MON

MON.1 Zeolite framework type and topology

The framework type code is named after the mineral **MON**tesommaite, $(K,Na)_9 \cdot Al_9Si_{23}O_{64} \cdot 10H_2O$, first found in the Monte Somma-Vesuvius volcanic complex at Pollena, Italy, and described in [90Rou1]. The crystal structure was solved in space group $I4_1/amd$ although optical investigations indicated orthorhombic symmetry. Combined optical and X-ray diffraction studies lead to space group $Fdd2$ as most probable symmetry. However, all refinements were done in the substructure. A synthetic aluminogermanate analogue was synthesized and described by [2002Tri1] crystallizing in subgroup $I\bar{4}2d$ The framework structure (Fig. MON.1.1) can be described as being built from *kaj* ($5^2 8^2 8^1$) units as shown in Fig. MON.1.2 forming a two-dimensional channel system parallel **a** and **b**.

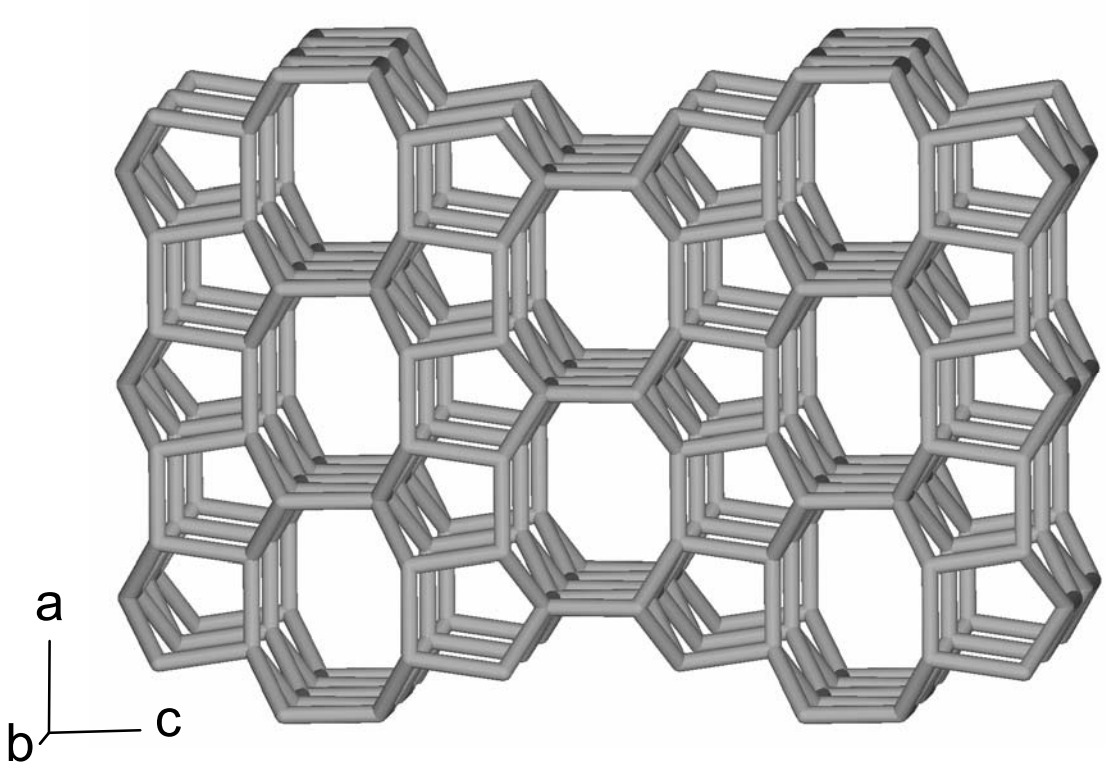
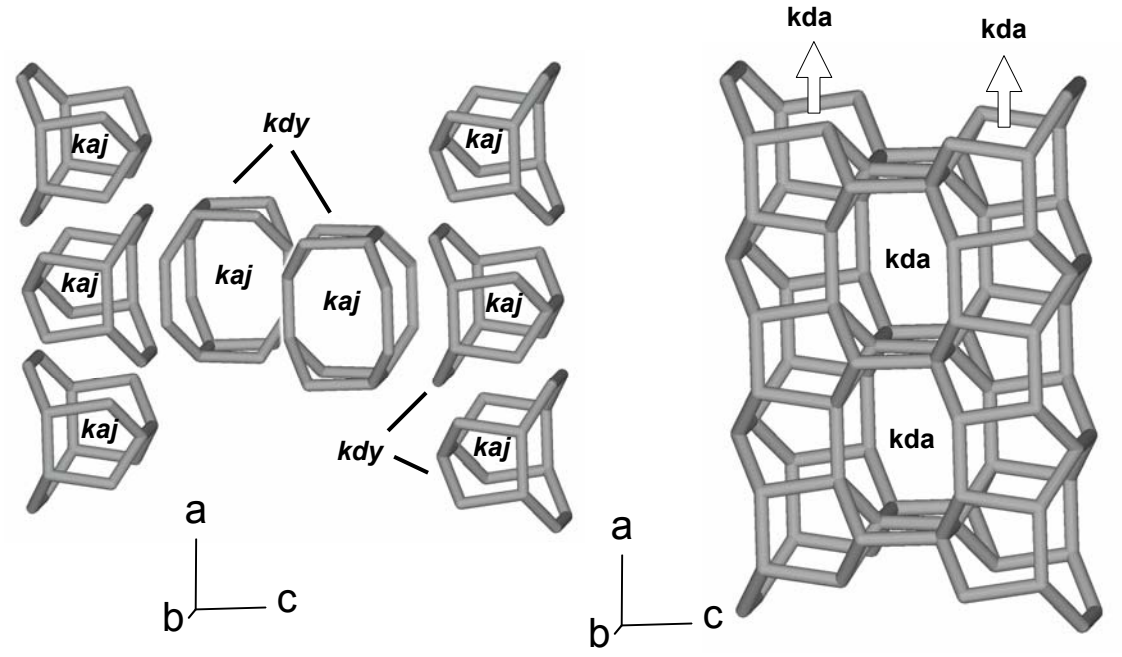


Fig. MON.1.1. The framework structure of MON-type compounds in the highest possible topological symmetry $I4_1/amd$ (MON1990a01, 90Rou1). View parallel **b** rotated by 5° about **a** and **c**.



a Linkage of *kaj* units. Two *kaj* units, respectively, form a *kdy* unit.

b The assemblage shown in a) extended parallel **a** by consecutive stacking of *kaj* (*kdy*) units. Arrows indicate the directions of the 8-ring channels (**kda** units).

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

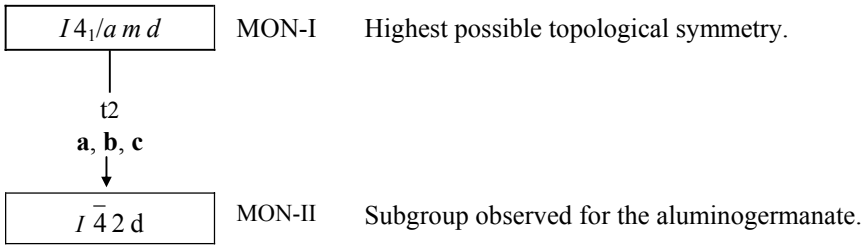


Fig. MON.1.2 The Bärnighausen tree illustrating the symmetry relationship of the MON types.

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

MON-I $I\,4_1/a\,m\,d$		MON-II $I\,\bar{4}\,2\,d$	
T1 [16(h), . *m* .]	→	T1	[16(e), 1]
O1 [16(g), . . 2]	→	O1	[16(e), 1]
O2 [8(e), 2 *mm* .]	→	O2	[8(c), 2 . .]
O3 [8(c), . 2/*m* .]	→	O3	[8(d), . 2 .]

MON.2 Compounds and crystal data

Table MON.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
MON-I ***I*** **4$_1$/*a m d***								
MON1990a01	$Al_5Si_{11}O_{32} \cdot 5H_2O$	18.4	T	-	-	-	-	90Rou1
MON1990a02	$K_5 \cdot Al_5Si_{11}O_{32} \cdot 5H_2O$	18.1	M	-	H_2O	-	-	90Rou1
MON-II ***I*** $\bar{4}$ **2 d**								
MON2002a01	$K_{6.2} \cdot Al_{6.2}Ge_{9.8}O_{32} \cdot 4H_2O$	16.8	S	-	H_2O	-	-	2002Tri1

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

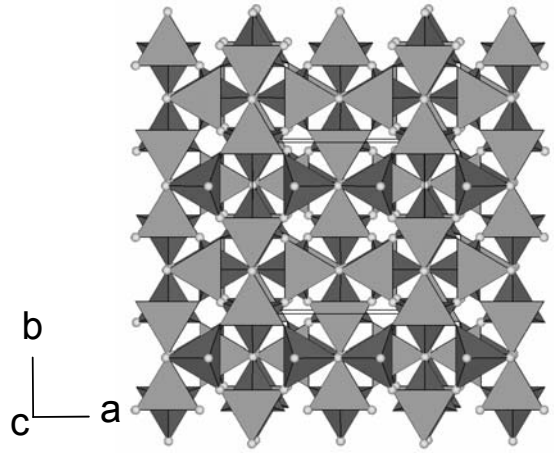
code	*a* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
MON-I ***I*** **4$_1$/*a m d***								
MON1990a01	7.09	17.33	871	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	90Rou1
MON1990a02	7.141	17.307	883	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Rou1
MON-II ***I*** $\bar{4}$ **2 *d***								
MON2002a01	7.373(1)	17.513(4)	952	0, -1/4, -3/8	**a**, **b**, **c**	*x*, *y*+1/4, *z*+3/8	RT	2002Tri1

MON.3 Framework structures

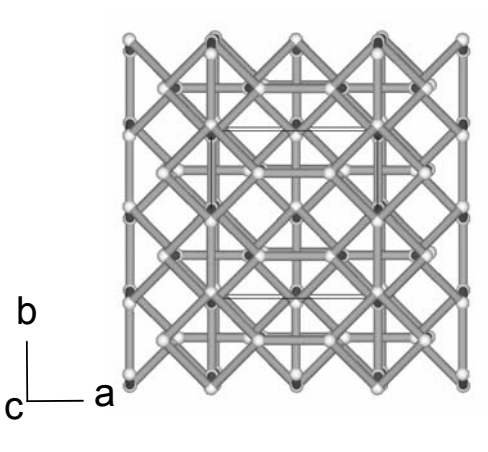
MON.3.1 MON-I compounds (*I* 4$_1$/*a m d* , IT #141)

Table MON.3.1.1 Atomic coordinates and site definitions for montesommaite, $K_5 \cdot Al_5Si_{11}O_{32} \cdot 5H_2O$ (MON1990a02, 90Rou1).

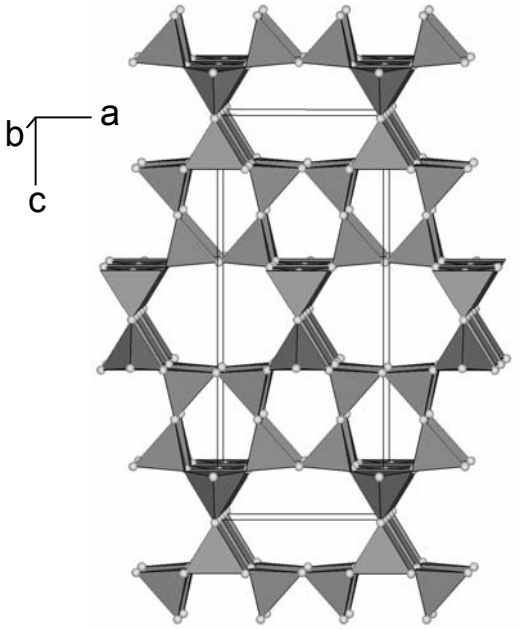
Atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0	0.463(4)	0.090(2)	0.39	. *m* .	16(h)	11.2 / 4.8
O1	0.186(7)	*x*+¼	7/8	1.18	. . 2	16(g)	16
O2	0	¼	0.116(8)	1.18	2 *mm* .	8(e)	8
O3	0	0	0	1.18	. 2/m .	8(c)	8
K1	0	0	½	1.97	. 2/m .	8(d)	8
OW1	0	¼	0.34(2)	1.18	2 *mm* .	8(e)	8



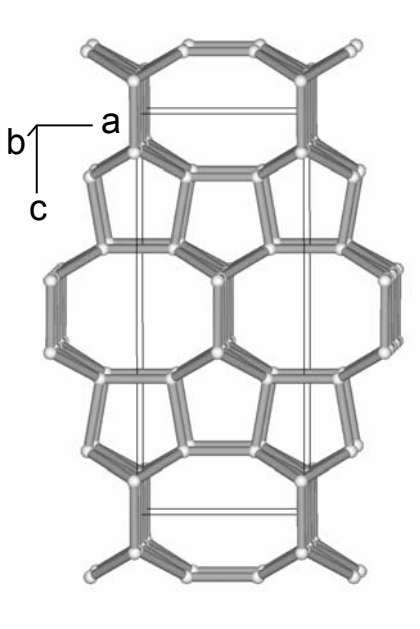
a Polyhedral representation. View parallel **c** rotated by 0.5° about **a** and **b**.



b Ball and stick model corresponding to a).



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



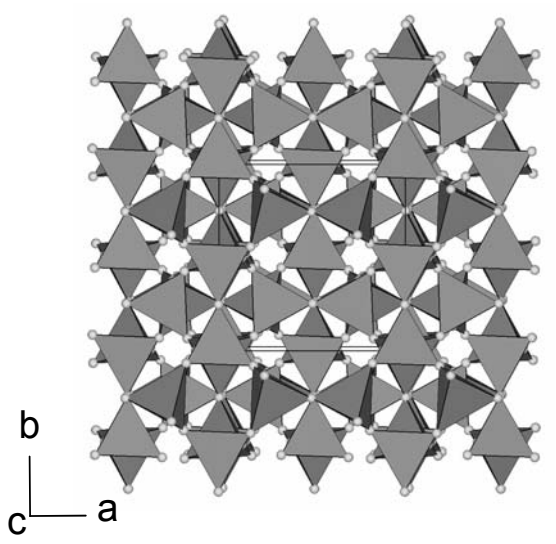
d Ball and stick model corresponding to c).

Fig. MON.3.1.1 Projections of the MON-I crystal structure of montesommaite, $K_5 \cdot Al_5Si_{11}O_{32} \cdot 5H_2O$ (MON1990a02, 90Rou1).

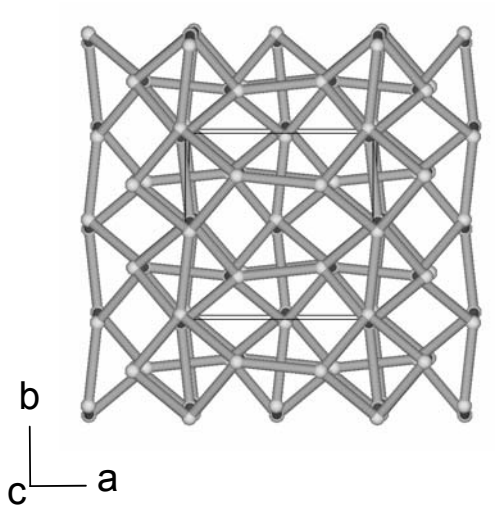
Table MON.3.1.2 Selected interatomic distances and angles for montesommaite, $K_5 \cdot Al_5Si_{11}O_{32} \cdot 5H_2O$ (MON1990a02, 90Rou1).

	T - O [Å]	T - O - T [°]
(Si,Al)1 - O3	1.58(3)	180
(Si,Al)1 - O2	1.59(5)	147(10)
(Si.Al)1 - O1	1.63(5)	149(4)
(Si,Al)1 - O1	1.63(5)	149(4)
mean	1.61	156

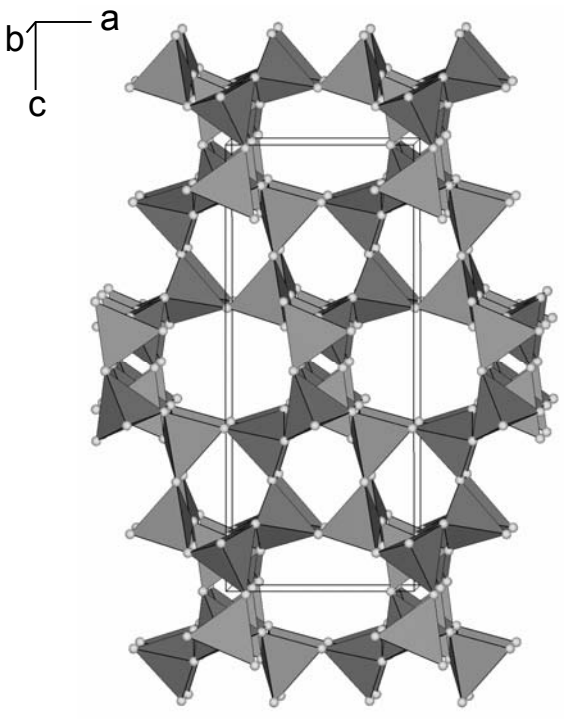
MON.3.2 MON-II compounds ($I\bar{4}2d$, IT #122)



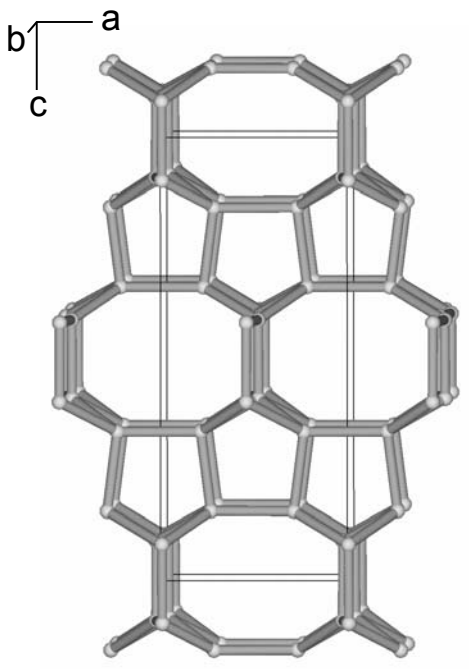
a Polyhedral representation. View parallel **c** rotated by 0.5° about **a** and **b**.



b Ball and stick model corresponding to a).



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



d Ball and stick model corresponding to c).

Fig. MON.3.2.1 Projections of the MON-II crystal structure of $K_{6.2} \cdot Al_{6.2}Ge_{9.8}O_{32} \cdot 4H_2O$ (MON2002a01, 2002Tri1).

Table MON.3.2.1 Atomic coordinates and site definitions for MON-II, $K_{6.2} \cdot Al_{6.2}Ge_{9.8}O_{32} \cdot 4H_2O$ (MON2002a01, 2002Tri1).

Atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Ge,Al)1	0.0241(1)	0.4731(1)	0.0896(1)	0.87	1	16(e)	9.84 / 6.16
O1	0.1727(3)	0.4369(3)	0.8424(1)	1.82	1	16(e)	16
O2	0	¼	0.1183(2)	2.66	2 . .	8(c)	8
O3	-0.1226(4)	0	0	1.68	. 2 .	8(d)	8
K1	-0.0117(3)	½	½	8.16	. 2 .	8(d)	6.16
OW1	0.0063(8)	0.251(1)	0.3850(6)	1.37	1	16(e)	4.00

Nonstandard setting, origin at 1 2 d, at 0, -1/4, -3/8 from $\bar{4}$.
Symmetry operators: *x*, *y* ,*z* *y*-¼ , -*x*+¼, -*z*-¼ -*x*, -*y*+½, *z* -*y*+¼, *x*+¼, -*z*-¼
x, -*y*, -*z* *y*-¼ , *x*-¼, *z*+¼ -*x*, *y*+½, -*z* -*y*+¼, -*x*-¼, *z*+¼
and equivalent positions related by I-centering (½, ½, ½)+

Table MON.3.2.2 Selected interatomic distances and angles for MON-II, $K_{6.2} \cdot Al_{6.2}Ge_{9.8}O_{32} \cdot 4H_2O$ (MON2002a01, 2002Tri1).

	T - O [Å]	T - O - T [°]
(Ge,Al)1 - O2	1.729(1)	146.2(2)
(Ge,Al)1 - O1	1.736(2)	129.5(1)
(Ge.Al)1 - O3	1.740(2)	130.7(2)
(Ge,Al)1 - O1	1.749(2)	129.5(1)
mean	1.739	134.0

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

MON.5 Flexibility and apertures

There is insufficient information about the MON-type framework to deduce anything about its flexibility.

The 8-ring openings parallel [100] are elliptical with free diameters above and below 4 Å. The 8-ring openings parallel [001] are buckled with diameters about 3.5 Å.

MON.6 Other Information

No useful properties of MON-type frameworks have been reported.

MON.7 References

90Rou1 Rouse, R.C., Dunn, P.J., Grice, J.D., Schlenker, J.L., Higgins, J.B.: Amer. Mineral. **75** (1990) 1415.

2002Tri1 Tripathi, A., Parise, J.B.: Microporous Mesoporous Mater. **52** (2002) 65.

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