I	PAU-II
$Im\bar{3}m$	$I\bar{4}3m$	$Im\bar{3}m$	$I\bar{4}3m$
T1 [96(l), 1]	T11 [48(h), 1] T12 [48(h), 1]	T2 [96(l), 1]	T21 [48(h), 1] T22 [48(h), 1]
T3 [96(l), 1]	T31 [48(h), 1] T32 [48(h), 1]	T4 [96(l), 1]	T41 [48(h), 1] T42 [48(h), 1]
T5 [96(l), 1]	T51 [48(h), 1] T52 [48(h), 1]	T6 [96(l), 1]	T61 [48(h), 1] T62 [48(h), 1]
T7 [48(i), . . 2]	T7 [48(h), 1]	T8 [48(i), . . 2]	T8 [48(h), 1]
O1 [96(l), 1]	O11 [48(h), 1] O12 [48(h), 1]	O2 [96(l), 1]	O21 [48(h), 1] O22 [48(h), 1]
O3 [96(l), 1]	O31 [48(h), 1] O32 [48(h), 1]	O4 [96(l), 1]	O41 [48(h), 1] O42 [48(h), 1]
O5 [96(l), 1]	O51 [48(h), 1] O52 [48(h), 1]	O6 [96(l), 1]	O61 [48(h), 1] O62 [48(h), 1]
O7 [96(l), 1]	O71 [48(h), 1] O72 [48(h), 1]	O8 [96(l), 1]	O81 [48(h), 1] O82 [48(h), 1]
O9 [48(k), . . *m*]	O91 [24(g), . . *m*] O92 [24(g), . . *m*]	O10[48(k), . . *m*]	O101[24(g), . . *m*] O102[24(g), . . *m*]
O11[48(k), . . *m*]	O111[24(g), . . *m*] O111[24(g), . . *m*]	O12[48(k), . . *m*]	O121[24(g), . . *m*] O122[24(g), . . *m*]
O13[48(k), . . *m*]	O131[24(g), . . *m*] O132[24(g), . . *m*]	O14[48(k), . . *m*]	O141[24(g), . . *m*] O142[24(g), . . *m*]
O15[48(j), *m* . .]	O15 [48(h), 1]	O16[48(j), *m* . .]	O16 [48(h), 1]
O17[48(j), *m* . .]	O17 [48(h), 1]	O18[48(j), *m* . .]	O18 [48(h), 1]
O19[48(j), *m* . .]	O19 [48(h), 1]	O20[48(j), *m* . .]	O20 [48(h), 1]

PAU.2 Compounds and crystal data

Table PAU.2.1 Chemical data.

FD = framework density CE = cation exchange TT = thermal treatment REF = reference
SM = source of material SR = sorbate T = temperature of thermal treatment [K]

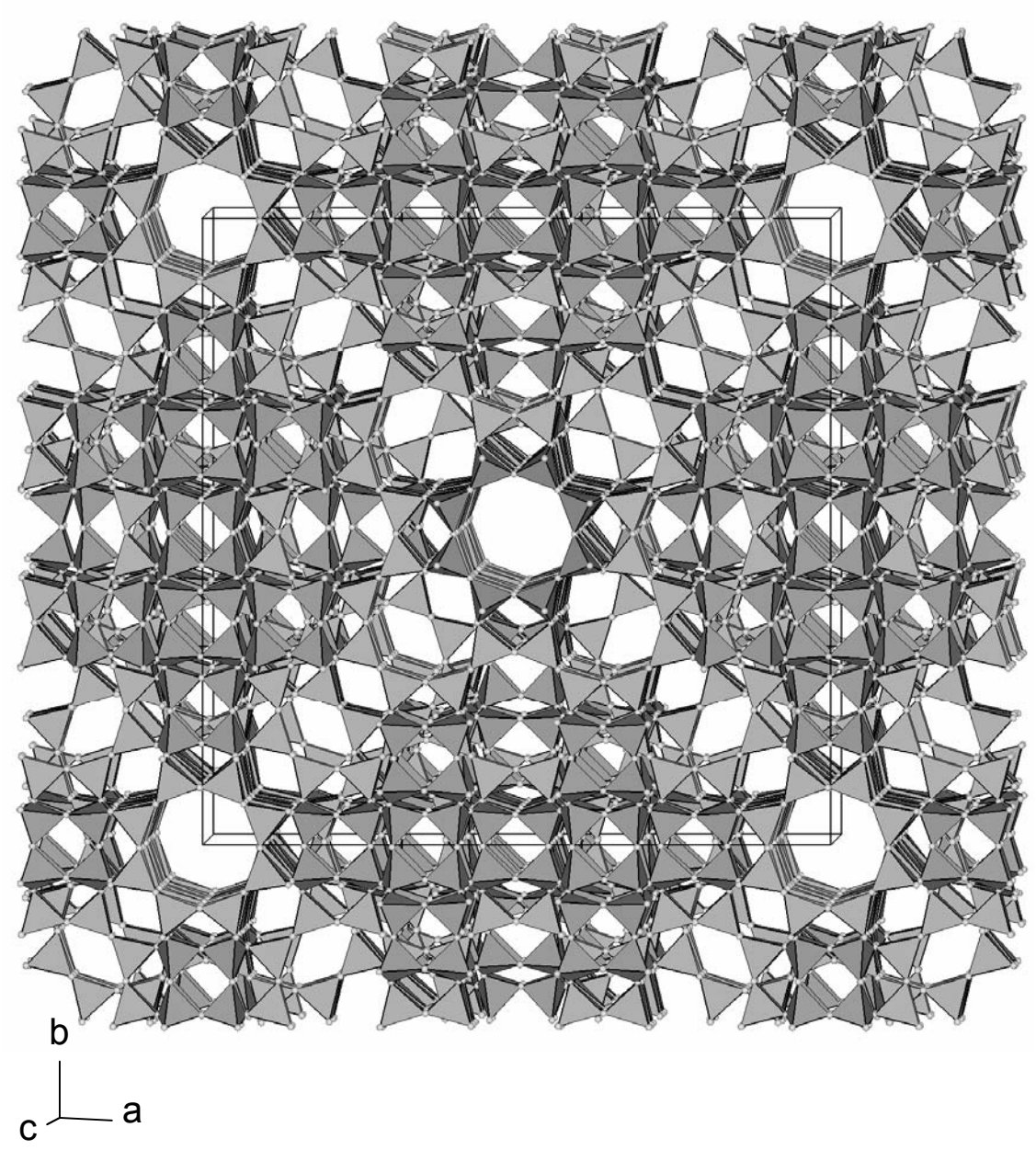
code	chemical composition	FD	SM	CE	SR	TT	T	REF
PAU-I ***I m*** $\bar{3}$ ***m***								
PAU1966a01	$K_{68}Ba_{1.5}Ca_{36}Na_{13} \cdot Al_{152}Si_{520}O_{1344} \cdot 705H_2O$	15.5	M	-	H_2O	-	-	66Gor1
PAU1996a01	$Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 550H_2O$	15.5	M	-	H_2O	-	-	96Bie1
PAU1996a02	$Ba_{13}Ca_{37}K_{57}Na_9SrMg_2 \cdot Al_{171}FeSi_{500}O_{1344} \cdot 527H_2O$	15.5	M	-	H_2O	-	-	96Bie1
PAU1997a01	$Ba_{22.2}Ca_{41.1}Fe_{0.6}K_{36.5}Mg_{0.8}Mn_{0.2}Na_{6.1}Sr_{2.1} \cdot Al_{184.8}Si_{489.4}O_{1344} \cdot 432H_2O$	15.5	M	-	H_2O	-	-	97Len1
PAU-II ***I*** $\bar{4}$ **3** ***m***								
PAU2000a01	$Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 100H_2O$	17.4	M	-	H_2O	D	373	2000Bie1

Table PAU.2.2 Structural parameters of the PAU-type compounds.

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
PAU-I ***I m*** $\bar{3}$ ***m***				
PAU1966a01	35.093(2)	43218	n.s.	66Gor1
PAU1996a01	35.120(9)	43318	n.s.	96Bie1
PAU1996a02	35.103(4)	43255	n.s.	96Bie1
PAU1997a01	35.1231(5)	43329	n.s.	97Len1
PAU-II ***I*** $\bar{4}$ **3** ***m***				
PAU2000a01	33.88(5)	38889	373	2000Bie1

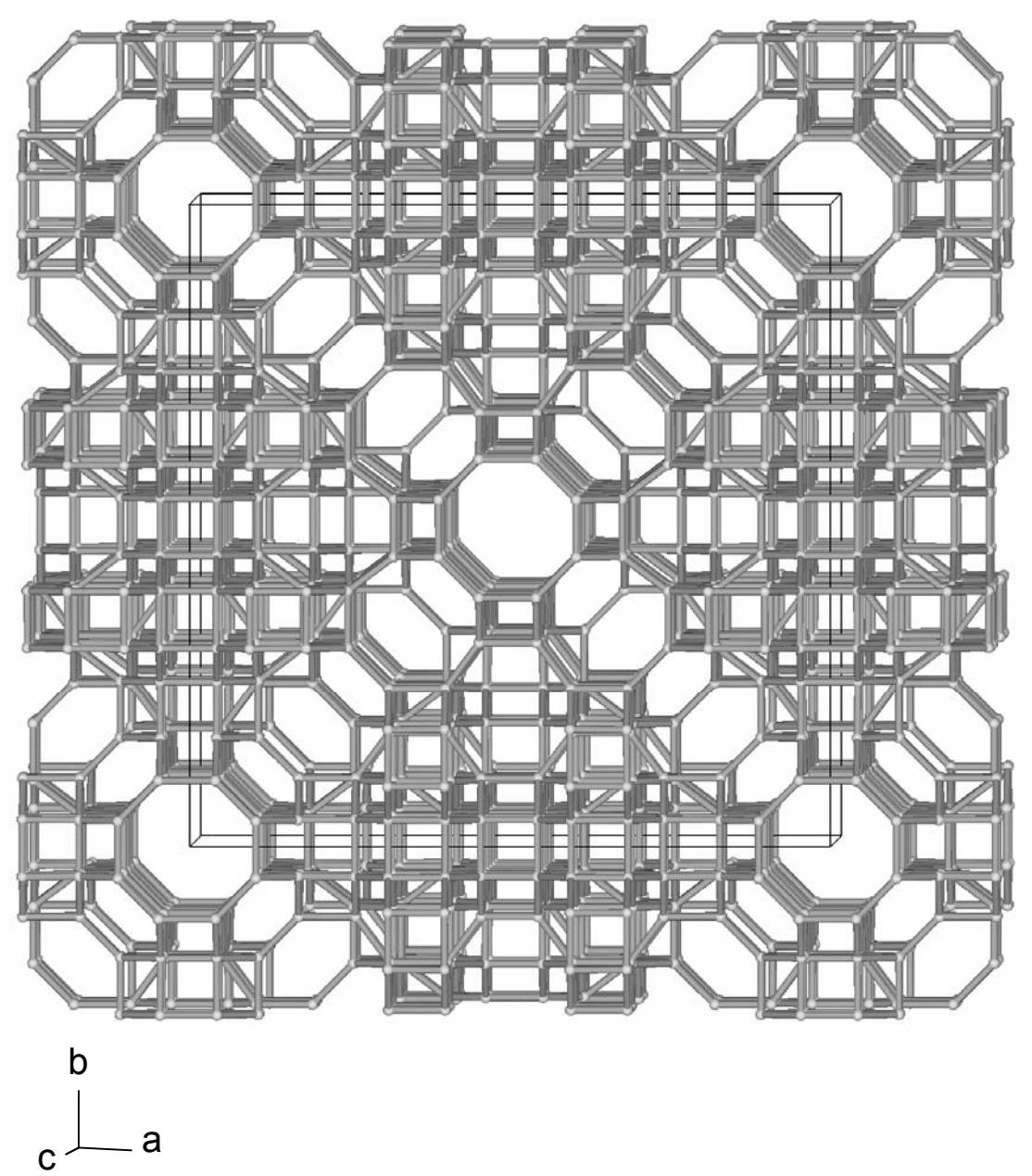
PAU.3 Framework structures

PAU.3.1 PAU-I compound ($Im\bar{3}m$, IT #229)



a Polyhedral representation.

Fig. PAU.3.1.1 Projections of the PAU-I crystal structure of paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 550H_2O$ (PAU1996a01, 96Bie1). View parallel **c** rotated by 1° about **a** and **b**.



b Ball and stick model corresponding to a).

Fig. PAU.3.1.1 (continued) Projections of the PAU-I crystal structure of paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 550H_2O$ (PAU1996a01, 96Bie1). View parallel **c** rotated by 1° about **a** and **b**.

Table PAU.3.1.1 Atomic coordinates and site definitions for PAU-I, paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 550H_2O$ (PAU1996a01, 96Bie1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0.3133(1)	0.2499(1)	0.0980(1)	1.03(8)	1	96(l)	71.33 / 24.67
(Si,Al)2	0.4556(1)	0.1072(1)	0.0441(1)	1.18(8)	1	96(l)	71.33 / 24.67
(Si,Al)3	0.4018(1)	0.1783(1)	0.0444(1)	1.11(8)	1	96(l)	71.33 / 24.67
(Si,Al)4	0.3128(1)	0.1784(1)	0.0448(1)	1.11(8)	1	96(l)	71.33 / 24.67
(Si,Al)5	0.2594(1)	0.1076(1)	0.0445(1)	1.03(8)	1	96(l)	71.33 / 24.67
(Si,Al)6	0.1709(1)	0.1074(1)	0.0439(1)	0.95(8)	1	96(l)	71.33 / 24.67
(Si,Al)7	¼	0.1861(1)	-*y* + ½	1.03(8)	. . 2	48(i)	35.66 / 12.34
(Si,Al)8	¼	0.0981(1)	-*y* + ½	1.11(8)	. . 2	48(i)	35.66 / 12.34
O1	0.2152(2)	0.1216(2)	0.0497(2)	1.9(2)	1	96(l)	96
O2	0.2874(2)	0.1415(2)	0.0586(2)	2.4(2)	1	96(l)	96
O3	0.3571(2)	0.1676(2)	0.0526(2)	2.5(2)	1	96(l)	96
O4	0.4282(2)	0.1424(2)	0.0568(2)	2.9(2)	1	96(l)	96
O5	0.3006(2)	0.2159(2)	0.0695(2)	2.3(2)	1	96(l)	96
O6	0.4150(2)	0.2139(2)	0.0711(2)	2.6(2)	1	96(l)	96
O7	0.3575(2)	0.2618(2)	0.0906(2)	2.2(2)	1	96(l)	96
O8	0.3078(2)	0.2360(2)	0.1418(2)	1.7(2)	1	96(l)	96
O9	0.0713(2)	*x*	0.1599(3)	2.1(2)	. . *m*	48(k)	48
O10	0.4300(2)	*x*	0.2312(2)	2.4(2)	. . *m*	48(k)	48
O11	0.1441(2)	*x*	0.0548(2)	2.1(2)	. . *m*	48(k)	48
O12	0.2860(2)	*x*	0.1966(2)	2.1(2)	. . *m*	48(k)	48
O13	0.2873(2)	*x*	0.0887(2)	2.1(2)	. . *m*	48(k)	48
O14	0.4295(2)	*x*	0.0543(3)	2.9(2)	. . *m*	48(k)	48
O15	0	0.1631(2)	0.0931(2)	2.1(2)	*m* . .	48(j)	48
O16	0	0.2689(2)	0.0961(2)	2.0(2)	*m* . .	48(j)	48
O17	0	0.3046(2)	0.1885(3)	2.2(2)	*m* . .	48(j)	48
O18	0	0.4086(3)	0.1902(3)	2.5(2)	*m* . .	48(j)	48
O19	0	0.4476(3)	0.0950(3)	2.8(2)	*m* . .	48(j)	48
O20	0	0.4490(3)	0.3793(3)	2.5(2)	*m* . .	48(j)	48
Ca1	0.1788(1)	*x*	*x*	3.55(8)	. 3 *m*	16(f)	16
K1	0.1041(2)	*x*	0.3539(3)	6.9(2)	. . *m*	48(k)	31.2(5)
K2	0	0.2527(2)	*y*	7.7(2)	*m.m*2	24(h)	24
OW1	0.1399(4)	*x*	*x*	6.6(4)	. 3 *m*	16(f)	16
OW2	0.2170(4)	*x*	*x*	6.1(3)	. 3 *m*	16(f)	16
OW3	0.2151(5)	*x*	0.1336(6)	2.8(2)	. . *m*	48(k)	48
OW4	0.1423(6)	*x*	0.2231(7)	2.1(2)	. . *m*	48(k)	39(2)
OW5	0.1501(3)	*x*	0.3030(6)	9.1(6)	. . *m*	48(k)	48
OW6	0.1480(4)	*x*	0.4114(9)	15.0(8)	. . *m*	48(k)	48
OW7	0.3578(8)	0.077(1)	0.043(3)	55(2)	1	96(l)	42(3)
OW8	0.2078(3)	*x*	0.0520(6)	8.5(6)	. . *m*	48(k)	48
OW9	0	0.338(2)	0.2802(9)	39(4)	*m* . .	48(j)	48
OW10	0.253(1)	0	0	14(2)	4*m* . *m*	12(e)	12
OW11	0.0287(6)	*x*	0.1259(8)	1.3(7)	. . *m*	48(k)	12(1)
OW12	0.178(1)	0	0	10(2)	4*m* . *m*	12(e)	12
OW13	0.459(4)	0	0	30(7)	4*m* . *m*	12(e)	12
OW14	0.036(1)	*x*	0.090(1)	58(6)	. . *m*	48(k)	48
OW15	0	0.444(2)	0.281(1)	32(3)	*m* . .	48(j)	48
OW16	0	0.6378(6)	*y*	19(2)	*m* .*m* 2	24(h)	24
OW17	0.4676(8)	0.1811(8)	0.1104(8)	10.3(8)	1	96(l)	48(29)

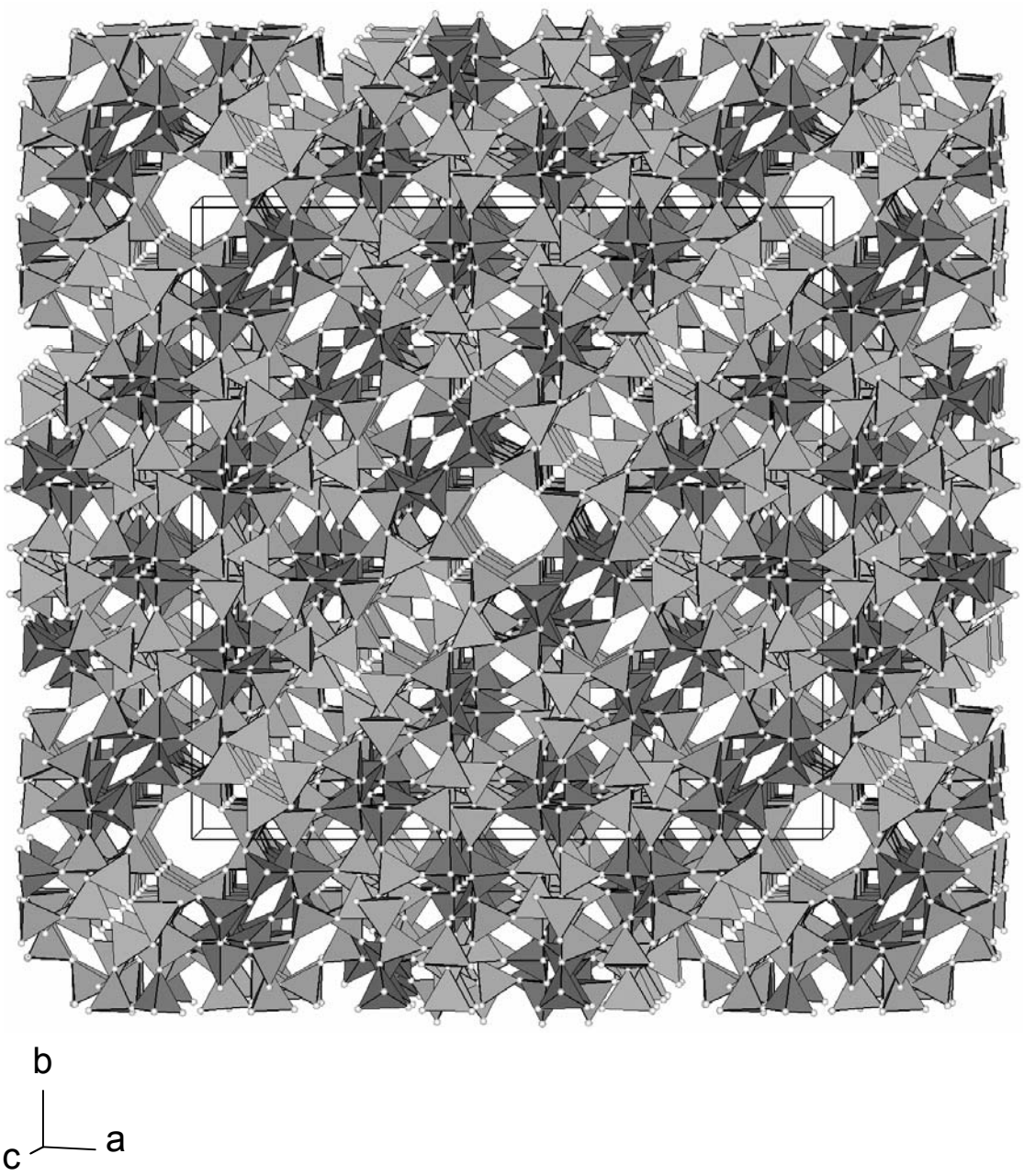
Table PAU.3.1.1 (continued)

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
OW18	0.0257(9)	*x*	0.317(2)	28(3)	. . *m*	48(k)	38(3)
OW19	0.032(1)	*x*	0.382(2)	58(6)	. . *m*	48(k)	48

Table PAU.3.1.2 Selected interatomic distances and angles for PAU-I, paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 550H_2O$ (PAU1996a01, 96Bie1).

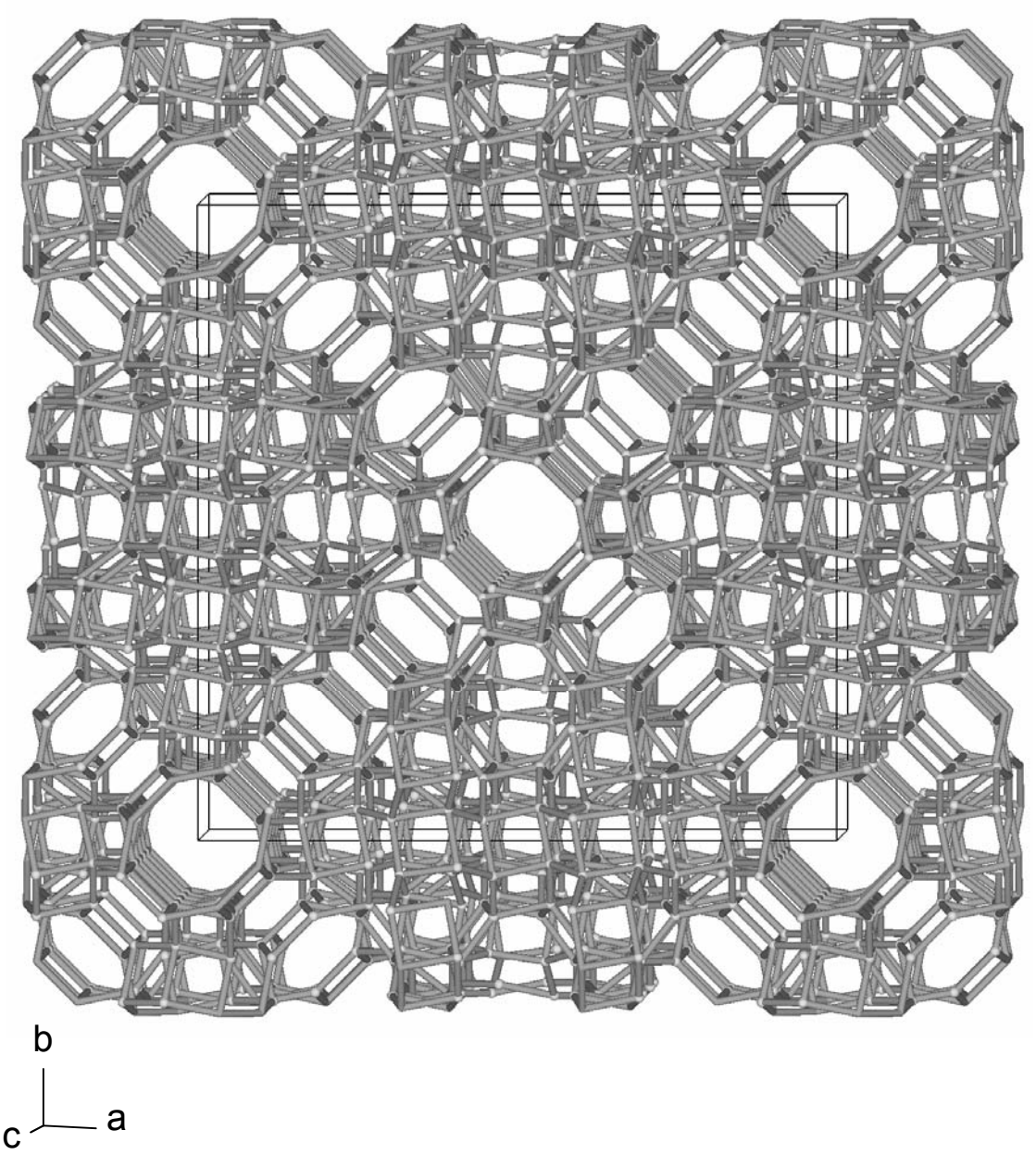
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)1 - O5	1.621(8)	148.2(5)	(Si,Al)2 - O14	1.625(8)	149.2(7)
(Si,Al)1 - O8	1.625(8)	142.1(5)	(Si,Al)2 - O4	1.629(8)	148.5(5)
(Si,Al)1 - O7	1.628(8)	144.9(5)	(Si,Al)2 - O19	1.631(5)	143.4(7)
(Si,Al)1 - O13	1.633(8)	149.3(5)	(Si,Al)2 - O20	1.648(5)	142.3(7)
mean	1.627	146.1	mean	1.633	145.9
(Si,Al)3 - O4	1.624(8)	148.5(5)	(Si,Al)4 - O3	1.625(8)	146.5(5)
(Si,Al)3 - O6	1.630(8)	147.3(5)	(Si,Al)4 - O5	1.634(8)	148.2(5)
(Si,Al)3 - O18	1.632(5)	145.7(7)	(Si,Al)4 - O17	1.638(4)	147.6(7)
(Si,Al)3 - O3	1.640(8)	146.5(5)	(Si,Al)4 - O2	1.646(8)	144.8(5)
mean	1.632	147.0	mean	1.636	146.8
(Si,Al)5 - O2	1.622(8)	144.8(5)	(Si,Al)6 - O9	1.638(8)	148.6(7)
(Si,Al)5 - O10	1.629(8)	148.2(5)	(Si,Al)6 - O11	1.641(8)	147.8(5)
(Si,Al)5 - O1	1.639(8)	142.2(5)	(Si,Al)6 - O15	1.644(4)	139.3(5)
(Si,Al)5 - O16	1.648(4)	142.9(5)	(Si,Al)6 - O1	1.646(8)	142.2(5)
Mean	1.634	144.5	Mean	1.643	144.5
(Si,Al)7 - O12	1.642(7)	150.4(5)	(Si,Al)8 - O7	1.635(8)	144.9(5)
(Si,Al)7 - O12	1.642(7)	150.4(5)	(Si,Al)8 - O7	1.635(8)	144.9(5)
(Si,Al)7 - O8	1.646(8)	142.1(5)	(Si,Al)8 - O6	1.649(7)	147.3(5)
(Si,Al)7 - O8	1.646(8)	142.1(5)	(Si,Al)8 - O6	1.649(7)	147.3(5)
mean	1.644	146.3	mean	1.642	146.1

PAU.3.2 PAU-II compound ($I\bar{4}3m$, IT #217)



a Polyhedral representation.

Fig. PAU.3.2.1 Projections of the PAU-II crystal structure of partly dehydrated paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 100H_2O$ (PAU2000a01, 2000Bie1). View parallel **c** rotated by 1° about **a** and **b**.



b Ball and stick model corresponding to a).

Fig. PAU.3.2.1 (continued) Projections of the PAU-II crystal structure of partly dehydrated paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 100H_2O$ (PAU2000a01, 2000Bie1). View parallel **c** rotated by 1° about **a** and **b**.

Table PAU.3.2.1 Atomic coordinates and site definitions for PAU-II, partly dehydrated paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 100H_2O$ (PAU2000a01, 2000Bie1).

atom	*x*	*y*	*z*	*B* [Å²]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11	0.3219(4)	0.2583(4)	0.0897(5)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)12	0.3063(4)	0.2402(4)	0.8948(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)21	0.4476(4)	0.0983(4)	0.0341(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)22	0.4637(4)	0.1175(4)	0.9465(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)31	0.3945(4)	0.1691(4)	0.0515(5)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)32	0.4095(4)	0.1896(4)	0.9618(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)41	0.3062(4)	0.1871(4)	0.0379(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)42	0.3190(4)	0.1691(4)	0.9496(5)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)51	0.2515(4)	0.1164(4)	0.0510(5)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)52	0.2686(4)	0.0997(5)	0.9643(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)61	0.1627(4)	0.0982(4)	0.0329(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)62	0.1818(4)	0.1166(4)	0.9465(4)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)7	0.2422(4)	0.1783(4)	0.3063(5)	0.71(8)	1	48(h)	35.66 / 12.34
(Si,Al)8	0.2402(5)	0.1049(4)	0.4090(4)	0.71(8)	1	48(h)	35.66 / 12.34
O11	0.2030(9)	0.1209(9)	0.0487(8)	1.6(2)	1	48(h)	48
O12	0.2317(8)	0.1234(9)	0.9527(9)	1.6(2)	1	48(h)	48
O21	0.2684(8)	0.1619(9)	0.0565(9)	1.6(2)	1	48(h)	48
O22	0.3050(8)	0.1227(9)	0.9461(9)	1.6(2)	1	48(h)	48
O31	0.3467(8)	0.1666(9)	0.052(1)	1.6(2)	1	48(h)	48
O32	0.3691(8)	0.1707(8)	0.9472(9)	1.6(2)	1	48(h)	48
O41	0.4115(8)	0.1233(8)	0.0533(9)	1.6(2)	1	48(h)	48
O42	0.4457(9)	0.1632(8)	0.9443(9)	1.6(2)	1	48(h)	48
O51	0.3050(9)	0.2330(9)	0.0527(9)	1.6(2)	1	48(h)	48
O52	0.2993(9)	0.1945(9)	0.9129(9)	1.6(2)	1	48(h)	48
O61	0.412(1)	0.1921(9)	0.0886(9)	1.6(2)	1	48(h)	48
O62	0.4144(9)	0.2348(9)	0.9496(9)	1.6(2)	1	48(h)	48
O71	0.3722(9)	0.2632(9)	0.0892(9)	1.6(2)	1	48(h)	48
O72	0.3452(9)	0.2625(9)	0.9124(9)	1.6(2)	1	48(h)	48
O81	0.3087(9)	0.2343(9)	0.1313(9)	1.6(2)	1	48(h)	48
O82	0.3075(9)	0.2371(9)	0.8465(9)	1.6(2)	1	48(h)	48
O91	0.0508(9)	*x*	0.158(1)	1.6(2)	. . *m*	24(g)	24
O92	0.0951(9)	*x*	0.828(1)	1.6(2)	. . *m*	24(g)	24
O101	0.4074(8)	*x*	0.765(1)	1.6(2)	. . *m*	24(g)	24
O102	0.4478(9)	*x*	0.234(1)	1.6(2)	. . *m*	24(g)	24
O111	0.1256(9)	*x*	0.044(1)	1.6(2)	. . *m*	24(g)	24
O112	0.1598(9)	*x*	0.952(1)	1.6(2)	. . *m*	24(g)	24
O121	0.2665(9)	*x*	0.193(1)	1.6(2)	. . *m*	24(g)	24
O122	0.3007(9)	*x*	0.805(1)	1.6(2)	. . *m*	24(g)	24
O131	0.3032(9)	*x*	0.091(1)	1.6(2)	. . *m*	24(g)	24
O132	0.2652(9)	*x*	0.907(1)	1.6(2)	. . *m*	24(g)	24
O141	0.4075(8)	*x*	0.048(1)	1.6(2)	. . *m*	24(g)	24
O142	0.4472(8)	*x*	0.948(1)	1.6(2)	. . *m*	24(g)	24
O15	-0.0146(9)	0.1628(9)	0.088(1)	1.6(2)	1	48(h)	48
O16	0.0128(9)	0.2716(9)	0.0942(9)	1.6(2)	1	48(h)	48
O17	-0.0113(9)	0.3041(9)	0.1862(9)	1.6(2)	1	48(h)	48
O18	0.0123(9)	0.4127(9)	0.1871(9)	1.6(2)	1	48(h)	48
O19	-0.0129(9)	0.4425(9)	0.0943(8)	1.6(2)	1	48(h)	48
O20	-0.0107(8)	0.4506(9)	0.3785(8)	1.6(2)	1	48(h)	48

Table PAU..3.2.1 (continued)

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Ca1	0.224(2)	*x*	*x*	3	. 3 *m*	8(c)	2.2(4)
K1	0.094(1)	*x*	0.347(2)	5(2)	. . *m*	24(g)	9.1(7)
K11	0.402(1)	*x*	0.138(2)	3(2)	. . *m*	24(g)	7.2(7)
K2	0.266(1)	*x*	0.992(2)	6(2)	. . *m*	24(g)	9.1(5)
K22	0.220(1)	*x*	0.967(2)	9(2)	. . *m*	24(g)	14.9(5)
K3	0.239(2)	0	0	17(4)	2 *.m m*	12(e)	9.4(6)
K4	0.363(1)	*x*	0.122(2)	24(2)	. . *m*	24(g)	16.8(7)
K5	0	½	½	5(2)	$\bar{4}$ 2. *m*	6(b)	2.9(3)
K6	0.665(2)	0.335(2)	0.073(2)	32(16)	1	48(h)	11(1)
K7	0.481(1)	*x*	0.057(2)	3	. . *m*	24(g)	5.8(5)
OW1	0.834(3)	0	0	8(2)	2. *m m*	12(e)	12
OW2	0.141(1)	*x*	0.332(1)	5(2)	. . *m*	24(g)	24
OW3	0.210(3)	*x*	0.005(4)	3	. . *m*	24(g)	9.1(5)
OW4	0.159(1)	*x*	0.707(2)	9(2)	. . *m*	24(g)	24
OW5	0.033(4)	*x*	0.317(5)	22(6)	. . *m*	24(g)	13(3)
OW6	0.039(3)	*x*	0.631(5)	12(7)	. . *m*	24(g)	11(2)
OW7	0.313(3)	*x*	*x*	16	. 3 *m*	8(c)	6.2(6)

Table PAU.3.2.2 Selected interatomic distances and angles for PAU-II, partly dehydrated paulingite, $Ba_2Ca_{59}K_{36}Na_{14} \cdot Al_{173}Si_{499}O_{1344} \cdot 100H_2O$ (PAU2000a01, 2000Bie1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11 - O51	1.62(3)	137(2)	(Si,Al)12 - O72	1.63(3)	139(2)
(Si,Al)11 - O131	1.65(3)	135(2)	(Si,Al)12 - O82	1.64(3)	146(2)
(Si,Al)11 - O81	1.69(3)	139(2)	(Si,Al)12 - O52	1.68(3)	134(2)
(Si,Al)11 - O71	1.71(3)	138(2)	(Si,Al)12 - O132	1.69(3)	140(3)
mean	1.67	137	mean	1.66	140
(Si,Al)21 - O19	1.61(3)	135(2)	(Si,Al)22 - O20	1.60(3)	144(2)
(Si,Al)21 - O41	1.62(3)	137(2)	(Si,Al)22 - O141	1.62(3)	143(2)
(Si,Al)21 - O142	1.67(3)	135(2)	(Si,Al)22 - O42	1.67(3)	140(2)
(Si,Al)21 - O20	1.70(3)	144(2)	(Si,Al)22 - O19	1.74(3)	135(2)
mean	1.65	138	mean	1.66	141
(Si,Al)31 - O18	1.59(3)	146(2)	(Si,Al)32 - O32	1.59(3)	149(2)
(Si,Al)31 - O61	1.60(4)	134(2)	(Si,Al)32 - O62	1.60(3)	129(2)
(Si,Al)31 - O31	1.62(3)	146(2)	(Si,Al)32 - O42	1.63(3)	140(2)
(Si,Al)31 - O41	1.66(3)	137(2)	(Si,Al)32 - O18	1.72(3)	146(2)
mean	1.62	141	mean	1.64	141
(Si,Al)41 - O31	1.61(3)	146(2)	(Si,Al)42 - O17	1.53(4)	149(2)
(Si,Al)41 - O51	1.63(3)	137(2)	(Si,Al)42 - O22	1.65(3)	132(2)
(Si,Al)41 - O21	1.66(3)	135(2)	(Si,Al)42 - O52	1.65(3)	134(2)
(Si,Al)41 - O17	1.67(3)	149(2)	(Si,Al)42 - O32	1.70(3)	149(2)
mean	1.64	142	mean	1.63	141

Table PAU.3.2.2 (continued)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)51 - O16	1.65(3)	135(2)	(Si,Al)52 - O12	1.54(3)	140(2)
(Si,Al)51 - O11	1.65(3)	142(2)	(Si,Al)52 - O22	1.58(3)	132(2)
(Si,Al)51 - O21	1.66(3)	135(2)	(Si,Al)52 - O16	1.66(3)	135(2)
(Si,Al)51 - O102	1.68(3)	137(2)	(Si,Al)52 - O101	1.71(3)	128(2)
Mean	1.66	137	Mean	1.62	134
(Si,Al)61 - O111	1.61(3)	147(3)	(Si,Al)62 - O92	1.62(3)	138(2)
(Si,Al)61 - O15	1.65(3)	128(2)	(Si,Al)62 - O112	1.65(3)	142(2)
(Si,Al)61 - O11	1.66(3)	142(2)	(Si,Al)62 - O12	1.72(3)	140(2)
(Si,Al)61 - O91	1.73(3)	130(2)	(Si,Al)62 - O15	1.76(3)	128(2)
Mean	1.66	137	Mean	1.69	137
(Si,Al)7 - O82	1.61(3)	146(2)	(Si,Al)8 - O71	1.56(3)	138(2)
(Si,Al)7 - O81	1.62(3)	139(2)	(Si,Al)8 - O72	1.70(3)	139(2)
(Si,Al)7 - O122	1.62(3)	142(2)	(Si,Al)8 - O61	1.72(3)	134(2)
(Si,Al)7 - O121	1.66(4)	136(3)	(Si,Al)8 - O62	1.74(3)	129(2)
mean	1.63	141	mean	1.68	135

PAU.4 Chemical composition

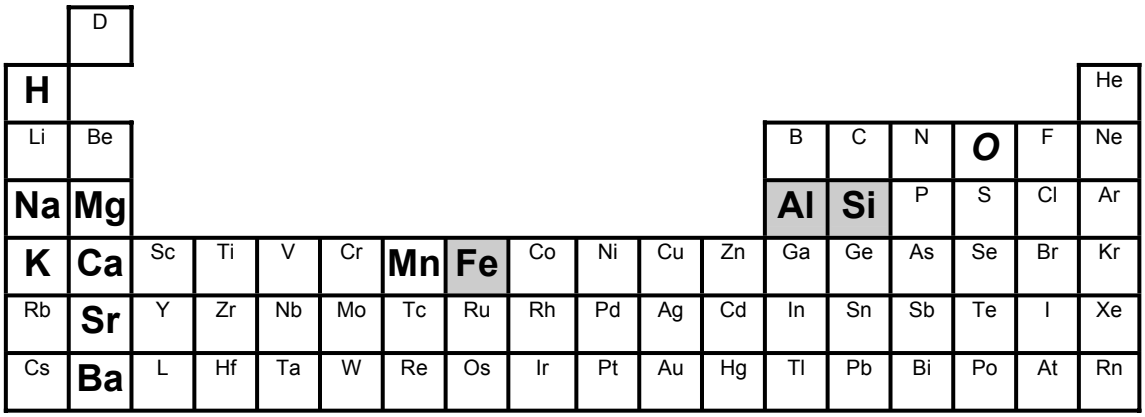


Fig. PAU.4.1 Chemical elements (highlighted) occurring in PAU-type compounds. Framework cations are in grey fields.

PAU.5 Flexibility and apertures

The mean T-O-T angle in hydrated paulingite (PAU1996a01) measures 146°. Upon partial dehydration the unit cell constant shrinks by 3.7% (Table PAU.2.2, the reduction in volume is 11%) and the overall mean T-O-T angle is reduced to 138°. This is a clear indication that the PAU-type framework is collapsible [92Bau1]. The individual T-O-T angles corotate as the volume of the unit cell is reduced. This

makes the PAU-type fundamentally different from the FAU-, KFI- and LTA-type frameworks (see the respective chapters for details). The PAU-type is most likely similar to the GIS-, NAT- or RHO-types, but so far we do not have enough experimental data to document it the same way as it can be done for the other mentioned types. All we can do now is to compare the partly dehydrated phase with hydrated paulingite. The relationship of the PAU-type framework to the GIS-type framework has been emphasized by [83And1], who describe it as an interpenetrating sixling of parts of the GIS-type structure.

The 8-rings in the hydrated framework of PAU-type are more compressed, with openings of about 3.5 Å by 3.5 Å, than in the LTA-type (more than 4 Å by 4 Å).

PAU.6 Other information

Useful properties have not been reported for PAU-type compounds.

The varied chemistry of the pore filling of paulingites from different localities has been studied by [82Tsc1]. Paulingite has been synthesized successfully (ECR-18) analogously to the natural form [99Vau1] and as a gallium silicate [2005Kim1].

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