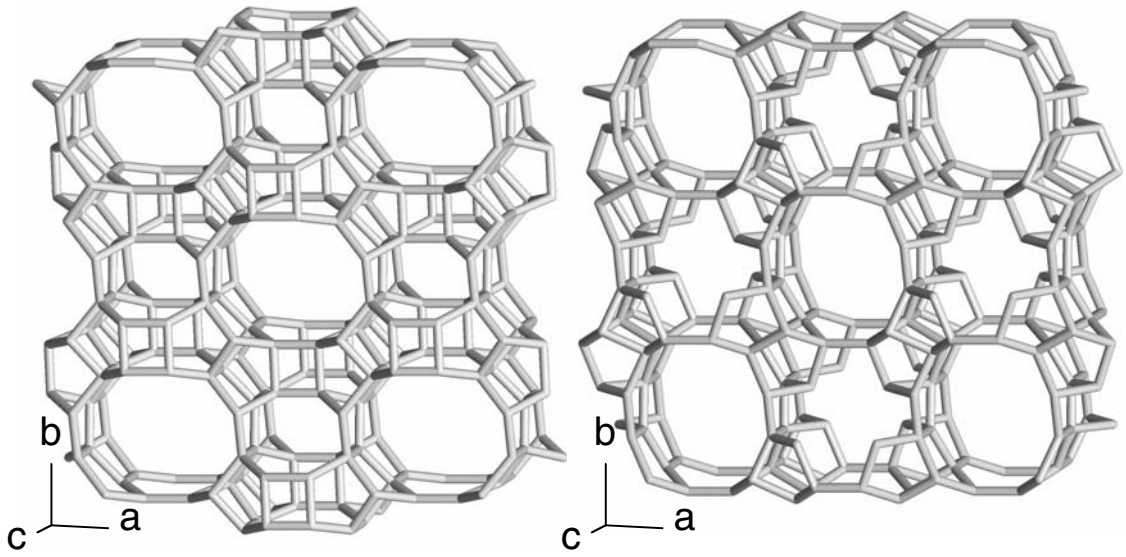
MOR

MOR.1 Zeolite framework type and topology

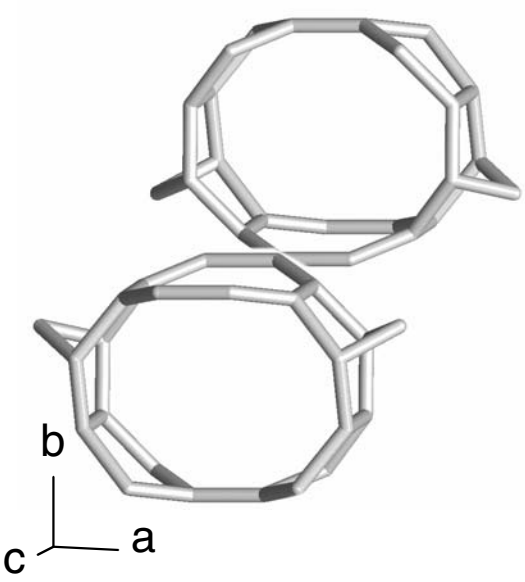
The framework type code is named after the mineral **MOR**denite, $(Na,K,Ca_{0.5})_8 \cdot Al_8Si_{40}O_{96} \cdot 28H_2O$, first found at the shore of Bay of Fundy, close to Morden, King's County, Nova Scotia, Canada, and described by How [1864How1, cited after 98Coo1]. Another mineral named ptilolite [1886Cro1, cited after 85Got1] was shown to be identical to mordenite [58Dav1]. Consequently, the name ptilolite has been discredited as well as the mordenite analogues arduinite, ashtonite, flokite, pseudonatrolite, and steelite [98Coo1]. The first synthesis of mordenite is mentioned in [27Leo1, cited after 89Szo1] and reliably reported by [48Bar1]. The crystal structure was solved by Meier [61Mei1] on Na exchanged mordenite in space group *C m c m* representing the aristotypic framework geometry.
The framework structure (Fig. MOR.1.1a) can be described as being built from *bb45* ($5^2 5^2 5^2 8^1 12^2$) units forming the 12-ring channel (**mdn** unit, Figs. MOR.1.2a,b and MOR.1.3) crosslinked by composite units formed by *kaj* ($5^2 8^2 8^1$, **csh** channel, Fig. MOR.1.4a) *dah* ($4^2 5^4 5^4 8^2$) and *tes* (5^4) units as shown in Fig. MOR.1.2.



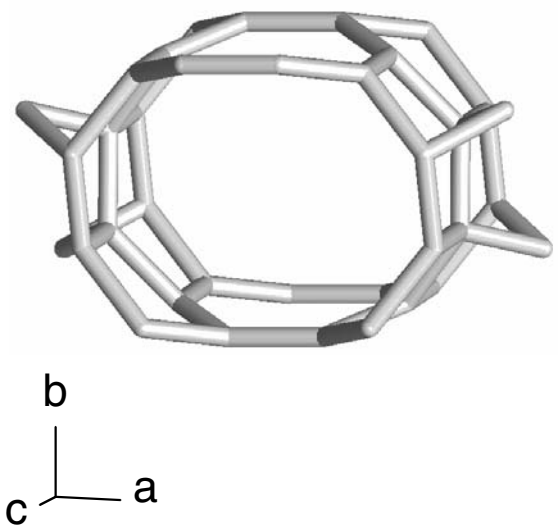
a The framework structure of MOR-type compounds in the highest possible topological symmetry *C m c m*.

b The framework structure of maricopaite in *C m* 2 *m* (MOR1994b01, 94Rou1).

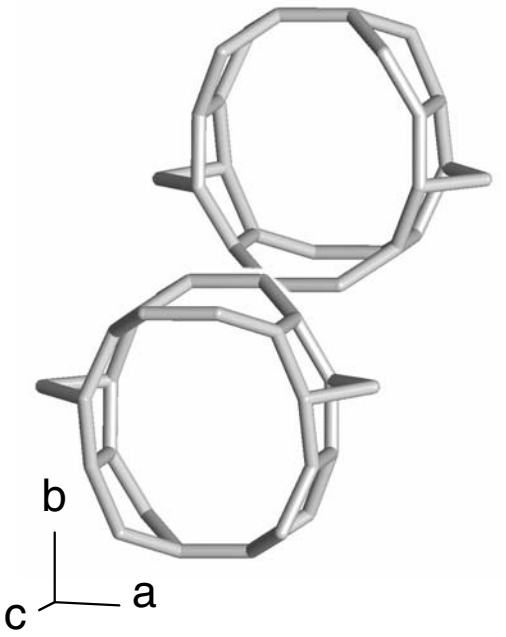
Fig. MOR.1.1. The framework structures of MOR-type compounds. View parallel **c** rotated by 10° about **a** and 15° about **b**. The 4-ring in the aristotypic MOR-framework visible at the front of diagram **a** is interrupted in maricopaite, diagram **b**, between atoms O91' and O92'.



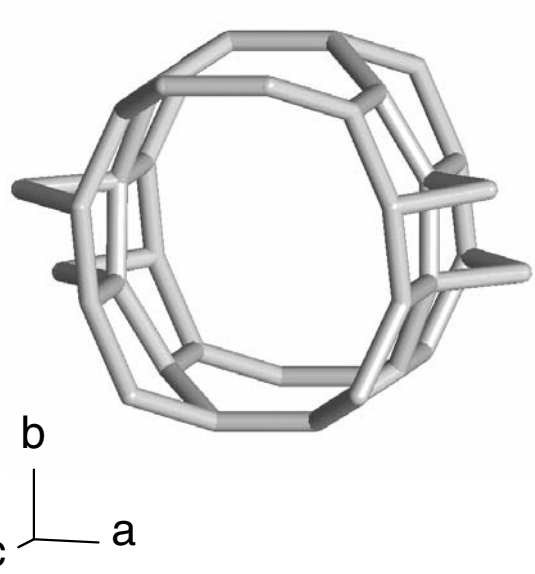
a Linkage of *bb45* units in the aristotype structure forming the **mdn** channels.



b The complete assemblage shown in a).

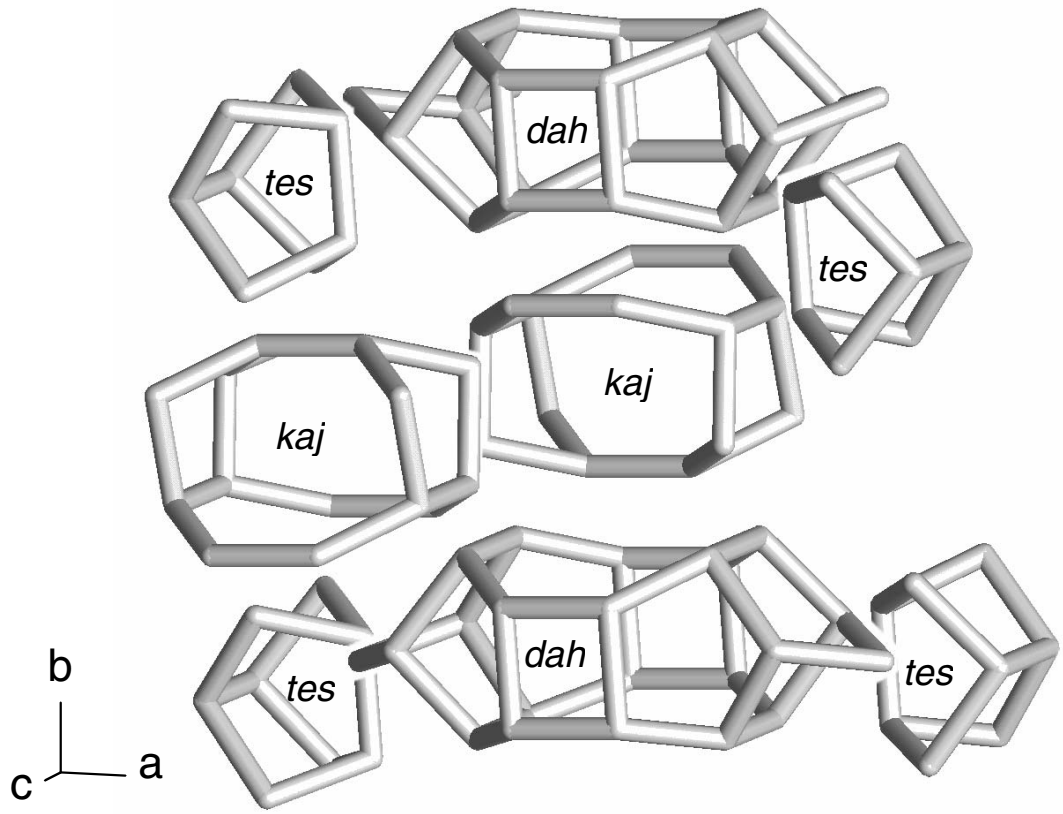


c Linkage of *bb45* units in maricopaite forming the **mdn** channels.

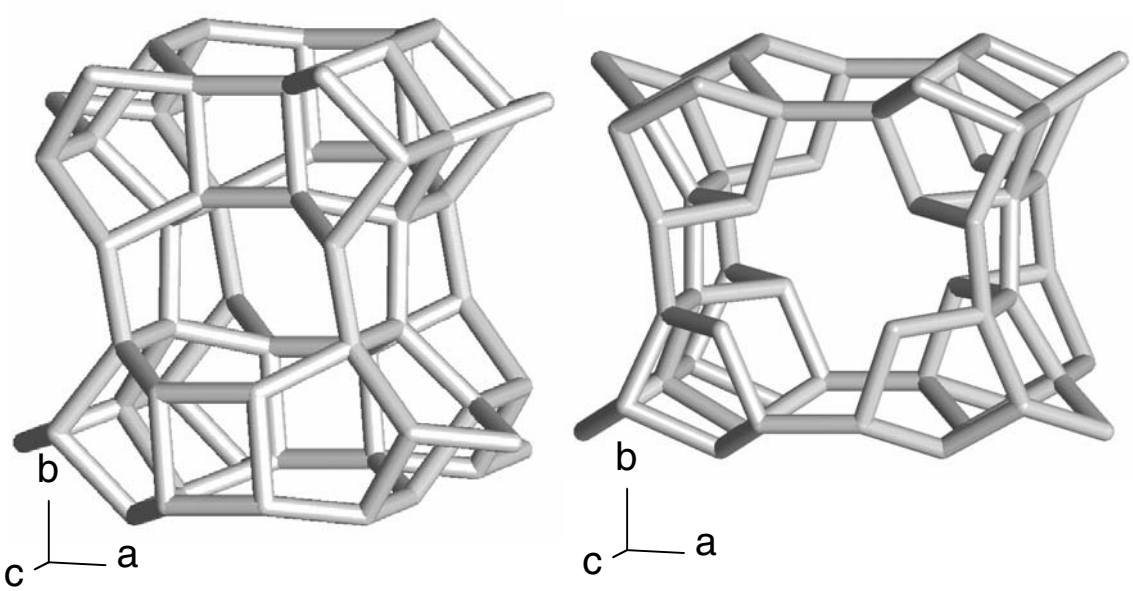


d The complete assemblage shown in c).

Fig. MOR.1.2. Building scheme of the MOR-type framework corresponding to the models shown in Fig. MOR.1.1. View parallel **c** rotated by 10° about **a** and 15° about **b**. The 4-ring in the aristotypic MOR-framework visible at the front of diagrams **f** and **h** is interrupted in maricopaite, diagrams **g** and **i**, between atoms O91' and O92'.



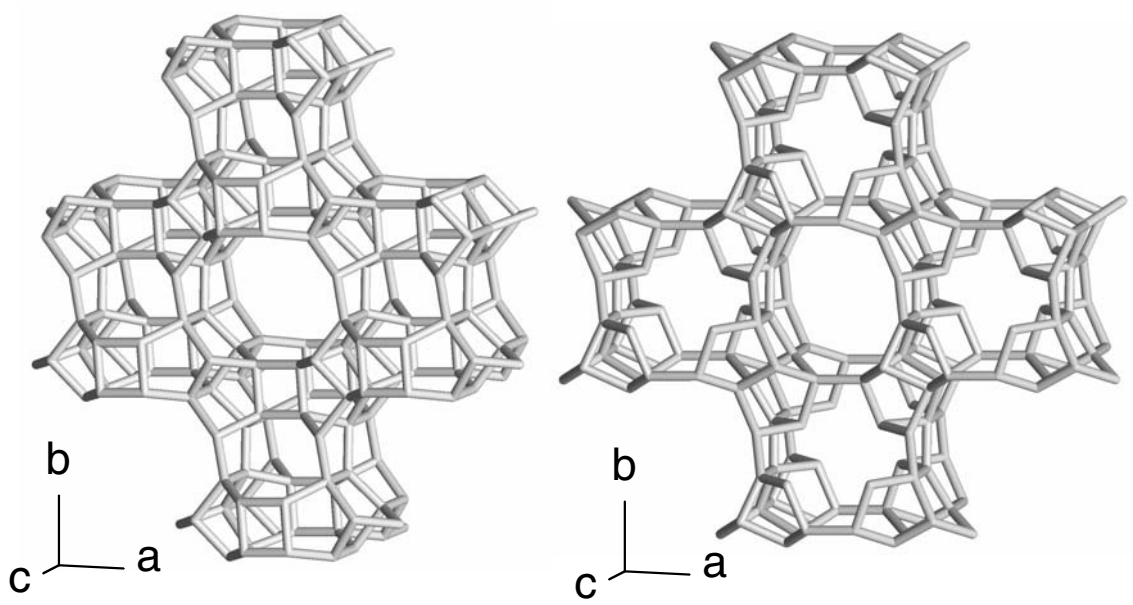
e Linkage between *dah* and *tes* units around the central *kaj* units forming the **csh** channels.



f The complete assemblage shown in e).

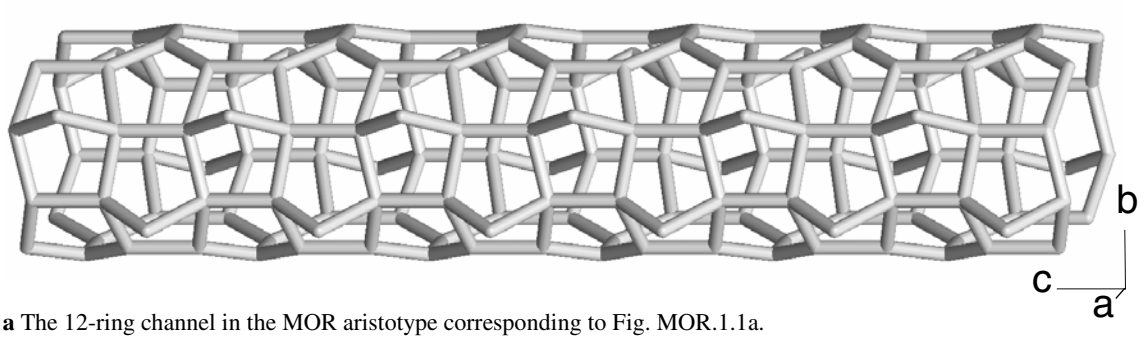
g The corresponding environment in maricopaite.

Fig. MOR.1.2. (continued) Building scheme of the MOR-type framework corresponding to the models shown in Fig. MOR.1.1. View parallel **c** rotated by 10° about **a** and 15° about **b**. The 4-ring in the aristotypic MOR-framework visible at the front of diagrams **f** and **h** is interrupted in maricopaite, diagrams **g** and **i**, between atoms O91' and O92'.

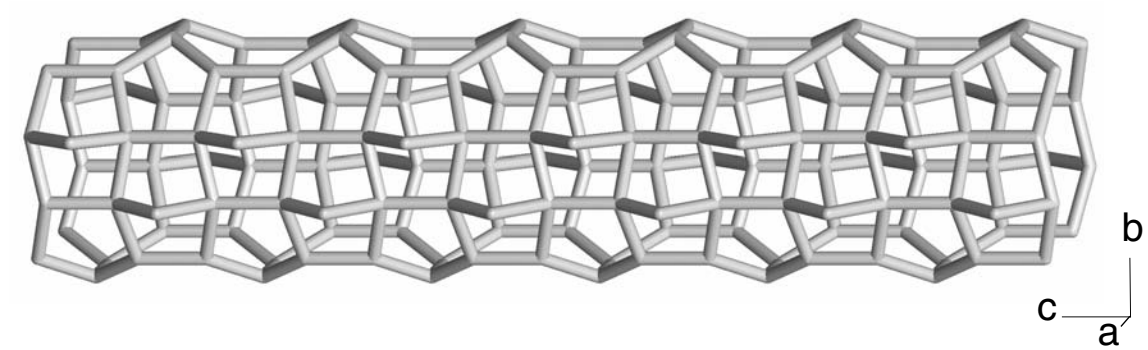


h Framework structure of the MOR aristotype. **i** Framework structure of maricopaite.

Fig. MOR.1.2. (continued) Building scheme of the MOR-type framework corresponding to the models shown in Fig. MOR.1.1. View parallel **c** rotated by 10° about **a** and 15° about **b**. The 4-ring in the aristotypic MOR-framework visible at the front of diagrams **f** and **h** is interrupted in maricopaite, diagrams **g** and **i**, between atoms O91' and O92'.

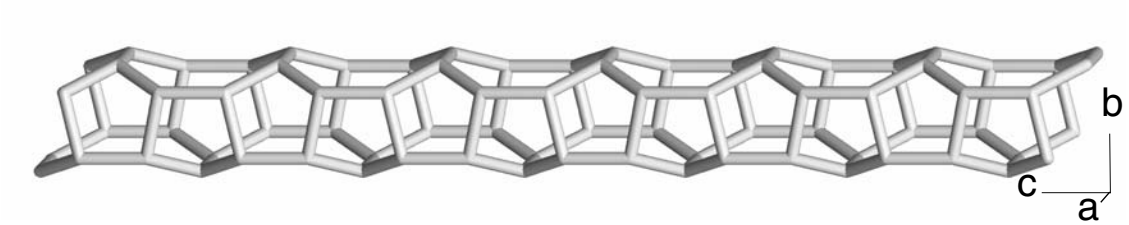


a The 12-ring channel in the MOR aristotype corresponding to Fig. MOR.1.1a.

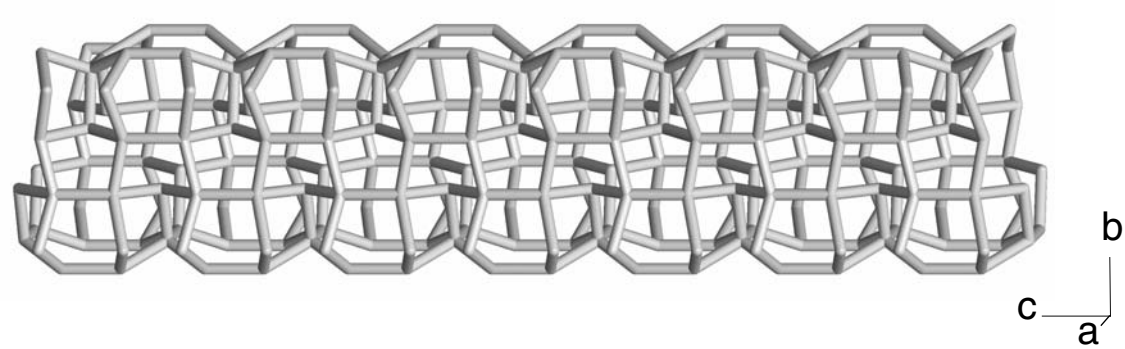


b The 12-ring cahnnel in maricopaite (MOR1994b01, 94Rou1) corresponding to Fig. MOR.1.1b.

Fig. MOR.1.3 The 12-ring channel (**mdn** unit) in ½, ½, *z*. View parallel **a** rotated by 10° about **b** and **c**.



a The 8-ring channel in the MOR aristotype corresponding to Fig. MOR.1.1a.



b The 12-ring channel in maricopaite (MOR1994b01, 94Rou1). Some bonds in *tes* units are omitted for clarity.

Fig. MOR.1.4 The channels in ½, 0, *z*. View parallel **a** rotated by 10° about **b** and **c**.

The subgroup relationships of MOR-type compounds are shown in Fig. MOR.1.5. In addition there are several structure descriptions of mordenites in lower symmetry space groups like *C m c* 2_1 and *C* 1 *c* 1 (see Table MOR.2.1) probably representing refinements in unnecessarily low symmetries as discussed in [86Bau1] and [2003Bau1]. In all these low-symmetry refinements the authors constrained part of the framework atoms to remain in space group *C m c m* avoiding high correlations between the corresponding atomic parameters in the crystal structure refinements. These entries are listed in Tables MOR.2.1 and MOR.2.2 but they are not considered in the symmetry derivations in Fig. MOR.1.5 and they are not further described in chapter 3. Natural mordenite contains stacking faults which are modeled by additional atomic sites of low occupancies (see, e.g., [75Mor2] and [78Mor1]).

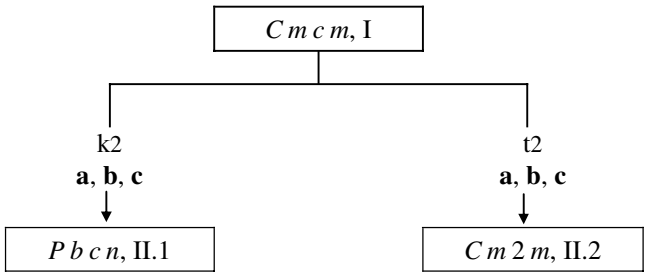


Fig. MOR.1.5 The Bärnighausen tree illustrating the symmetry relationship of the MOR types.

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

MOR-I *C m c m*		MOR-II.1 *P b c n*		MOR-I *C m c m*		MOR-II.2 *C m* 2 *m*	
T1	[16(h), 1]	T11	[8(d), 1]	T1	[16(h), 1]	T11	[8(f), 1]
		T12	[8(d), 1]			T12	[8(f), 1]
T2	[16(h), 1]	T21	[8(d), 1]	T2	[16(h), 1]	T21	[8(f), 1]
		T22	[8(d), 1]			T22	[8(f), 1]
T3	[8(g), . . *m*]	T3	[8(d), 1]	T3	[8(g), . . *m*]	T31	[4(e), . . *m*]
						T32	[4(d), . . *m*]
T4	[8(g), . . *m*]	T4	[8(d), 1]	T4	[8(g), . . *m*]	T41	[4(e), . . *m*]
						T42	[4(d), . . *m*]
O1	[16(h), 1]	O11	[8(d), 1]	O1	[16(h), 1]	O11	[8(f), 1]
		O12	[8(d), 1]			O12	[8(f), 1]
O2	[16(h), 1]	O21	[8(d), 1]	O2	[16(h), 1]	O21	[8(f), 1]
		O22	[8(d), 1]			O22	[8(f), 1]
O3	[16(h), 1]	O31	[8(d), 1]	O3	[16(h), 1]	O31	[8(f), 1]
		O32	[8(d), 1]			O32	[8(f), 1]
O4	[8(g), . . *m*]	O4	[8(d), 1]	O4	[8(g), . . *m*]	O41	[4(e), . . *m*]
						O42	[4(d), . . *m*]
O5	[8(g), . . *m*]	O5	[8(d), 1]	O5	[8(g), . . *m*]	O51	[4(e), . . *m*]
						O52	[4(d), . . *m*]
O6	[8(g), . . *m*]	O6	[8(d), 1]	O6	[8(g), . . *m*]	O61	[4(e), . . *m*]
						O62	[4(d), . . *m*]
O7	[8(e), 2 . .]	O7	[8(d), 1]	O7	[8(e), 2 . .]	O7	[8(f), 1]
O8	[8(d), $\bar{1}$]	O8	[8(d), 1]	O8	[8(d), $\bar{1}$]	O8	[8(f), 1]
O9	[4(c), *m* 2 *m*]	O9	[4(c), . 2 .]	O9	[4(c), *m* 2 *m*]	O91	[2(b), *m* 2 *m*]
						O92	[2(a), *m* 2 *m*]
O10	[4(c), *m* 2 *m*]	O10	[4(c), . 2 .]	O10	[4(c), *m* 2 *m*]	O101	[2(b), *m* 2 *m*]
						O102	[2(a), *m* 2 *m*]

MOR.2 Compounds and crystal data

Table MOR.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
MOR-I ***C m c m***									
MOR1961a01	$Na_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$	[mordenite]	17.2	M	Na	H_2O	-	-	61Mei1
MOR1971a01	$Na_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$	[mordenite]	17.1	M	Na	H_2O	-	-	71Gra1
MOR1975a01	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96}$	[mordenite]	17.6	M	Ca	-	D	773	75Mor1
MOR1975b01	$H_{7.41}K_{0.10}Na_{0.39} \cdot Al_{7.9}Si_{40.1}O_{96}$	[mordenite]	17.1	M	NH_4	-	C	593	75Mor2
MOR1976a01	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96} \cdot 34.43H_2O$	[mordenite]	17.2	M	Ca	H_2O	-	-	76Mor1
MOR1977a01	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96}$	[mordenite]	17.6	M	Ca	-	D	773	77Mor1
MOR1977a02	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96} \cdot 2.61H_20$	[mordenite]	17.5	M	Ca	H_2O	D	773	77Mor1
MOR1977a03	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96}$	[mordenite]	17.5	M	Ca	-	D	773	77Mor1
MOR1977a04	$Ca_{3.33} \cdot Al_{7.82}Si_{40.2}O_{96}$	[mordenite]	17.8	M	Ca	H_2O	D	773	77Mor1
MOR1978a01	$K_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$	[mordenite]	17.0	M	K	H_2O	D	783	78Mor1
MOR1978b01	$Rb_8 \cdot Al_8Si_{40}O_{96}$	[mordenite]	17.4	M	Rb	-	D	613	78Sch1
MOR1978d01	$Cs_{7.40} \cdot Al_8Si_{40}O_{96}$	[mordenite]	17.2	M	Cs	-	D	573	78Sch3
MOR1979b01	$Na_{2.4} \cdot Al_{8.4}Si_{39.6}O_{96}$	[mordenite]	17.3	M	Na	-	D	573	79Sch2
MOR1979c01	$Ca_{1.8}K_{0.1}Na_{0.2} \cdot Al_{8.5}Si_{39.5}O_{96}$	[mordenite]	17.5	M	H	-	D	573	79Sch3
MOR1985a01	$Ca_{2.9}Na_{1.4} \cdot Al_{7.2}Si_{40.8}O_{96} \cdot 24H_2O$	[mordenite]	17.3	M	H	H_2O	-	-	85Ito1
MOR1987a01	$Ca_{3.36} \cdot Al_{7.84}Si_{40.24}O_{96} \cdot 26.88H_2O$	[mordenite]	17.3	M	Ca	H_2O	-	-	87Els1
MOR1987a02	$Ca_{3.36} \cdot Al_{7.84}Si_{40.24}O_{96} \cdot 15.16H_2O$	[mordenite]	17.7	M	Ca	H_2O	-	-	87Els1
MOR1987a03	$Ca_{3.36} \cdot Al_{7.84}Si_{40.24}O_{96} \cdot 3.72H_2O$	[mordenite]	17.6	M	Ca	H_2O	-	-	87Els1
MOR1987a04	$Ca_{3.36} \cdot Al_{7.84}Si_{40.24}O_{96} \cdot 1.68H_2O$	[mordenite]	17.7	M	Ca	H_2O	-	-	87Els1
MOR1988a01	$Si_{48}O_{96}$	-	17.1	T	-	-	-	-	88van1
MOR1989a01	$Na_{7.79} \cdot Al_{7.87}Si_{40.13}O_{96} \cdot 10.16H_2O$	(mordenite)	17.1	S	-	H_2O	-	-	89Shi1
MOR1989a02	$Na_{5.81} \cdot Al_{5.75}Si_{42.25}O_{96} \cdot 5.92H_2O$	(mordenite)	17.2	S	-	H_2O	-	-	89Shi1
MOR1989a03	$Na_{4.60} \cdot Al_{4.55}Si_{43.45}O_{96} \cdot 8.36H_2O$	(mordenite)	17.1	S	-	H_2O	-	-	89Shi1
MOR1989a04	$Na_{0.31} \cdot Al_{3.55}Si_{42.72}O_{96} \cdot 4H_2O$	(mordenite)	17.5	S	H	H_2O	-	-	89Shi1
MOR1989b01	$Si_{48}O_{96}$	-	17.1	T	-	-	-	-	89Uyt1

Table MOR.2.1 (MOR-I, *C m c m* continued).

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MOR1994a01	$Na_6 \cdot Al_6Si_{42}O_{96} \cdot 18.4H_2O$	(mordenite)	17.4	S	-	H_2O	-	-	94Rud1
MOR1994a02	$Na_8 \cdot Al_8Si_{40}O_{96} \cdot 12H_2O$	(mordenite)	17.4	S	-	H_2O	-	-	94Rud1
MOR1994a03	$Na_{5.9} \cdot Al_{5.9}Si_{42.1}O_{96} \cdot 20H_2O$	(mordenite)	17.5	S	-	H_2O	-	-	94Rud1
MOR1994a04	$Na_{4.4} \cdot Al_{4.4}Si_{43.9}O_{96} \cdot 18H_2O$	(mordenite)	17.5	S	-	H_2O	-	-	94Rud1
MOR1994a05	$Si_{48}O_{96} \cdot 6.8H_2O$	(mordenite)	17.2	S	H	H_2O	-	-	94Rud1
MOR1994a06	$Si_{48}O_{96} \cdot 8H_2O$	(mordenite)	17.2	S	H	H_2O	-	-	94Rud1
MOR1995a01	$Ca_{1.6}K_{2.6}Na_{2.2} \cdot Al_8Si_{40}O_{96} \cdot 27.8H_2O$	mordenite	17.2	M	-	H_2O	-	-	95Pas1
MOR1997a01	$Cu_{1.39} \cdot Al_{3.12}Si_{44.88}O_{96} \cdot 27.98H_2O$	(mordenite)	17.3	S	Cu	H_2O	-	-	97Att1
MOR1997a02	$Cu_{1.49} \cdot Al_{1.92}Si_{46.08}O_{96} \cdot 4.03H_2O$	(mordenite)	17.5	S	Cu	H_2O	D	783	97Att1
MOR2000a01	$D_{3.2} \cdot Al_{7.42}Si_{40.58}O_{96} \cdot 2.8H_2O$	[mordenite]	17.4	M	ND_4	H_2O	C	823	2000Mar1
MOR2000a02	$D_{3.5} \cdot Al_{7.33}Si_{40.67}O_{96} \cdot 2.48H_2O$	[mordenite]	17.4	S	ND_4	H_2O	C	823	2000Mar1
MOR2000a03	$D_{2.8} \cdot Al_{4.34}Si_{43.66}O_{96} \cdot 2.36H_2O$	[mordenite]	17.4	S	ND_4	H_2O	C	823	2000Mar1
MOR2000b01	$Si_{48}O_{96}$	-	17.2	T	-	-	-	-	2000Dem1
MOR2000b02	$Si_{48}O_{96}$	-	16.7	T	-	-	-	-	2000Dem1
MOR2003a01	$Ca_{1.89}K_{0.14}Mg_{0.09}Na_{3.51} \cdot Al_{7.4}Fe_{0.03}Si_{40.53}O_{96} \cdot 27.26H_2O$	mordenite	17.2	M	-	H_2O	-	-	2003Mar1
MOR2003a02	$Ca_{1.89}K_{0.14}Mg_{0.09}Na_{3.51} \cdot Al_{7.4}Fe_{0.03}Si_{40.53}O_{96} \cdot 13.66H_2O$	[mordenite]	17.3	M	-	H_2O	-	-	2003Mar1
MOR2003a03	$Ca_{1.89}K_{0.14}Mg_{0.09}Na_{3.51} \cdot Al_{7.4}Fe_{0.03}Si_{40.53}O_{96} \cdot 7.76H_2O$	[mordenite]	17.4	M	-	H_2O	-	-	2003Mar1
MOR2003a04	$Ca_{1.89}K_{0.14}Mg_{0.09}Na_{3.51} \cdot Al_{7.4}Fe_{0.03}Si_{40.53}O_{96} \cdot 0.83H_2O$	[mordenite]	17.5	M	-	H_2O	-	-	2003Mar1
MOR2003b01	$Na_{7.45} \cdot Al_{7.76}Si_{40.24}O_{96} \cdot 32H_2O$	(mordenite)	17.2	S	-	H_2O	-	-	2003Kat1
MOR2003b02	$Na_{5.33} \cdot Al_{5.55}Si_{42.45}O_{96} \cdot 32H_2O$	(mordenite)	17.3	S	-	H_2O	-	-	2003Kat1
MOR2003b03	$Na_{4.67} \cdot Al_{4.8}Si_{43.2}O_{96} \cdot 32H_2O$	(mordenite)	17.3	S	-	H_2O	-	-	2003Kat1
MOR-II.1 ***P b c n***									
MOR1978a02	$K_8 \cdot Al_8Si_{40}O_{96}$	[mordenite]	17.5	M	K	-	D	783	78Mor1
MOR1978c01	$Ba_{3.33}Ca_{0.35} \cdot Al_{8.6}Si_{39.9}O_{96}$	[mordenite]	17.7	M	Ba	-	D	573	78Sch2
MOR1979a01	$Ca_{0.03}K_{0.2}Na_{7.3} \cdot Al_{8.3}Si_{39.9}O_{96}$	[mordenite]	17.6	M	Na	-	D	573	79Sch1
MOR-II.2 ***C m* 2 *m***									
MOR1994b01	$Ca_{2.2}Pb_{7.2} \cdot Al_{11.6}Si_{36.4}O_{99.6} \cdot 31.8H_2O$	maricopaite	16.6	M	-	H_2O	-	-	94Rou1

Table MOR.2.1 (continued).

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
	MOR-II.3 *C m c* 2$_1$								
MOR1986a01	$Ca_{2.05}K_{2.8}Mg_{0.04}Na_{1.49}Sr_{0.05} \cdot Al_{8.98}Si_{39.13}O_{96} \cdot 29.07H_2O$	mordenite	17.2	M	-	H_2O	-	-	86Alb1
MOR2004a01	$Ca_{1.85}K_{2.99}Na_{1.06} \cdot Al_{7.89}Si_{40.15}O_{96} \cdot 28H_2O$	mordenite	17.2	M	-	H_2O	-	-	2004Sim1
MOR2004a02	$Na_6 \cdot Al_{6.02}Si_{42.02}O_{96} \cdot 19H_2O$	(mordenite)	17.2	S	-	H_2O	-	-	2004Sim1
	MOR-IV.3 *C* 1 *c* 1								
MOR1971a02	$Al_8Si_{40}O_{96}$	-	17.1	T	-	-	-	-	71Gra1
MOR2004b01	$Na_6 \cdot Al_6Si_{42}O_{96} \cdot Se_{7.9} \cdot 10.04H_2O$	(mordenite)	17.2	S	Se	Se, H_2O	-	-	2004Sim2
MOR2004c01	$Na_{5.5}(C_{12}H_{10}N_3S)_{0.4} \cdot Al_{5.88}Si_{42.02}O_{96} \cdot 9.76H_20$	(mordenite)	17.3	S	-	[1]), H_2O		-	2004Sim3
MOR2004d01	$Na_6 \cdot Al_6Si_{42}O_{96} \cdot 26.48H_2O$	(mordenite)	17.3	S	-	H_2O		-	2004Sim4
MOR2004d02	$Na_{5.52}(C_{16}H_{18}N_3S)_{0.28} \cdot Al_{5.8}Si_{42.2}O_{96} \cdot 9.44H_20$	(mordenite)	17.3	S	-	[2]), H_2O		-	2004Sim4
MOR2005a01	$Na_{5.52}(C_{16}H_{18}N_3S)_{0.28} \cdot Al_{5.8}Si_{42.2}O_{96} \cdot 9.44H_20$	(mordenite)	17.3	S	-	[2]), H_2O		-	2005Sim1

[1]) thionin blue [2]) methylene blue

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

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
MOR-I *C m c m*						
MOR1961a01	18.13(2)	20.49(2)	7.52(3)	2794	n.s.	61Mei1
MOR1971a01	18.11(1)	20.53(1)	7.528(3)	2799	n.s.	71Gra1
MOR1975a01	18.01(1)	20.27(1)	7.465(4)	2725	RT	75Mor1
MOR1975b01	18.223(7)	20.465(9)	7.531(4)	2809	RT	75Mor2
MOR1976a01	18.122(8)	20.46(1)	7.515(4)	2786	RT	76Mor1
MOR1977a01	18.009(5)	20.248(5)	7.461(3)	2721	298	77Mor1
MOR1977a02	18.061(7)	20.331(7)	7.490(4)	2750	623	77Mor1
MOR1977a03	18.05(1)	20.28(1)	7.483(4)	2739	618	77Mor1
MOR1977a04	17.881(7)	20.189(8)	7.479(3)	2700	908	77Mor1
MOR1978a01	18.167(9)	20.61(2)	7.529(6)	2819	RT	78Mor1
MOR1978b01	18.127(7)	20.408(6)	7.463(3)	2761	RT	78Sch1
MOR1978d01	18.19(2)	20.47(2)	7.506(9)	2795	n.s.	78Sch3
MOR1979b01	18.178(7)	20.394(6)	7.488(4)	2776	n.s.	79Sch2
MOR1979c01	18.058(3)	20.297(3)	7.484(2)	2743	RT	79Sch3
MOR1985a01	18.089(3)	20.412(4)	7.504(1)	2771	n.s.	85Ito1
MOR1987a01	18.091(4)	20.418(4)	7.508(1)	2773	293	87Els1
MOR1987a02	17.964(5)	20.273(7)	7.467(3)	2719	423	87Els1
MOR1987a03	17.955(7)	20.295(9)	7.468(4)	2721	573	87Els1
MOR1987a04	17.979(7)	20.229(9)	7.456(4)	2721	723	87Els1
MOR1988a01	18.16	20.55	7.54	2814	-	88van1
MOR1989a01	18.121(5)	20.517(4)	7.544(1)	2805	n.s.	89Shi1
MOR1989a02	18.136(3)	20.490(2)	7.531(1)	2799	n.s.	89Shi1
MOR1989a03	18.168(4)	20.467(3)	7.528(1)	2799	n.s.	89Shi1
MOR1989a04	18.122(3)	20.256(2)	7.473(1)	2743	n.s.	89Shi1

Table MOR.2.2 (continued).

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
MOR1989b01	18.16	20.55	7.54	2814	n.s.	89Uyt1
MOR1994a01	18.1073(5)	20.3820(4)	7.4950(1)	2766	n.s.	94Rud1
MOR1994a02	18.1048(5)	20.3801(4)	7.4938(1)	2765	n.s.	94Rud1
MOR1994a03	18.0748(7)	20.2740(5)	7.4678(2)	2737	n.s.	94Rud1
MOR1994a04	18.0807(7)	20.2770(5)	7.4682(2)	2738	n.s.	94Rud1
MOR1994a05	18.1088(7)	20.4609(6)	7.5312(2)	2790	n.s.	94Rud1
MOR1994a06	18.1132(6)	20.4616(6)	7.5305(2)	2791	n.s.	94Rud1
MOR1995a01	18.109(3)	20.485(6)	7.523(9)	2791	n.s.	95Pas1
MOR1997a01	18.1659(4)	20.375(1)	7.495(1)	2774	RT	97Att1
MOR1997a02	18.0546(7)	20.298(2)	7.4772(3)	2740	RT	97Att1
MOR2000a01	18.125(1)	20.312(1)	7.489(1)	2757	2	2000Mar1
MOR2000a02	18.125(1)	20.298(1)	7.477(1)	2751	2	2000Mar1
MOR2000a03	18.126(1)	20.299(1)	7.478(1)	2751	2	2000Mar1
MOR2000b01	18.101	20.501	7.526	2793	-	2000Dem1
MOR2000b02	18.260	20.706	7.606	2876	-	2000Dem1
MOR2003a01	18.120(1)	20.494(1)	7.531(1)	2797	298	2003Mar1
MOR2003a02	18.074(1)	20.446(1)	7.521(1)	2779	473	2003Mar1
MOR2003a03	18.024(1)	20.386(1)	7.503(1)	2757	723	2003Mar1
MOR2003a04	18.029(1)	20.308(1)	7.493(1)	2743	1103	2003Mar1
MOR2003b01	18.112(5)	20.475(5)	7.523(2)	2790	n.s.	2003Kat1
MOR2003b02	18.108(3)	20.428(3)	7.504(1)	2776	n.s.	2003Kat1
MOR2003b03	18.110(2)	20.404(2)	7.494(1)	2769	n.s.	2003Kat1
MOR-II.1 ***P b c n***						
MOR1978a02	18.030(7)	20.41(1)	7.457(5)	2744	RT	78Mor1
MOR1978c01	17.974(7)	20.320(8)	7.419(4)	2710	n.s.	78Sch2
MOR1979a01	17.92(1)	20.31(1)	7.480(7)	2722	n.s.	79Sch1
MOR-II.2 ***C m* 2 *m***						
MOR1994b01	19.434(2)	19.702(2)	7.538(1)	2886	n.s.	94Rou1
MOR-II.3 ***C m c* 2$_1$**						
MOR1986a01	18.094(1)	20.516(1)	7.524(1)	2793	n.s.	86Alb1
MOR2004a01	18.096(4)	20.473(4)	7.515(2)	2784	293	2004Sim1
MOR2004a02	18.131(2)	20.507(2)	7.522(5)	2797	293	2004Sim1
MOR-IV.3 ***C* 1 *c* 1**						
MOR1971a02	18.11(1)	20.53(1)	7.528(3)	90 2799	-	71Gra1
MOR2004b01	18.077(3)	20.509(2)	7.5172(9)	90.03(2) 2787	120	2004Sim2
MOR2004c01	18.126(3)	20.403(2)	7.499(1)	90.02(2) 2773	120	2004Sim3
MOR2004d01	18.073(3)	20.463(3)	7.5145(9)	90.05(1) 2779	120	2004Sim4
MOR2004d02	18.159(4)	20.349(4)	7.492(1)	90.03(2) 2768	120	2004Sim4
MOR2005a01	18.159(4)	20.349(4)	7.492(1)	90.03(2) 2768	120	2005Sim1

Table MOR.2.3 Transformation matrices. Entries not listed are not transformed.

code	shift	matrix	coord. transform.	reference
MOR-I ***C m c m***				
MOR1997a01	½, 0, 0	**-a**, **-b**, **c**	*-x*+½, *-y*, *z*	97Att1
MOR1997a02	½, 0, 0	**-a**, **-b**, **c**	*-x*+½, *-y*, *z*	97Att1
MOR-II.2 ***C m* 2 *m***				
MOR1994b01	½, 0, ¼	**a**, **b**, **c**	*x*-½, *y*, *z*-¼	94Rou1

Table MOR.2.3 (continued)

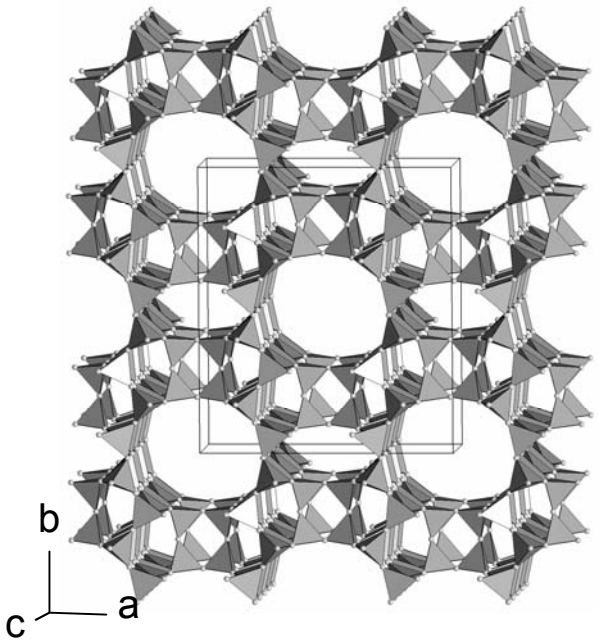
code	shift	matrix	coord. transform.	reference
MOR-IV.3 *C* 1 *c* 1				
MOR2004b01	0, 0, 1/8	**a**, **b**, **c**	*x*, *y*, *z*-1/8	2004Sim2
MOR2004c01	0, 0, 1/8	**a**, **b**, **c**	*x*, *y*, *z*-1/8	2004Sim3
MOR2004d01	0, 0, 1/8	**a**, **b**, **c**	*x*, *y*, *z*-1/8	2004Sim4
MOR2004d02	0, 0, 1/8	**a**, **b**, **c**	*x*, *y*, *z*-1/8	2004Sim4
MOR2005a01	0, 0, 1/8	**a**, **b**, **c**	*x*, *y*, *z*-1/8	2005Sim1

MOR.3 Framework structures

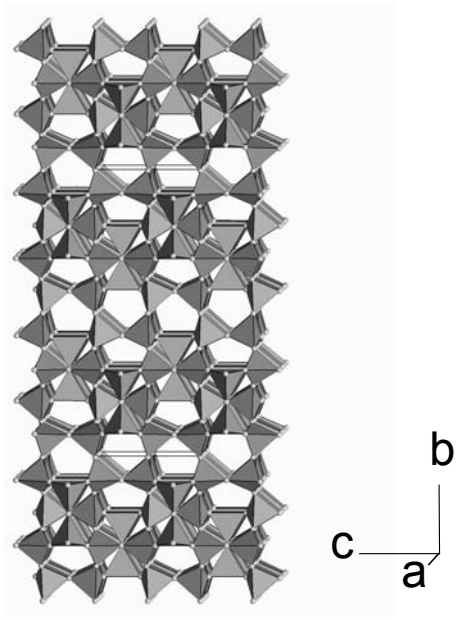
MOR.3.1 MOR-I compound (*C m c m*, IT #63)

Table MOR.3.1.1 Atomic coordinates and site definitions for MOR-I, mordenite, $Na_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$ (MOR1971a01, 71Gra1).

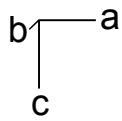
atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0.30103(9)	0.07229(7)	0.0418(3)	1.37	1	16(h)	13.328/2.672
(Si,Al)2	0.30344(9)	0.30908(9)	0.0454(2)	1.49	1	16(h)	13.328/2.672
(Si,Al)3	0.0871(2)	0.3840(1)	¼	1.21	. . *m*	8(g)	6.664/1.336
(Si,Al)4	0.0866(2)	0.2280(1)	¼	1.32	. . *m*	8(g)	6.664/1.336
O1	0.1232(2)	0.4170(2)	0.4292(5)	3.09	1	16(h)	16
O2	0.1226(2)	0.1946(2)	0.4262(5)	2.95	1	16(h)	16
O3	0.2632(2)	0.3776(2)	0.4887(5)	3.63	1	16(h)	16
O4	0.0974(3)	0.3057(3)	¼	3.61	. . *m*	8(g)	8
O5	0.8306(3)	0.8054(3)	¼	3.61	. . *m*	8(g)	8
O6	0.8231(3)	0.5788(3)	¼	2.66	. . *m*	8(g)	8
O7	0.7324(3)	0	0	2.35	2 . .	8(e)	8
O8	¼	¼	0	4.72	$\bar{1}$	8(d)	8
O9	0	0.4071(3)	¼	2.17	*m* 2 *m*	4(c)	4
O10	0	0.2061(4)	¼	3.00	*m* 2 *m*	4(c)	4
Ow1	0	½	0	2.50	2/*m* . .	4(b)	4
Ow2	0	0.4335(4)	¾	4.95	*m* 2 *m*	4(c)	4
Ow3	0.040(1)	0.303(1)	¾	16.32	. . *m*	8(g)	4
Ow4	0	0.181(1)	¾	13.84	*m* 2 *m*	4(c)	4
Ow5	0	0.094(1)	0.502(2)	21.32	*m* . .	8(f)	8
Ow6	0.109(1)	0.030(1)	¾	82.17	. . *m*	8(g)	8
Ow7	0	-0.009(3)	¼	22.84	*m* 2 *m*	4(c)	1

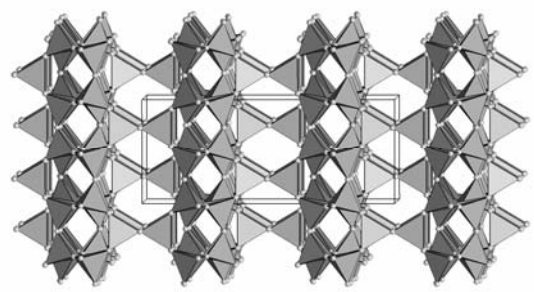


a View parallel **c** rotated by 5° about **a** and **b**.

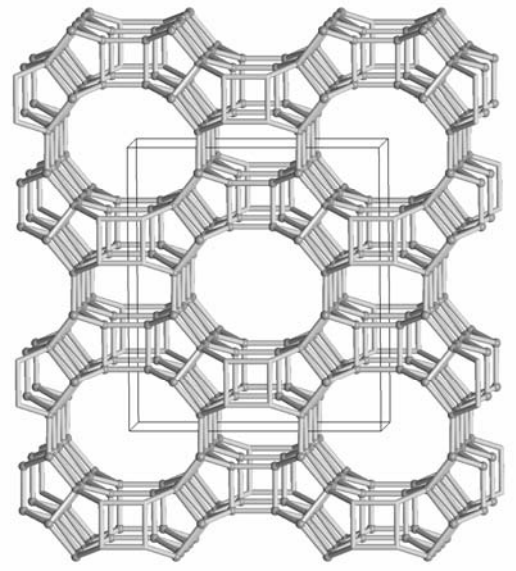


b View parallel **a** rotated by 1° about **b** and **c**.





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



d Ball and stick model corresponding to a).

Fig. MOR.3.1.1 Projections of the MOR-I crystal structure of mordenite, $Na_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$ (MOR1971a01, 71Gra1).

Table MOR.3.1.2 Selected interatomic distances and angles for MOR-I, mordenite, $Na_8 \cdot Al_8Si_{40}O_{96} \cdot 24H_2O$ (MOR1971a01, 71Gra1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)1 - O3	1.603(4)	158.7(3)	(Si,Al)2 - O8	1.589(2)	180
(Si,Al)1 - O6	1.623(3)	149.9(4)	(Si,Al)2 - O3	1.605(4)	158.7(3)
(Si,Al)1 - O1	1.628(4)	144.9(3)	(Si,Al)2 - O2	1.614(4)	143.6(3)
(Si,Al)1 - O7	1.633(4)	136.5(4)	(Si,Al)2 - O5	1.619(2)	144.2(4)
mean	1.622	147.5	mean	1.607	156.6
(Si,Al)3 - O4	1.618(6)	166.4(4)	(Si,Al)4 - O4	1.607(6)	166.4(4)
(Si,Al)3 - O1	1.645(4)	144.9(3)	(Si,Al)4 - O2	1.629(4)	143.6(3)
(Si,Al)3 - O1	1.645(4)	144.9(3)	(Si,Al)4 - O2	1.629(4)	143.6(3)
(Si,Al)3 - O9	1.647(4)	146.5(4)	(Si,Al)4 - O10	1.632(4)	148.0(6)
mean	1.639	150.7	mean	1.624	150.4

MOR.3.2 MOR-II.1 compound (*Pbcn*, IT #60)

Crystal structure projections are essentially identical with Fig. MOR.3.1.1.

Table MOR.3.2.1 Atomic coordinates and site definitions for MOR-II.1, K-exchanged and dehydrated mordenite, $K_8 \cdot Al_8Si_{40}O_{96}$ (MOR1978a02, 78Mor1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11	0.31019(9)	0.07653(7)	0.0800(2)	1.59	1	8(d)	6.664 / 1.336
(Si,Al)12	0.79836(9)	0.56916(7)	0.0049(2)	1.70	1	8(d)	6.664 / 1.336
(Si,Al)21	0.30800(9)	0.31581(7)	0.0682(2)	1.77	1	8(d)	6.664 / 1.336
(Si,Al)22	0.79679(8)	0.80451(7)	0.0176(2)	1.56	1	8(d)	6.664 / 1.336
(Si,Al)3	0.08488(8)	0.38184(7)	0.2839(2)	1.34	1	8(d)	6.43 / 1.29(4)
(Si,Al)4	0.08472(8)	0.22444(7)	0.2767(2)	1.30	1	8(d)	6.50 / 1.30(4)
O11	0.1102(2)	0.4137(2)	0.4775(5)	3.21	1	8(d)	8
O12	0.6346(3)	0.9122(3)	0.3738(6)	5.61	1	8(d)	8
O21	0.1136(2)	0.1921(2)	0.4646(5)	3.39	1	8(d)	8
O22	0.6322(2)	0.6970(2)	0.3895(5)	4.11	1	8(d)	8
O31	0.2475(2)	0.3680(2)	0.5233(6)	4.02	1	8(d)	8
O32	0.7738(2)	0.8865(2)	0.4710(6)	3.90	1	8(d)	8
O4	0.0896(2)	0.3034(2)	0.2885(6)	3.97	1	8(d)	7.76
O5	0.8293(2)	0.8087(2)	0.2205(5)	3.40	1	8(d)	8
O6	0.8298(2)	0.5788(2)	0.2070(5)	3.07	1	8(d)	8
O7	0.7252(2)	-0.0062(2)	-0.0265(5)	2.70	1	8(d)	8
O8	0.2512(2)	0.2607(2)	0.0031(6)	3.38	1	8(d)	8
O9	0	0.4078(3)	¼	3.67	. 2 .	4(c)	3.88
O10	0	0.1999(3)	¼	2.96	. 2 .	4(c)	3.88
K2	0.0125(4)	0.4517(2)	0.8090(9)	8.08	1	8(d)	3.34(3)
K4	0.0128(4)	0.1823(3)	0.8007(9)	7.16	1	8(d)	3.04(3)
K6	0.1606(7)	0.024(1)	0.791(2)	6.93	1	8(d)	0.91(3)
(Si,Al)13	0.0849	0.3818	0.78390(0)	1.30	1	8(d)	0.20 / 0.04
(Si,Al)14	0.0847	0.2244	0.77670(0)	1.30	1	8(d)	0.20 / 0.04
O14	0.0896	0.3034	0.78850(0)	3.80	1	8(d)	0.24
O19	0	0.4078	¾	3.20	. 2 .	4(c)	0.12
O20	0	0.1999	¾	3.20	. 2 .	4(c)	0.12

Table MOR.3.2.2 Selected interatomic distances and angles for MOR-II.1, K-exchanged and dehydrated mordenite, $K_8 \cdot Al_8Si_{40}O_{96}$ (MOR1978a02, 78Mor1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11 - O31	1.594(4)	171.0(3)	(Si,Al)12 - O12	1.600(5)	164.2(4)
(Si,Al)11 - O7	1.620(4)	141.0(3)	(Si,Al)12 - O32	1.605(4)	148.4(3)
(Si,Al)11 - O6	1.628(4)	145.8(3)	(Si,Al)12 - O7	1.612(4)	141.0(3)
(Si,Al)11 - O11	1.638(4)	134.4(3)	(Si,Al)12 - O6	1.622(4)	145.8(3)
mean	1.620	148.1	mean	1.610	149.9
(Si,Al)21 - O32	1.596(4)	148.4(3)	(Si,Al)22 - O8	1.595(4)	164.8(3)
(Si,Al)21 - O8	1.597(4)	164.8(3)	(Si,Al)22 - O22	1.598(4)	153.5(3)
(Si,Al)21 - O21	1.619(4)	136.7(3)	(Si,Al)22 - O31	1.600(4)	171.0(3)
(Si,Al)21 - O5	1.628(4)	145.2(3)	(Si,Al)22 - O5	1.625(4)	145.2(3)
mean	1.610	148.8	mean	1.604	158.6
(Si,Al)3 - O12	1.603(5)	164.2(4)	(Si,Al)4 - O22	1.607(4)	153.5(3)
(Si,Al)3 - O4	1.603(4)	172.5(3)	(Si,Al)4 - O4	1.616(4)	172.5(3)
(Si,Al)3 - O9	1.639(2)	142.3(4)	(Si,Al)4 - O10	1.620(2)	144.0(4)
(Si,Al)3 - O11	1.648(4)	134.4(4)	(Si,Al)4 - O21	1.634(4)	136.7(3)
mean	1.623	153.4	mean	1.619	151.7

MOR.3.3 MOR-II.2 compound (*Cm*2*m*, IT #38)

Table MOR.3.3.1 Atomic coordinates and site definitions for MOR-II.2, maricopaite, $Ca_{2.2}Pb_{7.2} \cdot Al_{11.6}Si_{36.4}O_{99.6} \cdot 31.8H_2O$ (MOR1994b01, 94Rou1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11	0.2446(3)	0.0779(2)	0.0385(6)	1.26(9)	1	8(f)	6.06 / 1.94
(Si,Al)12	0.7546(3)	0.9283(2)	0.9576(6)	1.18(9)	1	8(f)	6.06 / 1.94
(Si,Al)21	0.3210(3)	0.2907(2)	0.0456(6)	1.17(9)	1	8(f)	6.06 / 1.94
(Si,Al)22	0.6789(3)	0.7169(2)	0.9543(6)	1.38(9)	1	8(f)	6.06 / 1.94
(Si,Al)31	0.1395(3)	0.4238(3)	¼	1.0(1)	. . *m*	4(e)	3.03 / 0.97
(Si,Al)32	0.8658(4)	0.5843(3)	¾	1.1(1)	. . *m*	4(d)	3.03 / 0.97
(Si,Al)41	0.0817(3)	0.2763(3)	¼	1.1(1)	. . *m*	4(e)	3.03 / 0.97
(Si,Al)42	0.9206(4)	0.7311(3)	¾	1.6(1)	. . *m*	4(d)	3.03 / 0.97
O11	0.1861(7)	0.4200(6)	0.425(2)	2.9(3)	1	8(f)	8
O12	0.8180(6)	0.5864(5)	0.569(2)	1.7(2)	1	8(f)	8
O21	0.1168(7)	0.2424(6)	0.428(2)	3.3(3)	1	8(f)	8
O22	0.8836(6)	0.7604(7)	0.574(2)	3.0(3)	1	8(f)	8
O31	0.3135(6)	0.3708(6)	0.486(2)	2.0(2)	1	8(f)	8
O32	0.6866(6)	0.6342(5)	0.508(2)	2.3(2)	1	8(f)	8
O41	0.0862(8)	0.3586(8)	¼	1.4(3)	. . *m*	4(e)	4
O42	0.9190(9)	0.6441(9)	¾	2.3(4)	. . *m*	4(d)	4
O51	0.839(1)	0.777(1)	¼	3.5(5)	. . *m*	4(e)	4
O52	0.1557(9)	0.2307(8)	¾	2.2(4)	. . *m*	4(d)	4
O61	0.7660(9)	0.5838(8)	¼	2.0(4)	. . *m*	4(e)	4
O62	0.228(1)	0.4219(9)	¾	2.5(4)	. . *m*	4(d)	4
O7	0.2897(6)	0.5030(7)	0.504(2)	2.5(2)	1	8(f)	8
O8	0.2500(9)	0.2536(9)	0.499(2)	3.6(3)	1	8(f)	8
O91' [1])	0.093(1)	0.492(1)	¼	3.8(5)	. . *m*	4(e)	4
O92' [2])	0.086(1)	0.5162(9)	¾	2.4(4)	. . *m*	4(d)	4

Table MOR.3.3.1 (continued)

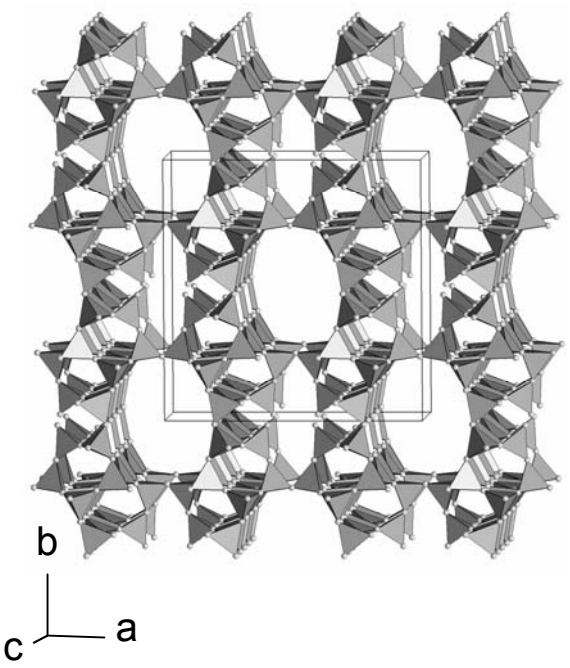
atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
O101	0	0.256(1)	¼	2.6(5)	*m* 2 *m*	2(b)	2
O102	0	0.753(1)	¾	2.5(5)	*m* 2 *m*	2(a)	2
Pb1	0.5975(1)	0.10440(0)	¼	2.25(2)	. . *m*	4(e)	3.32(1)
Pb2	0.5977(2)	0.8988(2)	¾	1.83(8)	. . *m*	4(d)	0.98(1)
Pb3	½	0.9662(1)	-0.0123(2)	2.29(3)	*m* . .	4(c)	2.49(1)
Pb4	½	0.0359(3)	0.002(1)	3.4(2)	*m* . .	4(c)	0.70(1)
Ow19	½	0.0828(9)	0.060(3)	2.2(4)	*m* . .	4(c)	3.7(1)
Ow20	½	0.231(1)	¼	2.60	*m* 2 *m*	2(b)	1.9(1)
Ow21	0.585(2)	0.561(1)	¾	2.60	. . *m*	4(d)	2.4(1)
Ow22	½	0.501(2)	0.849(5)	2.60	*m* . .	4(c)	2.0(1)
Ow23	0.561(3)	0.594(3)	¼	2.60	. . *m*	4(e)	1.1(1)
Ow24	0.577(4)	0.456(3)	-0.01(1)	2.60	1	8(f)	1.4(2)
Ow25	0.574(3)	0.457(3)	0.135(9)	2.60	1	8(f)	1.6(2)
Ow26	0.579(2)	0.871(2)	¾	2.60	. . *m*	4(d)	2.3(1)
Ow27	0.570(6)	0.151(6)	¼	2.60	. . *m*	4(e)	0.7(1)
Ow28	½	0.933(2)	-0.035(5)	2.60	*m* . .	4(c)	1.9(2)

[1]) (p. 189) This is an unshared oxygen atom bonded to (Si,Al)31, a T-atom with only three bridges to neighboring coordination tetrahedra.
[2]) (p. 189) This is an unshared oxygen atom bonded to (Si,Al)32, a T-atom with only three bridges to neighboring coordination tetrahedra.

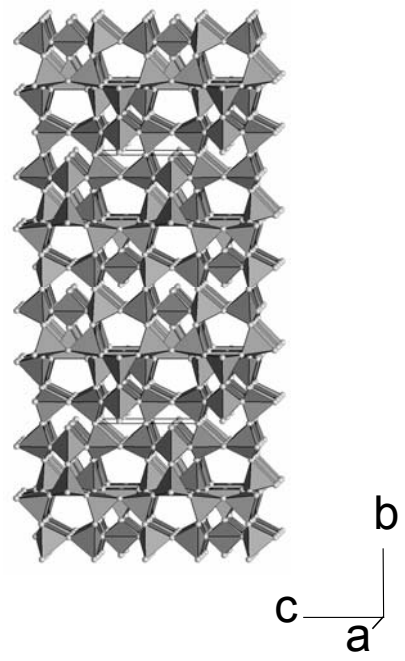
Nonstandard setting with origin in 0, 0, -¼ from . . *m*.
Symmetry operators : *x*, *y*, *z* -*x*, *y*, *z* -*x*, *y*, -*z*+½ *x*, *y*, -*z*+½
and equivalent positions related by C-centering (½, ½, 0)+

Table MOR.3.3.2 Selected interatomic distances and angles for MOR-II.2, maricopaite, $Ca_{2.2}Pb_{7.2} \cdot Al_{11.6}Si_{36.4}O_{99.6} \cdot 31.8H_2O$ (MOR1994b01, 94Rou1).

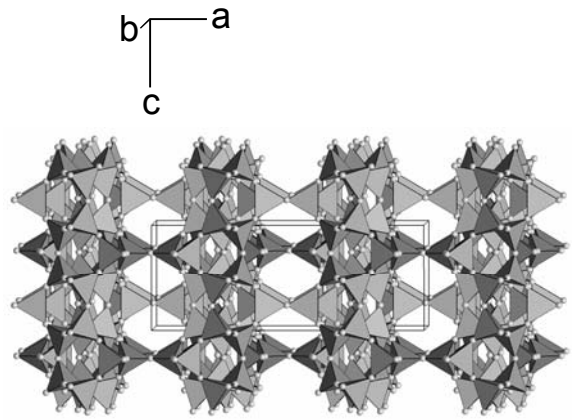
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11 - O32	1.62(1)	140(1)	(Si,Al)12 - O11	1.61(2)	157(1)
(Si,Al)11 - O12	1.65(1)	153(1)	(Si,Al)12 - O7	1.65(1)	132(1)
(Si,Al)11 - O7	1.65(1)	132(1)	(Si,Al)12 - O62	1.65(1)	142(1)
(Si,Al)11 - O61	1.65(1)	150(1)	(Si,Al)12 - O31	1.67(1)	140(1)
mean	1.64	144	mean	1.65	143
(Si,Al)21 - O8	1.60(2)	180	(Si,Al)22 - O21	1.58(2)	154(1)
(Si,Al)21 - O31	1.60(1)	140(1)	(Si,Al)22 - O8	1.60(2)	180
(Si,Al)21 - O51	1.60(1)	148(1)	(Si,Al)22 - O52	1.63(1)	142(1)
(Si,Al)21 - O22	1.63(1)	157(1)	(Si,Al)22 - O32	1.66(1)	140(1)
mean	1.61	156	mean	1.62	154
(Si,Al)31 - O11	1.60(1)	157(1)	(Si,Al)32 - O42	1.57(2)	140(1)
(Si,Al)31 - O11	1.60(1)	157(1)	(Si,Al)32 - O92’	1.63(2)	-
(Si,Al)31 - O91’	1.61(2)	-	(Si,Al)32 - O12	1.65(1)	153(1)
(Si,Al)31 - O41	1.65(2)	144(1)	(Si,Al)32 - O12	1.65(1)	153(1)
mean	1.62	153	mean	1.63	149
(Si,Al)41 - O41	1.62(2)	144(1)	(Si,Al)42 - O102	1.60(1)	149(2)
(Si,Al)41 - O101	1.64(1)	151(2)	(Si,Al)42 - O22	1.62(1)	157(1)
(Si,Al)41 - O21	1.65(2)	154(1)	(Si,Al)42 - O22	1.62(1)	157(1)
(Si,Al)41 - O21	1.65(2)	154(1)	(Si,Al)42 - O42	1.71(2)	140(1)
mean	1.64	151	mean	1.64	151



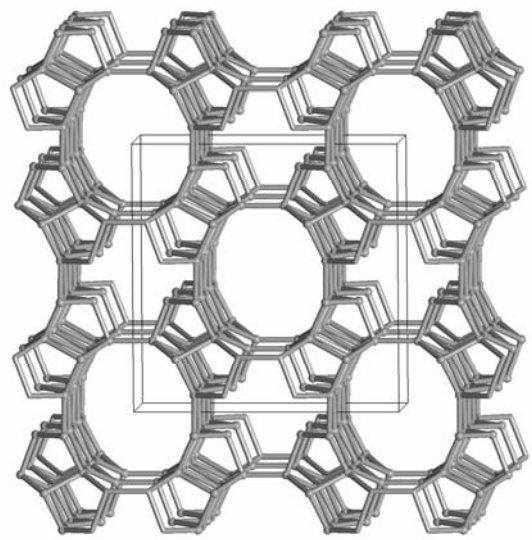
a View parallel **c** rotated by 5° about **a** and **b**.



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



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



d Ball and stick model corresponding to a).

Fig. MOR.3.3.1 Projections of the MOR-II.2 crystal structure of maricopaite, $Ca_{2.2}Pb_{7.2} \cdot Al_{11.6}Si_{36.4}O_{99.6} \cdot 31.8H_2O$ (MOR1994b01, 94Rou1).

MOR.4 Chemical composition

	D															
H																He
Li	Be										B	**C**	**N**	***O***	F	Ne
Na	**Mg**										**Al**	**Si**	P	**S**	Cl	Ar
K	**Ca**	Sc	Ti	V	Cr	Mn	**Fe**	Co	Ni	**Cu**	Zn	Ga	Ge	As	**Se**	Br	Kr
Rb	**Sr**	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	**Ba**	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	**Pb**	Bi	Po	At	Rn

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

MOR.5 Flexibility and apertures

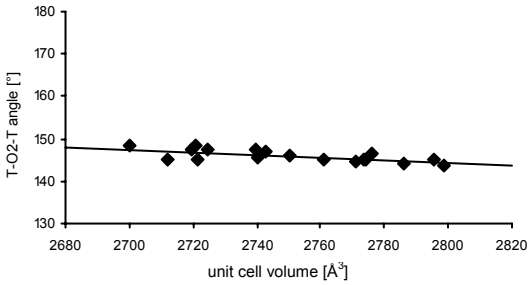


Fig. MOR.5.1 Individual T-O2-T angles from 18 crystal structure determinations of MOR-type compounds with silicoaluminate frameworks crystallizing in space group *C m c m* plotted against the unit cell volume. The plot shows 18 pairs of experimental values. The individual values of the cell volumes range from 2700Å^3 to 2799 Å^3, with a mean of 2750 Å^3. The values of the angles range from 143.6° to 148.3°, with a mean of 146°. The line is a least-squares fit to all points. Only precise single crystal structure determinations have been included in the data set: the mean e.s.d. of the individual T-O distances is 0.01 Å or less.

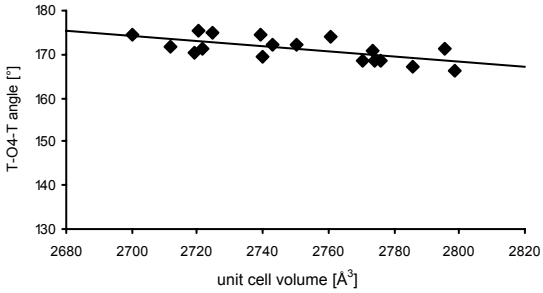


Fig. MOR.5.2 Individual T-O4-T angles from 18 crystal structure determinations of MOR-type compounds with silicoaluminate frameworks crystallizing in space group *Cm cm* plotted against the unit cell volume. The plot shows 18 pairs of experimental values. The values of the angles range from 166.4° to 175.6°, with a mean of 171°. The line is a least-squares fit to all points. Only precise single crystal structure determinations have been included in the data set: the mean e.s.d. of the individual T-O distances is 0.01Å or less.

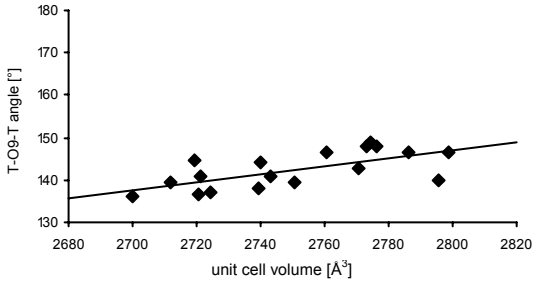


Fig. MOR.5.3 Individual T-O9-T angles from 18 crystal structure determinations of MOR-type compounds with silicoaluminate frameworks crystallizing in space group *C m c m* plotted against the unit cell volume. The plot shows 18 pairs of experimental values. The values of the angles range from 136.5° to 148.9°, with a mean of 142°. The line is a least-squares fit to all points. Only precise single crystal structure determinations have been included in the data set: the mean e.s.d. of the individual T-O distances is 0.01 Å or less.

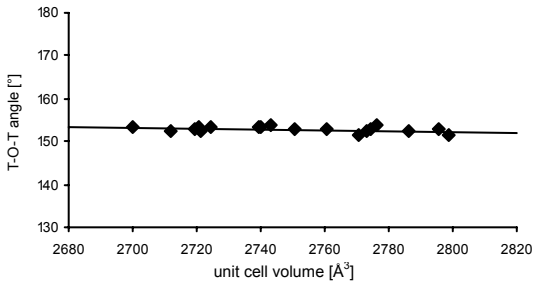


Fig. MOR.5.4 Mean T-O-T angles from 18 crystal structure determinations of MOR-type compounds with silicoaluminate frameworks crystallizing in space group *C m c m* plotted against the unit cell volume. The plot shows 18 pairs of experimental values. The values of the angles range from 151.5° to 153.9°, with a mean of 153°. The line is a least-squares fit to all points. Only precise single crystal structure determinations have been included in the data set: the mean e.s.d. of the individual T-O distances is 0.01 Å or less.

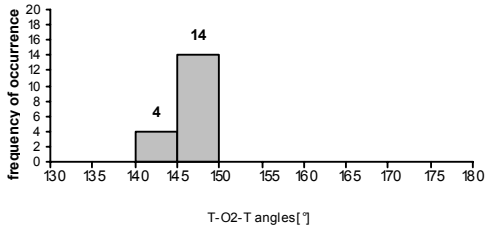


Fig. MOR.5.5 Histogram of individual T-O2-T angles from 18 experimental crystal structure determinations of MOR-type compounds with silicoaluminate frameworks. The individual values of the angles range from 144° to 148°, with a mean value of 146°.

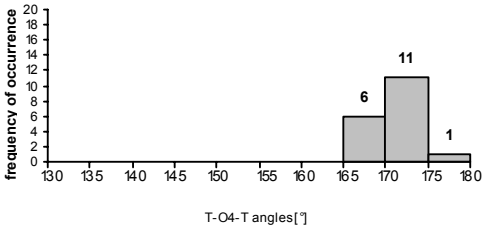


Fig. MOR.5.6 Histogram of individual T-O4-T angles from 18 experimental crystal structure determinations of MOR-type compounds with silicoaluminate frameworks. The individual values of the angles range from 166° to 176°, with a mean value of 171°.

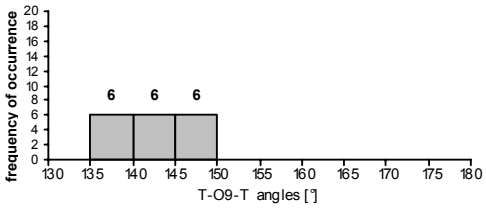


Fig. MOR.5.7 Histogram of individual T-O9-T angles from 18 experimental crystal structure determinations of MOR-type compounds with silicoaluminate frameworks. The individual values of the angles range from 136° to 149°, with a mean value of 142°.

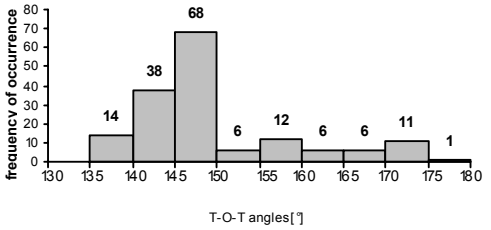


Fig. MOR.5.8 Distribution of all individual T-O-T angles from 18 experimental crystal structure determinations of MOR-type compounds with silicoaluminate frameworks. The individual values of the angles range from 136° to 180°, with an overall mean value of 153°.

The unit cell volumes of MOR-type silicoaluminate compounds crystallizing in space group Cmcm as shown in Table MOR.2.2 vary by about 4.4%. This is a small deviation, not only when compared with collapsible frameworks such as the natrolites [92Bau2], but also when compared with a rather stable framework, such as the noncollapsible framework of the LTA-type [92Bau2]. There the unit cell constants vary by about 4%. For a meaningful comparison we must contrast this with the ratio of the third root of the unit cell volumes of the MOR-type compounds, which is about 1.5%. It seems that the framework of MOR-type is relatively inflexible. This is also supported by the observation that the three unit cell constants of MOR-type silicoaluminate compounds in space group *C m c m* vary only by one to two percent, despite the wide array of exchanged cations in its pores (Table MOR.2.1 and Fig. MOR.4.1). That is a small range when compared to the *a* and *b* cell constants of NAT-type silicoaluminates which vary from 16.01 Å to 19.66 Å, or by 23% [92Bau2].

Figs. MOR.5.1 and MOR.5.2 show that as the angles T-O2-T and T-O4-T **decrease** in the MOR-I-type compounds in space group *C m c m*, their unit cell volumes **increase**. The slopes of T-O-T *vs*. V are negative. For the angles T-O9-T the reverse is true, the slope is positive (Fig. MOR.5.3). Of the ten crystallographically independent T-O-T angles in the MOR-I type a total of five, those around atoms O2, O3, O4, O5 and O7, have negative slopes, while the four around atoms O1, O6, O9 and O10 have positive slopes (the angle at O8 stays at 180° throughout). We show here the examples with the steepest slopes. The angles around O2 etc. antirotate [92Bau1, 92Bau2] to the other T-O-T angles (those with positive slopes) in the framework. As a consequence the framework is noncollapsible as opposed to such frameworks as NAT or SOD in which all T-O-T angle corotate and the frameworks become collapsible [95Bau1]. When the angles T-O-T open and close in concert upon volume change they are collapsible, while frameworks with antirotating hinges are noncollapsible. Among zeolites the only known noncollapsible frameworks known so far are FAU, KFI, LTA and MAZ (see Figs. FAU.5.8, KFI.5.1, KFI.5.2 in[2002Bau1], and Figs. LTA.5.6 and MAZ.5.2). The tetrahedral framework of feldspar is also noncollapsible [96Bau1].

The distributions for each crystallographically independent separate T-O-T angle are rather narrow (Figs. MOR.5.5, MOR.5.6 and MOR.5.7). The value of the overall mean T-O-T angles for 18 crystal structures of the MOR-type precisely determined by single crystal methods is about 153°, with individual angles ranging from 136° to 180°. This range of values T-O-T for the MOR-type is smaller than observed for the LTA-type compounds where it varies from 125° to 179° (see the LTA chapter and [92Bau1]). The full range of values displayed by numerous zeolite frameworks of different types is 115° to 180° as observed in a sample of 2436 T-O-T values [95Bau1]. The mean angle in MOR-type compounds is clearly larger than the maximum of the distribution of T-O-T angles in silicoaluminate zeolites (about 143° [95Bau1]).

The 12-ring opening in the framework of MOR has free diameters ranging from about 6.5 Å to 7 Å. This means that it is rather buckled compared with the opening in the FAU-type framework, which is almost 7.5 Å wide, but still more open than in the MTW framework (ca. 5.5 Å to 6 Å).

MOR.6 Other information

Next to FAU- and MFI-based catalysts MOR-type compounds may be the most important for applications in the chemical industry. Such uses involve among other things paraffin and xylene isomerization, ethylene production, methylamine synthesis and NO_x reduction. Numerous patents mentioning mordenite zeolites have been issued.

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