MER

MER.1 Zeolite framework type and topology

The framework type code is named after the mineral **MER**linoite, $K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$, first found in the nepheline melilitite from Cupaello, Italy, and described in [77Pas1]. The framework structure (Fig. MER.1.1), solved by Galli et al. [79Gal1], is isostructural with a synthetic barium chloroaluminosilicate [67Bel1, 72Sol1] and other synthetic analogues listed in Table MER.2.1. It can be described as being built from *opr* ($4^8 8^2$), *pau* ($4^8 4^4 8^4 8^2$), and *ste* ($4^2 8^4$) units as shown in Fig. MER.1.2 forming a three-dimensional channel system parallel to the basis vectors of the unit cell.

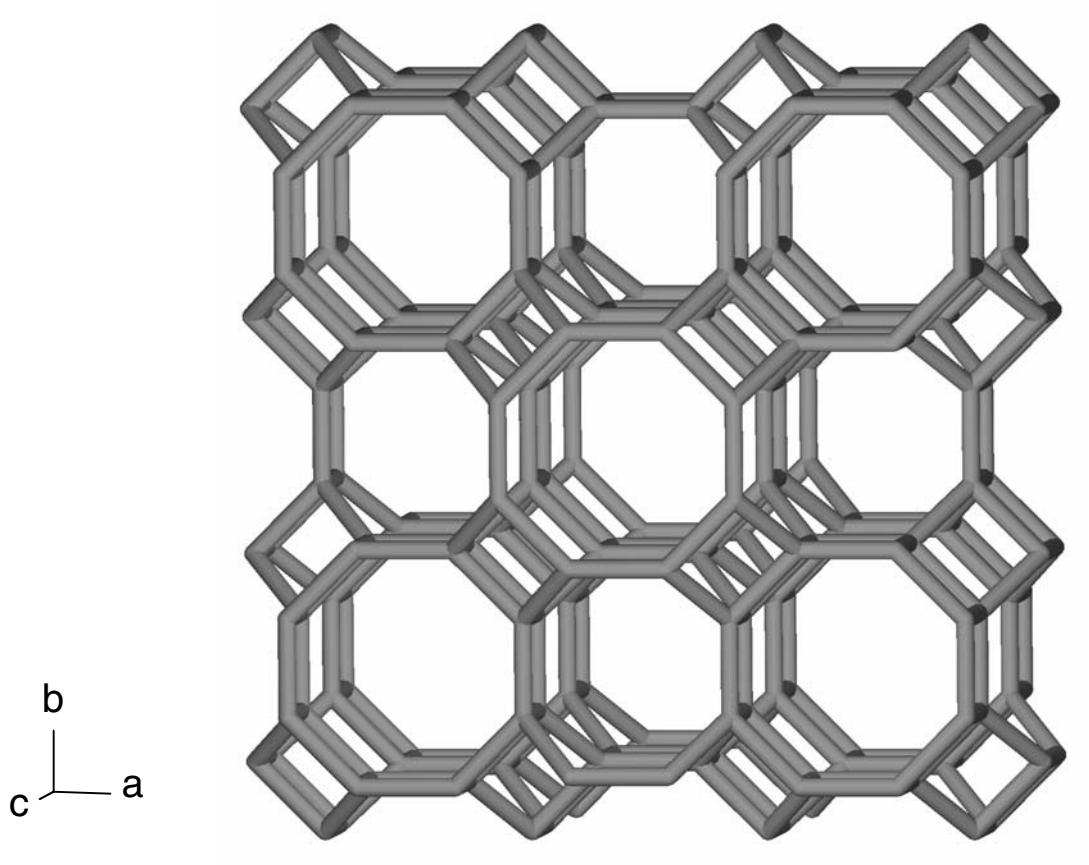
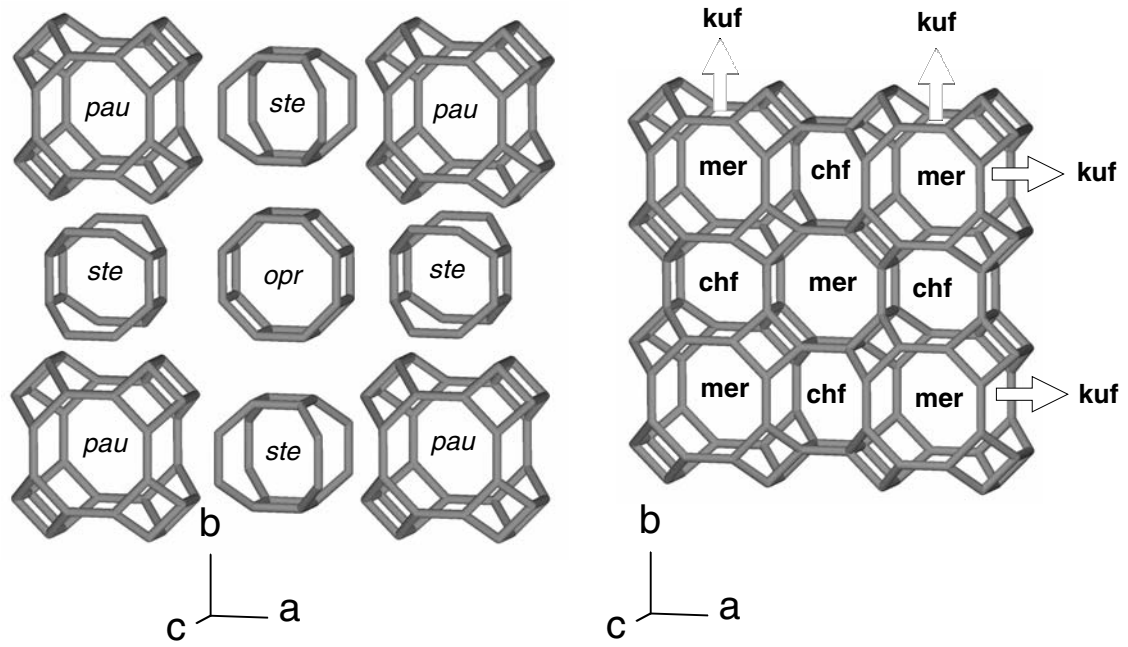


Fig. MER.1.1. The framework structure of MER-type compounds in the highest possible topological symmetry *I* 4/*m m m* (MER1988a01, 88van1). View parallel **c** rotated by 4° about **a** and 8° about **b**.



a Linkage of *opr*, *pau*, and *ste* units.

b The complete assemblage shown in a). The 8-ring channels are indicated by their 1D unit names.

Fig. MER.1.2 Building scheme of the MER-type framework. View parallel **c** rotated by 8° about **a** and 16° about **b**. Subsequent layers in front and in the rear are shifted by ½, ½, ½ according to the I-centering of the unit cell yielding an alternating sequence of *opr* and *pau* units (**mer** channel) parallel **c**.

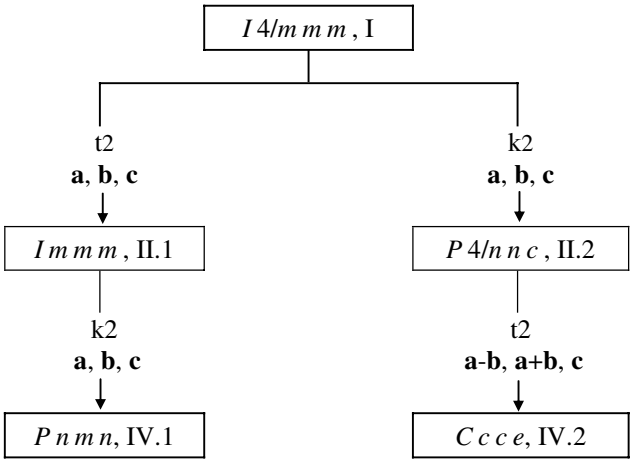


Fig. MER.1.3 The Bärnighausen tree illustrating the symmetry relationship of the MER types.

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

MER-I *I* 4/*m m m*	MER-II.1 *I m m m*	MER-IV.1 *P n m n*
T1 [32(o), 1]	T11 [16(o), 1]	T11a [8(h), 1] T11b [8(h), 1]
	T12 [16(o), 1]	T12a [8(h), 1] T12b [8(h), 1]
O1 [16(n), . *m* .]	O11 [8(l), *m* . .]	O11 [8(h), 1]
	O12 [8(m), . *m* .]	O12a [4(g), . *m* .] O12b [4(g), . *m* .]
O2 [16(m), . . *m*]	O2 [16(o), 1]	O21 [8(h), 1] O22 [8(h), 1]
O3 [16(l), *m* . .]	O31 [8(n), . . *m*]	O31 [8(h), 1]
	O32 [8(n), . . *m*]	O32 [8(h), 1]
O4 [16(k), . . 2]	O4 [16(o), 1]	O41 [8(h), 1] O42 [8(h), 1]

MER-I *I* 4/*m m m*	MER-II.2 *P* 4/*n n c*	MER-IV.2 *C c c e*
T1 [32(o), 1]	T11 [16(k), 1]	T11a [16(i), 1] T11b [16(i), 1]
	T12 [16(k), 1]	T12a [16(i), 1] T12b [16(i), 1]
O1 [16(n), . *m* .]	O1 [16(k), 1]	O11 [16(i), 1] O12 [16(i), 1]
O2 [16(m), . . *m*]	O2 [16(k), 1]	O21 [16(i), 1] O22 [16(i), 1]
O3 [16(l), *m* . .]	O3 [16(k), 1]	O31 [16(i), 1] O32 [16(i), 1]
O4 [16(k), . . 2]	O4 [16(k), 1]	O41 [16(i), 1] O42 [16(i), 1]

MER.2 Compounds and crystal data

Table MER.2.1 Chemical data.

M = mineral/compound name SM = source of material SR = sorbate TT = thermal treatment REF = reference
FD = framework density CE = cation exchange TE = template T = temperature of thermal treatment

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MER-I ***I 4/m m m***									
MER1972a01	$Ba_{12} \cdot Al_{12}Si_{20}O_{64} \cdot 8Cl\ 4OH$[1])		16.0	S	-	Cl, OH	-	-	72Sol1
MER1988a01	$Si_{32}O_{64}$	-	16.2	T	-	-	-	-	88van1
MER-II.1 ***I m m m***									
MER1979a01	$K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$	merlinoite	16.0	M	-	H_2O	-	-	79Gal1
MER1985a01	$K_5Ba_3Na \cdot Al_{12}Si_{20}O_{64} \cdot 20H_2O$	merlinoite	15.8	M	-	H_2O	-	-	85Bat1
MER1996a01	$K_{10} \cdot Al_{10}Si_{22}O_{64} \cdot 20H_2O$	zeolite W	15.9	S	-	H_2O	-	-	96Bie1
MER1998a01	$(C_8H_{20}N)_{0.8}\ H_{0.7}K_{5.2} \cdot Al_{6.7}Si_{25.3}O_{64} \cdot 12H_2O$		16.1	S	-	TEA	C	373	98Bar1
MER1999a01	$K_9Na_3 \cdot Al_{12}Si_{20}O_{64} \cdot 23H_2O$	merlinoite	16.3	M	-	H_2O	-	-	99Yak1
MER2001a01	$K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64} \cdot 15H_2O$		16.0	S	-	H_2O	-	-	2001Sko1
MER-IV.1 ***P n m n***									
MER2001a02	$K_{11.5} \cdot Al_{11.5}Si_{21.5}O_{64}$		18.2	S	-	-	D	523	2001Sko1
MER-II.2 ***P 4/n n c***									
MER1997a02	$(C_2N_2H_8)_4 \cdot Al_{3.36}Co_{12.64}P_{16}O_{64}$		15.5	S	-	EDA	-	-	97Fen1
MER-IV.2 ***C c c e***									
MER1997a01	$C_{6.3} \cdot Al_{11.2}Co_{20.8}P_{32}O_{128}$ [3])		15.4	S	-	[2])	-	-	97Fen1
MER1998b01	$(NH_4)_{32} \cdot Be_{32}P_{32}O_{128} \cdot 4H_2O$		20.9	S	-	H_2O	-	-	98Bu1

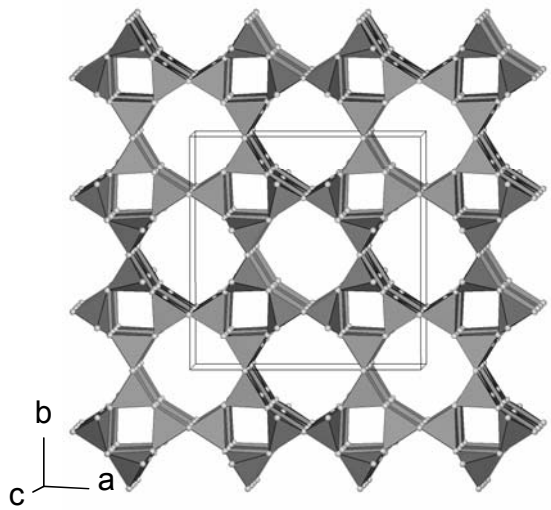
[1]) Chemical composition constrained to Ba : Al = 1 : 1.
[2]) The compound contains an unidentified organic species.
[3]) Chemical composition from personal communication from X. Bu.

Table MER.2.2 Structural parameters of MER-type compounds.

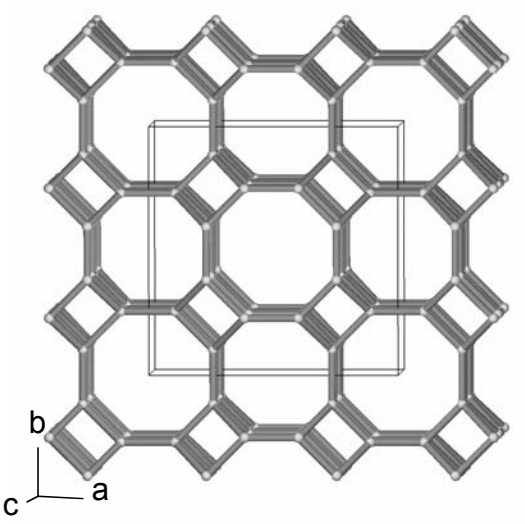
code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
MER-I ***I* 4/*m m m***									
MER1972a01	14.194(6)	14.194(6)	9.934(6)	2001	0, 0, ½	**a**, **b**, **c**	*x*, *y*, *z*-½	n.s.	72Sol1
MER1988a01	14.05	14.05	9.98	1970	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	88van1
MER-II.1 ***I m m m***									
MER1979a01	14.116	14.229	9.946	1998	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	79Gal1
MER1985a01	14.099(5)	14.241(5)	10.08(1)	2024	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	85Bat1
MER1996a01	14.0948(6)	14.2026(6)	10.0421(5)	2010	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	96Bie1
MER1998a01	14.129(1)	14.131(1)	9.9274(5)	1982	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	98Bar1
MER1999a01	13.863(3)	14.135(2)	10.047(2)	1969	½, 0, 0	**a**, **b**, **c**	*x*-½, *y*, *z*	120	99Yak1
MER2001a01	14.0716(6)	14.1978(5)	10.0291(3)	2004	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	2001Sko1
MER-IV.1 ***P n m n***									
MER2001a02	13.4160(6)	13.4118(5)	9.7970(2)	1763	0, 0, 0	**b**, **c**, **a**	*y*, *z*, *x*	n.s.	2001Sko1
MER-II.2 ***P* 4/*n n c***									
MER1997a02	14.6615(1)	14.6615(1)	9.6146(2)	2067	¼, ¼, ¼	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*-¼	293	97Fen1
MER-IV.2 ***C c c e***									
MER1997a01	20.147(1)	20.515(1)	10.0242(6)	4143	½, ¼, -¼	**a**, **b**, **c**	*x*-½, *y*-¼, *z*+¼	293	97Fen1
MER1998b01	18.0209(1)	17.9564(4)	9.4623(2)	3062	½, ¼, -¼	**a**, **b**, **c**	*x*-½, *y*-¼, *z*+¼	150	98Bu 1

MER.3 Framework structures

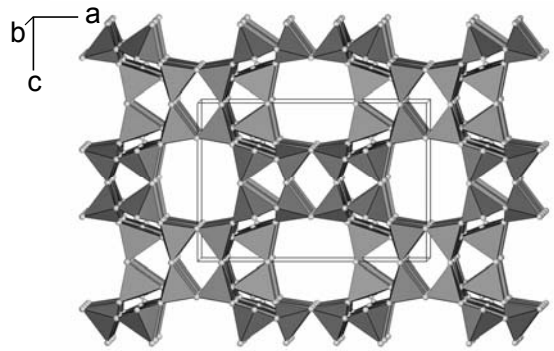
MER.3.1 MER-I compounds (*I 4/m m m* , IT #139)



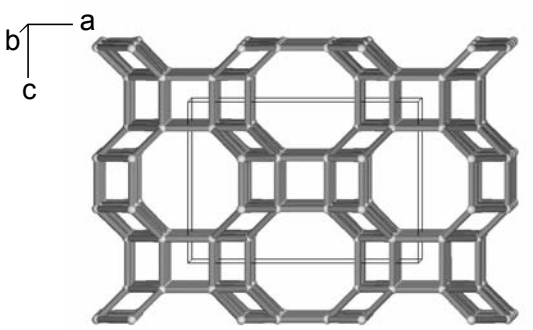
a Polyhedral representation. View parallel **c** rotated by 2° about **a** and **b**.



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel **b** rotated by 1° about **a** and **c**.



d Ball and stick model corresponding to c).

Fig. MER.3.1.1 Projections of the MER-I crystal structure of $Ba_{12} \cdot Al_{12}Si_{20}O_{64} \cdot 8Cl\ 4OH$ (MER1972a01, 72Sol1).

Table MER.3.1.2 Selected interatomic distances and angles for MER-I crystal structure of $Ba_{12} \cdot Al_{12}Si_{20}O_{64} \cdot 8Cl\ 4OH$ (MER1972a01,72Sol1).

	T - O [Å]	T - O - T [°]
(Si,Al)1- O4	1.63(1)	158(1)
(Si,Al)1- O1	1.66(2)	136(2)
(Si,Al)1- O2	1.69(1)	131(1)
(Si,Al)1- O3	1.69(2)	135(2)
mean	1.67	140

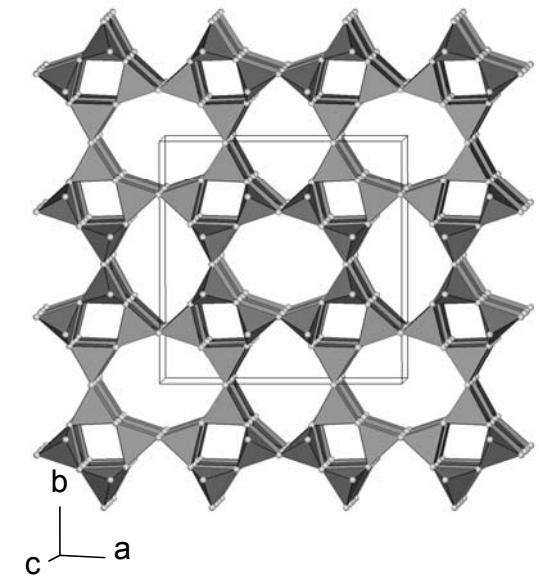
Table MER.3.1.1 Atomic coordinates and site definitions for MER-I crystal structure of $Ba_{12} \cdot Al_{12}Si_{20}O_{64} \cdot 8Cl\ 4OH$ (MER1972a01, 72Sol1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0.1083(7)	0.2614(7)	0.157(1)	2.2(2)	1	32(o)	20 / 12
O1	0	0.243(3)	0.213(3)	3(1)	. *m* .	16(n)	16
O2	0.150	0.150	0.156(3)	5(1)	. . *m*	16(m)	16
O3	0.110(2)	0.307(2)	0	4(1)	*m* . .	16(l)	16
O4	0.342	*x*+½	¼	7(1)	. . 2	16(k)	16
Ba1	0.1816(4)	½	0	5.0(2)	*m* 2 *m*.	8(j)	8
Ba2	½	½	0.788(1)	14.5(7)	4 *m m*	4(e)	4
Cl1	0.375	0.375	0	5.1(7)	*m*. 2 *m*	8(h)	8
OH1	0	½	¾	5(2)	$\bar{4}$ *m* 2	4(d)	4

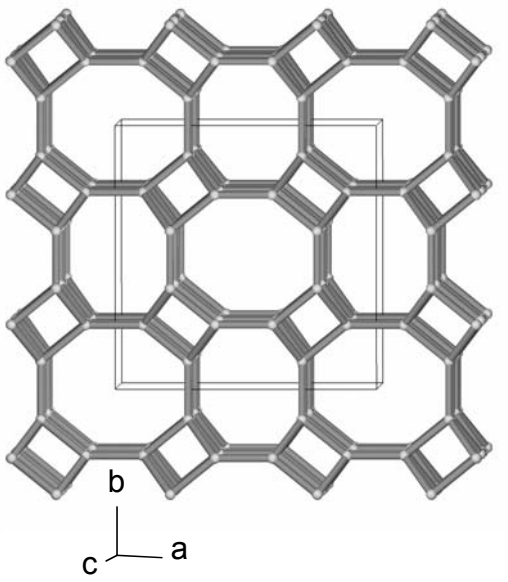
MER.3.2 MER-II.1 compounds (*I m m m* , IT #71)

Table MER.3.2.1 Atomic coordinates and site definitions for merlinoite, $K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$ (MER1979a01, 79Gal1).

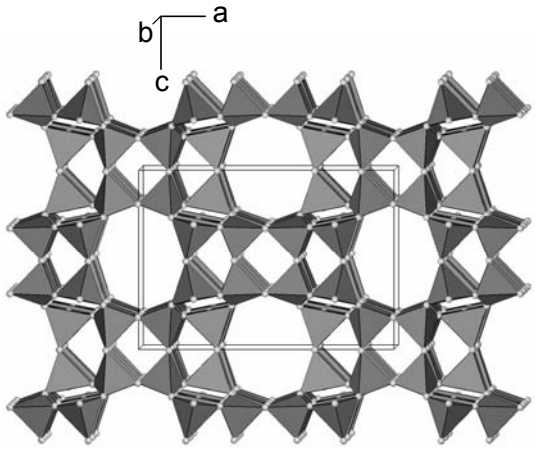
atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11	0.1097(2)	0.2473(2)	0.1563(4)	1.0(1)	1	16(o)	12.64/3.36
(Si,Al)12	0.2816(2)	0.1102(2)	0.1596(4)	1.0(1)	1	16(o)	12.64/3.36
O11	0	0.2155(9)	0.184(1)	1.8(4)	*m* . .	8(l)	8
O12	0.2767(9)	0	0.210(1)	1.9(4)	. *m* .	8(m)	8
O2	0.1765(6)	0.1568(6)	0.192(1)	2.3(3)	1	16(o)	16
O31	0.124(1)	0.2830(8)	0	1.8(4)	. . *m*	8(n)	8
O32	0.3089(9)	0.1177(8)	0	1.5(4)	. . *m*	8(n)	8
O4	0.3661(7)	0.8362(7)	0.245(1)	2.6(3)	1	16(o)	16
(K,Ba)1	0.156(1)	½	0	3.8(5)	2 *m m*	4(f)	1.68/ 0.16(8)
(K,Ba)2	½	0.192(1)	0	3.8(3)	*m* 2 *m*	4(h)	1.64/ 0.16(8)
(Ca,K, Na,Ba)3	½	½	0.275(7)	12(3)	*m m* 2	4(i)	0.60/0.36/ 0.20/0.04
(Ca,K, Na)4	0.390(9)	0.363(9)	0	12	. . *m*	8(n)	0.48/0.32/ 0.16
(Ca,K, Na,Ba)5	0.333(5)	0.380(5)	0	12	. . *m*	8(n)	0.80/0.48/ 0.32/0.08
OW1	½	0	0	7(2)	*m m m*	2(b)	2
OW2	0	½	0.158(3)	4.9(9)	*m m* 2	4(j)	4
OW3	0.385(3)	½	0.159(5)	10(2)	. *m* .	8(m)	4.80
OW4	½	½	0	4(4)	*m m m*	2(c)	0.40
OW5	0.459(7)	0.274(8)	0	6(4)	. . *m*	8(n)	1.6(4)
OW6	0.251(5)	0.464(5)	0	4(2)	. . *m*	8(n)	1.7(3)
OW7	0.446(6)	0.420(7)	0.062(9)	11(3)	1	16(o)	3.20
OW8	0.443(7)	½	½	12	2 *m m*	4(e)	1.76



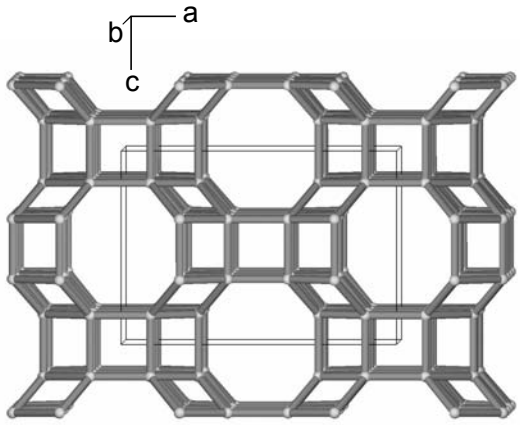
a Polyhedral representation. View parallel **c** rotated by 2° about **a** and **b**.



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel **b** rotated by 1° about **a** and **c**.



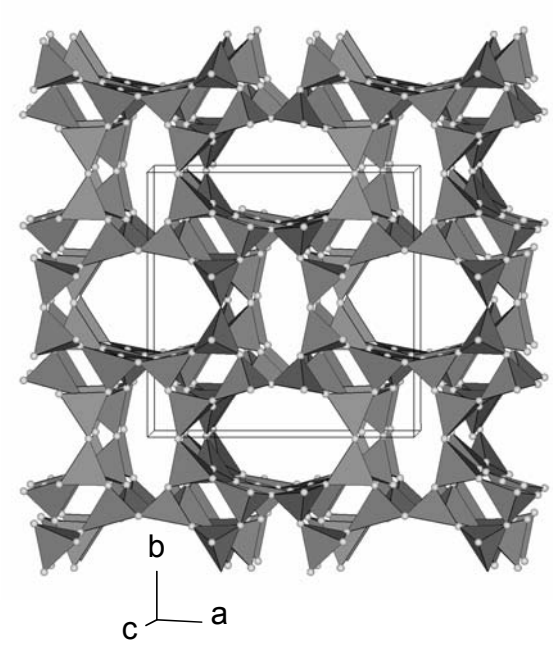
d Ball and stick model corresponding to c).

Fig. MER.3.2.1 Projections of the MER-II.1 crystal structure of $K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$ (MER1979a01, 79Gal1).

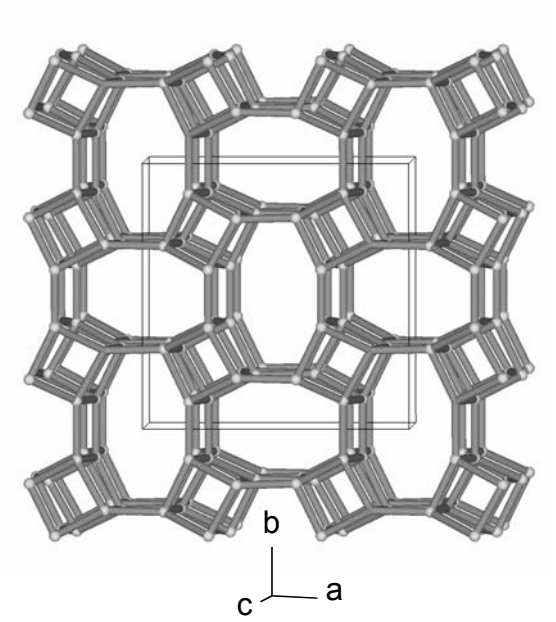
Table MER.3.2.2 Selected interatomic distances and angles for merlinoite, $K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$ (MER1979a01, 79Gal1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11 - O4	1.635(10)	144.7(7)	(Si,Al)12 - O32	1.637(5)	151.7(9)
(Si,Al)11 - O2	1.636(9)	142.0(6)	(Si,Al)12 - O12	1.646(5)	144.5(9)
(Si,Al)11 - O11	1.636(5)	142.3(9)	(Si,Al)12 - O4	1.653(10)	144.7(7)
(Si,Al)11 - O31	1.647(5)	141.4(8)	(Si,Al)12 - O2	1.657(9)	142.0(6)
mean	1.639	142.6	mean	1.648	145.7

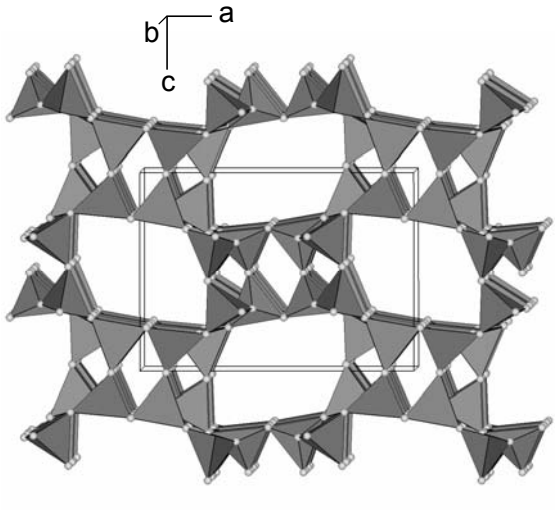
MER.3.3 MER-IV.1 compounds (*P n m n* , IT #58)



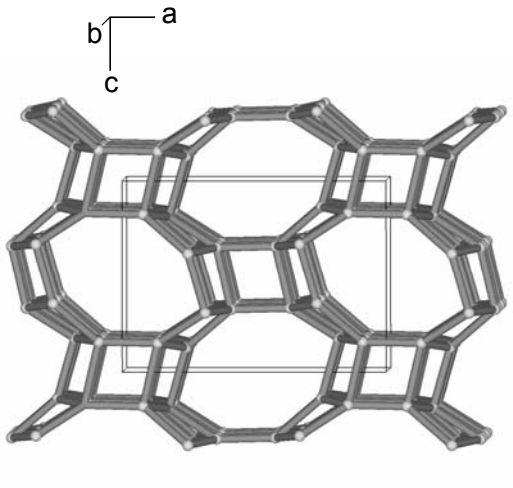
a Polyhedral representation. View parallel **c** rotated by 2° about **a** and **b**.



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel **b** rotated by 1° about **a** and **c**.



d Ball and stick model corresponding to c).

Fig. MER.3.3.1 Projections of the MER-IV.1 crystal structure of $K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64}$ (MER2001a02, 2001Sko1).

Table MER.3.2.1 Atomic coordinates and site definitions for MER-IV.1 crystal structure of $K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64}$ (MER2001a02, 2001Sko1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11a	0.084(2)	0.305(1)	0.166(2)	3.95	1	8(h)	5.12/2.88
(Si,Al)11b	0.139(2)	0.300(2)	0.840(3)	3.95	1	8(h)	5.12/2.88
(Si,Al)12a	0.179(1)	0.1090(5)	0.181(2)	3.95	1	8(h)	5.12/2.88
(Si,Al)12b	0.244(2)	0.1101(5)	0.868(2)	3.95	1	8(h)	5.12/2.88
O11	-0.028(2)	0.290(3)	0.225(4)	5.53	1	8(h)	8
O12a	0.119(2)	0	0.190(6)	5.53	. *m* .	4(g)	4
O12b	0.216(4)	0	0.810(4)	5.53	. *m* .	4(g)	4
O21	0.083(1)	0.183(2)	0.178(4)	5.53	1	8(h)	8
O22	0.143(1)	0.177(2)	0.843(5)	5.53	1	8(h)	8
O31	0.100(3)	0.306(3)	0.000(3)	5.53	1	8(h)	8
O32	0.245(3)	0.118(3)	0.037(2)	5.53	1	8(h)	8
O41	0.252(2)	0.852(3)	0.305(4)	5.53	1	8(h)	8
O42	0.326(3)	0.829(3)	0.776(4)	5.53	1	8(h)	8
K1	0	0	0	9.47	. 2/*m* .	2(a)	2
K2	0.220(2)	½	0.000(3)	9.47	. *m* .	4(g)	4
K3	0.403(2)	0.265(2)	0.060(2)	9.47	1	8(h)	6

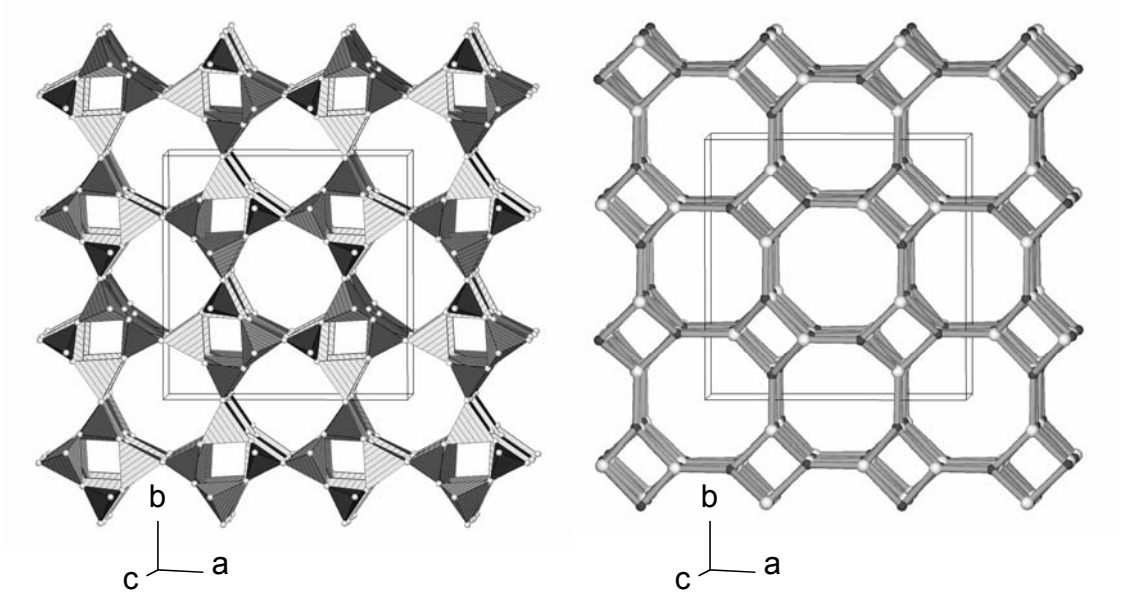
Table MER.3.2.2 Selected interatomic distances and angles for MER-IV.1 crystal structure of $K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64}$ (MER2001a02, 2001Sko1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11a - O11	1.63(3)	134(3)	(Si,Al)11b - O11	1.63(3)	134(3)
(Si,Al)11a - O21	1.63(3)	127(2)	(Si,Al)11b - O22	1.65(3)	125(2)
(Si,Al)11a - O42	1.65(4)	161(3)	(Si,Al)11b - O31	1.65(4)	169(3)
(Si,Al)11a - O31	1.65(4)	169(3)	(Si,Al)11b - O41	1.65(4)	144(3)
mean	1.64	148	mean	1.65	143
(Si,Al)12a - O21	1.63(3)	127(2)	(Si,Al)12b - O12b	1.63(2)	130(3)
(Si,Al)12a - O41	1.65(4)	144(3)	(Si,Al)12b - O42	1.64(4)	161(3)
(Si,Al)12a - O32	1.67(4)	146(3)	(Si,Al)12b - O22	1.65(3)	125(2)
(Si,Al)12a - O12a	1.67(2)	122(2)	(Si,Al)12b - O32	1.66(3)	146(3)
mean	1.66	135	mean	1.64	141

MER.3.4 MER-II.2 compounds (*P 4/n n c*, IT #126)

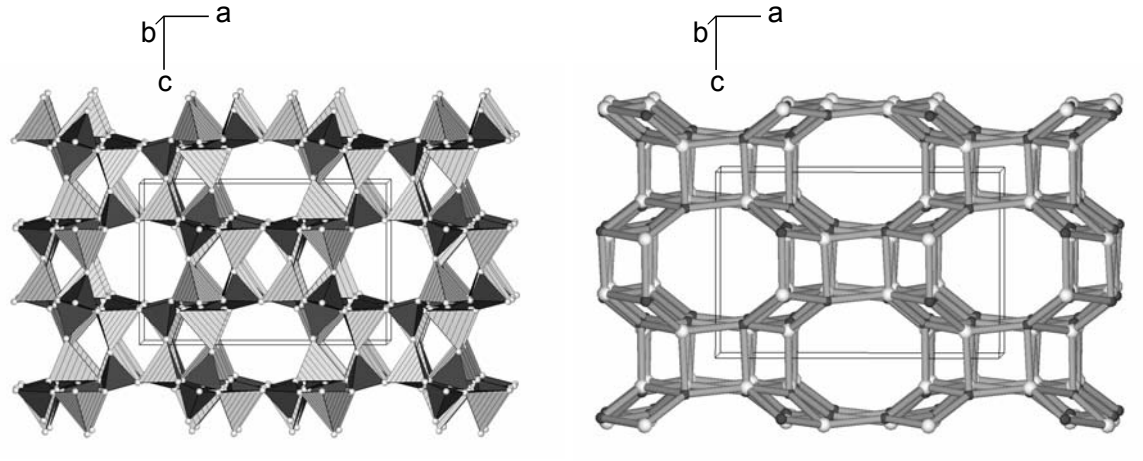
Table MER.3.4.2 Selected interatomic distances and angles for MER-II.2 crystal structure of $(C_2N_2H_8)_4 \cdot Al_{3.36}Co_{12.64}P_{16}O_{64}$ (MER1997a02, 97Fen1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Co,Al)11 - O2	1.866(8)	139.5(5)	P12 - O3	1.495(8)	143.1(7)
(Co,Al)11 - O1	1.869(8)	140.4(6)	P12 - O2	1.496(8)	139.5(5)
(Co,Al)11 - O4	1.870(11)	140.4(7)	P12 - O4	1.500(11)	140.4(7)
(Co,Al)11 - O3	1.910(8)	143.1(7)	P12 - O1	1.518(8)	140.4(6)
mean	1.879	140.9	mean	1.502	140.9



a Polyhedral representation. View parallel **c** rotated by 2° about **a** and **b**.

b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel **b** rotated by 1° about **a** and **c**.

d Ball and stick model corresponding to c).

Fig. MER.3.4.1 Projections of the MER-II.2 crystal structure of $(C_2N_2H_8)_4 \cdot Al_{3.36}Co_{12.64}P_{16}O_{64}$ (MER1997a02, 97Fen1).

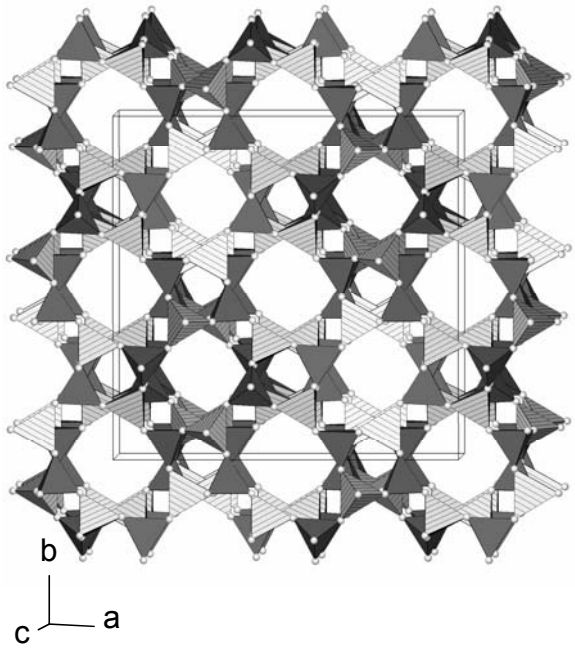
Table MER.3.4.1 Atomic coordinates and site definitions for MER-II.2 crystal structure of $(C_2N_2H_8)_4 \cdot Al_{3.36}Co_{12.64}P_{16}O_{64}$ (MER1997a02, 97Fen1). Origin choice 1 in IT #126, at 4 . . , at -¼, -¼, -¼ from $\bar{1}$.

atom	*x*	*y*	*z*	B_{eq} [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
(Co,Al)11	0.1140(1)	0.2576(1)	0.1499(2)	2.40	1	16(k)	3.36/12.64
P12	0.6022(1)	0.7612(2)	0.6858(2)	1.97	1	16(k)	16
O1	-0.0029(5)	0.2487(6)	0.2262(9)	5.42	1	16(k)	16
O2	0.1761(5)	0.1551(5)	0.2153(9)	5.11	1	16(k)	16
O3	0.1141(5)	0.2952(7)	-0.0403(8)	4.97	1	16(k)	16
O4	0.3656(7)	0.8359(7)	0.220(1)	7.40	1	16(k)	16
N1	0.3711(8)	0	½	3.32	. 2 .	8(j)	8
C1	0.470(1)	0.001(1)	0.565(2)	2.13	1	16(k)	8
N2	0.152(2)	-*x*	½	8.92	. . 2	8(h)	4
C2	-0.081(4)	-*x*	½	11.3	. . 2	8(h)	4
C3	0	0	0.647(8)	15.2	4 . .	4(e)	4
C4	-0.016(9)	0.081(3)	0.618(6)	33.1	1	16(k)	16

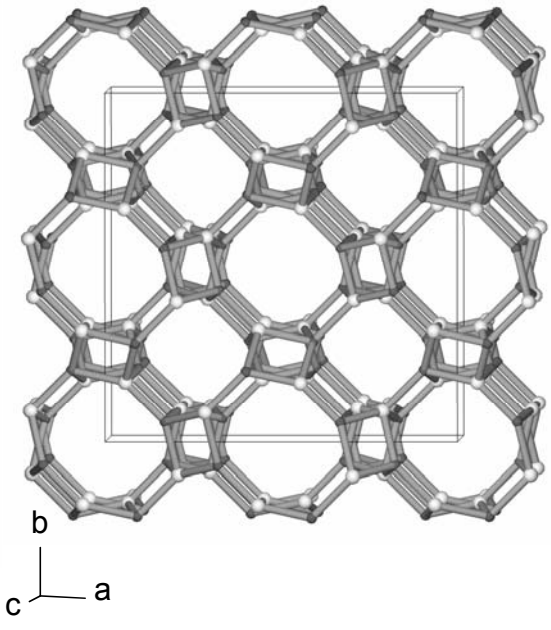
MER.3.5 MER-IV.2 compounds (*C c c e*, IT #68)

Table MER.3.5.1 Atomic coordinates and site definitions for MER-IV.2 crystal structure of $(NH_4)_{32} \cdot Be_{32}P_{32}O_{128} \cdot 4H_2O$ (MER1998b01, 98Bu1). Origin choice 1 in IT #68, at 2 2 2, at 0, -¼, -¼ from $\bar{1}$.

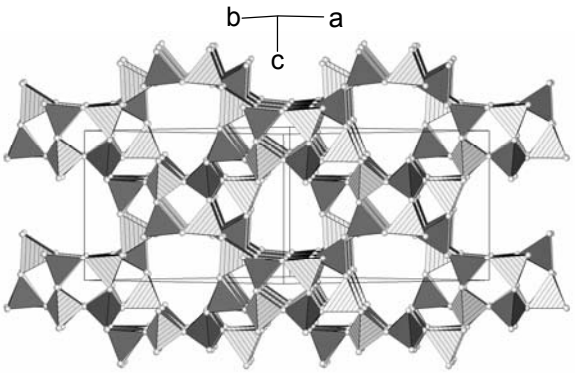
atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
P11a	0.9074(1)	0.2087(1)	0.1189(1)	0.79(8)	1	16(i)	16
P11b	0.1734(1)	0.9379(1)	0.8200(1)	0.71(8)	1	16(i)	16
Be12a	0.9393(2)	0.6750(2)	0.6720(4)	0.95(8)	1	16(i)	16
Be12b	0.7098(2)	0.9087(2)	0.3855(4)	0.95(8)	1	16(i)	16
O11	0.8346(1)	0.1689(1)	0.1606(2)	1.11(8)	1	16(i)	16
O12	0.0928(1)	0.9091(1)	0.8287(2)	1.11(8)	1	16(i)	16
O21	-0.0272(1)	0.1619(1)	0.1693(2)	1.26(8)	1	16(i)	16
O22	0.1660(1)	0.0224(1)	0.8178(2)	1.18(8)	1	16(i)	16
O31	0.9087(1)	0.2231(1)	-0.0409(2)	1.11(8)	1	16(i)	16
O32	0.2198(1)	0.9100(1)	-0.0552(2)	1.18(8)	1	16(i)	16
O41	0.9086(1)	0.2864(1)	0.1873(2)	1.26(8)	1	16(i)	16
O42	0.2068(1)	0.9071(1)	0.6823(2)	1.18(8)	1	16(i)	16
OW9	½	0	½	2.45(8)	2 2 2	4(a)	4
N1	½	0	0.1516(4)	1.03(8)	. . 2	8(g)	8
N2	¾	¼	0.3570(5)	1.42(8)	. . 2	8(h)	8
N3	0.6098(2)	0.3913(2)	0.4445(4)	1.82(8)	1	16(i)	16
H11	0.471(2)	0.972(2)	0.206(4)	3(1)	1	16(i)	16
H12	0.515(5)	0.957(2)	0.115(8)	13(3)	1	16(i)	16
H21	0.719(3)	0.279(3)	0.302(5)	5(1)	1	16(i)	16
H22	0.775(2)	0.283(2)	0.413(4)	2.0(8)	1	16(i)	16
H31	0.575(2)	0.421(2)	0.437(5)	2.4(9)	1	16(i)	16
H32	0.595(3)	0.335(4)	0.442(7)	8(2)	1	16(i)	16
H33	0.648(4)	0.403(3)	0.511(8)	8(2)	1	16(i)	16
H34	0.630(4)	0.400(4)	0.368(9)	9(2)	1	16(i)	16
H9	0.537(3)	0.966(3)	0.562(6)	0(1)	1	16(i)	16



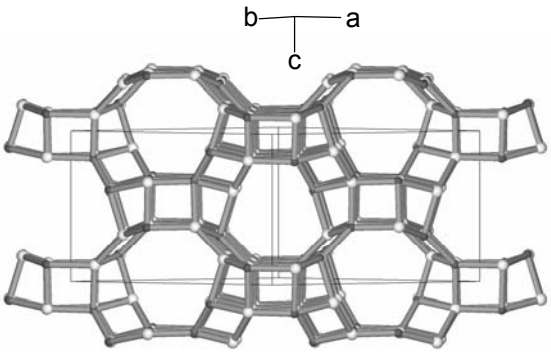
a Polyhedral representation. View parallel **c** rotated by 2° about **a** and **b**.



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel [110] rotated by 1° about [1 $\bar{1}$ 0] and [001].



d Ball and stick model corresponding to c).

Fig. MER.3.5.1 Projections of the MER-IV.2 crystal structure of $(NH_4)_{32} \cdot Be_{32}P_{32}O_{128} \cdot 4H_2O$ (MER1998b01, 98Bu1).

Table MER.3.5.2 Selected interatomic distances and angles for MER-IV.2 crystal structure of $(NH_4)_{32} \cdot Be_{32}P_{32}O_{128} \cdot 4H_2O$ (MER1998b01, 98Bu1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
P11a - O21	1.524(3)	133.5(2)	P11b - O22	1.523(3)	136.1(2)
P11a - O31	1.534(2)	132.4(2)	P11b - O32	1.531(2)	135.3(2)
P11a - O41	1.538(2)	138.4(2)	P11b - O42	1.538(2)	133.3(2)
P11a - O11	1.545(3)	136.7(2)	P11b - O12	1.544(3)	130.5(2)
mean	1.535	135.3	mean	1.534	133.8
Be12a - O41	1.600(4)	138.4(2)	Be12b - O22	1.601(4)	136.1(2)
Be12a - O21	1.602(4)	133.5(2)	Be12b - O32	1.616(4)	135.3(2)
Be12a - O31	1.609(4)	132.4(2)	Be12b - O42	1.634(4)	133.3(2)
Be12a - O12	1.617(4)	130.5(2)	Be12b - O11	1.665(4)	136.7(2)
mean	1.607	133.7	mean	1.629	135.4

MER.4 Chemical composition

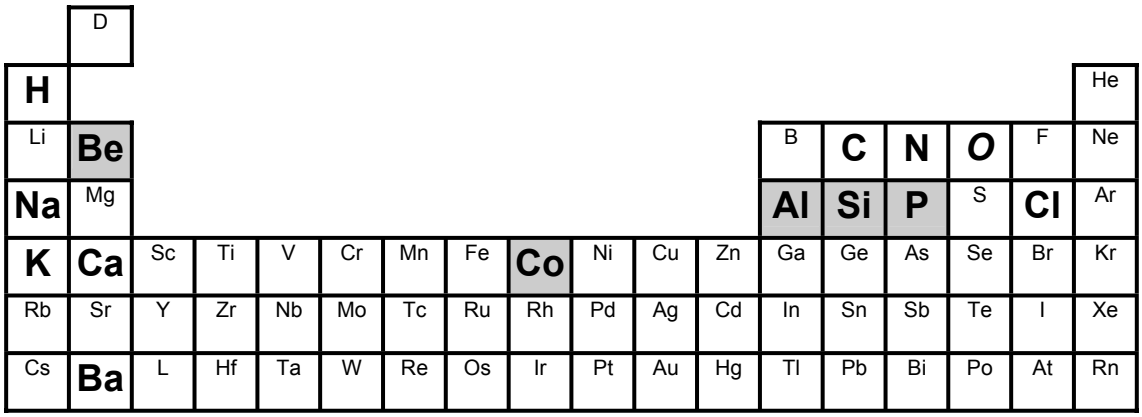


Fig. MER.4.1 Chemical elements (highlighted) occurring in MER-type compounds. Framework cations are in grey fields.

MER.5 Flexibility and apertures

The silicoaluminates with a MER-type framework of which the crystal structures have been determined have filled pores with the exception of the MER-IV.1-type crystal structure of $K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64}$ (MER2001a02, [2001Sko1]). We can compare this dehydrated form with the hydrated form (MER-II.1-type $K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64} \cdot 15H_2O$ (MER2001a01, [2001Sko1]). The unit cell volume of the hydrated form is 14% larger than of the unit cell of the dehydrated framework. This is much less of a volume change as we can observe for the collapsible NAT- and RHO-type frameworks, which are respectively 37% and 27% [92Bau2, 95Bau1]. It is more in line with the volume decrease shown by LTA-type

frameworks [92Bau1]. Whether or not this means that the MER-type framework is of the noncollapsible type cannot be decided on the basis of the evidence available now.

The 8-ring openings in merlinoite are strongly deformed and do not reach the diameter of slightly more than 4 Å, as seen in the LTA-type framework. In silicoaluminate MER-type frameworks one of the rings has an elliptical shape with diameters clearly smaller and clearly larger than 4 Å. The other 8-rings are buckled and have diameters of 3.6 Å or less.

MER.6 Other information

Useful properties of MER-type materials have not been reported so far.

A pure Ga,Si compound of the MER-type could not be synthesized. Instead it was possible to replace Al partly by Ga in the framework [2001Kim1]. The ion exchange equilibria of aluminosilicate MER-type compounds involving Na versus K^+, NH_4^+, Ba^{2+} and Ca^{2+} were studied at 298 K [2004Col1].

The tetrahedral framework of the crystal structure of $[C_2\ N_2H_{10}]_2[Co_4(PO_4)_4]H_2O$ [2000Nar1] is said by the authors to resemble very closely the MER-type framework. In fact it is of ACO-type [2002Bau1].

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Gone to press March 1, 2006