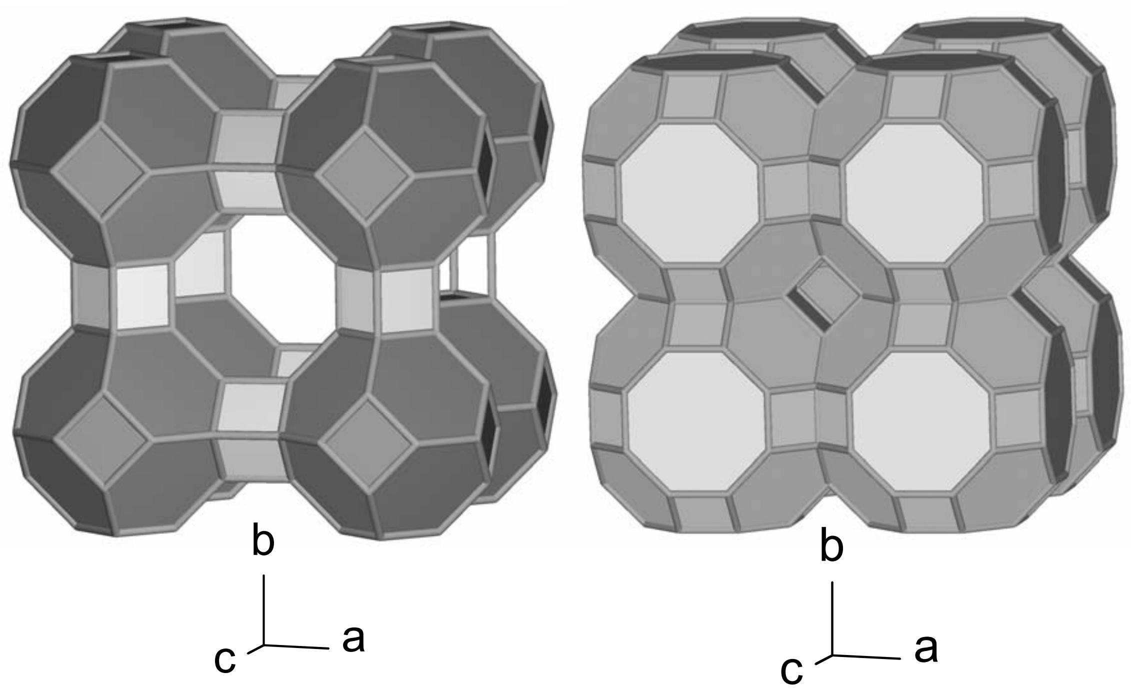
LTA

LTA.1 Zeolite framework type and topology

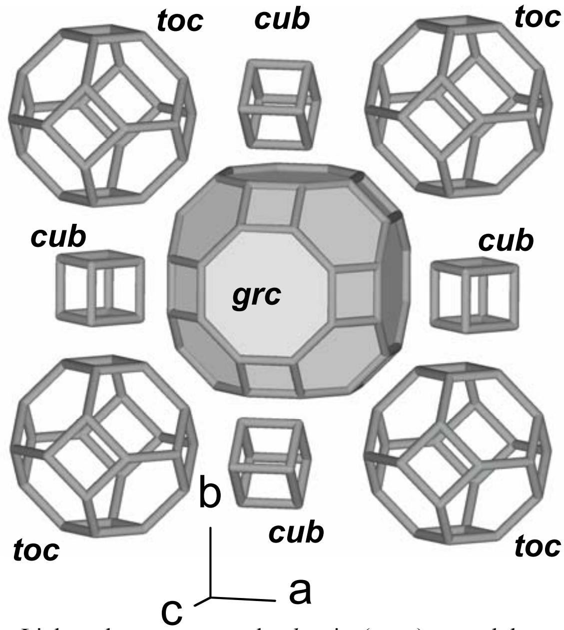
The designation of the FTC refers to **L**inde **T**ype **A**, a synthetic aluminosilicate with a composition of $Na_{12}Al_{12}Si_{12}O_{48} \cdot 27H_2O$, first synthesized and described in [56Bre1]. The crystal structure was solved by Reed and Breck [56Ree1] in space group $Pm\bar{3}m$ (a = 12.3 Å) but later on it has been shown that the compound is better described in space group $Fm\bar{3}c$ (a =24.6 Å) with eight formula units of the composition given above. The face centered supercell permits the ordering of Si and Al atoms which usually are in a ratio approximating 1 : 1. Common designations are also 4A for the Na zeolite which adsorbs only molecules smaller than propane, 5A for the partially exchanged Ca form which adsorbs molecules smaller in cross section than iso-paraffins or aromatics [60Bro1], and 3A for the K form of zeolite A.



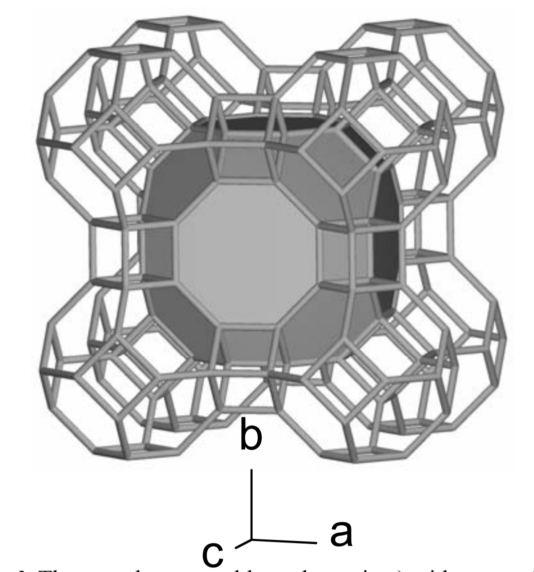
a Linkage of *toc* and *cub* units enclosing the *grc* unit. **b** Linkage of *grc* units enclosing *toc* and *cub* units.

Fig. LTA.1.1. The framework structure of LTA-type compounds in the highest possible topological symmetry $Pm\bar{3}m$ (LTA1968a02, 68Smi1). View parallel **c** rotated by 8° about **a** and 12° about **b**.

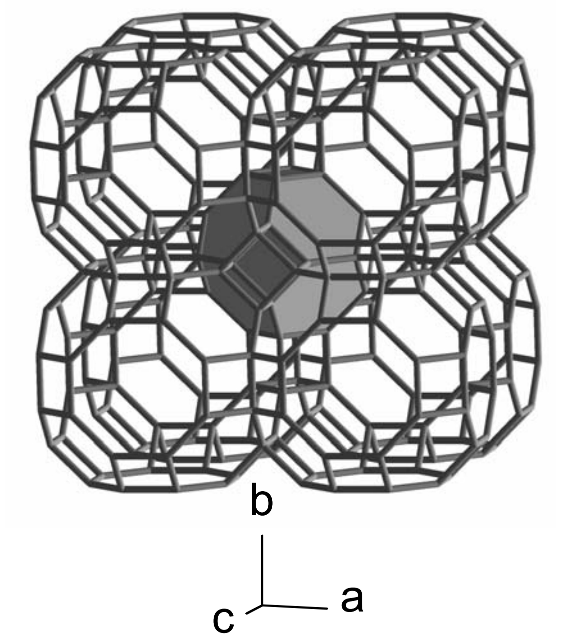
The crystal structure can be described as being built from *toc* ($4^6 6^8$) units (formerly called "sodalite cages") linked by *cub* (4^6) units via common 4-rings enclosing the big *grc* ($4^{12} 6^8 8^6$) cavities (also called α-cages in the early zeolite literature) as shown in Fig. LTA.1.1a and LTA.1.2a,b, or, vice versa, it can be described by linked *grc* units enclosing the *toc* and *cub* units (Figs. LTA.1.1b, LTA.1.2c,d).



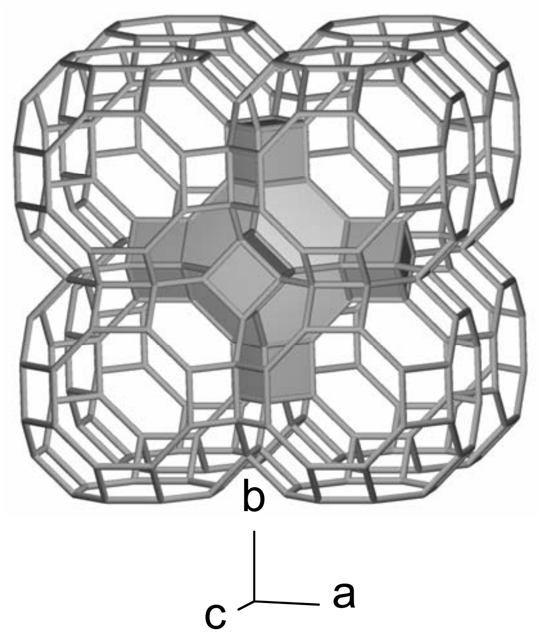
a Linkage between *toc* and *cub* units (open) around the central *grc* unit (solid).



b The complete assemblage shown in a) with rear and front units.



c Linkage of *grc* units (open) around central *toc* unit (solid).



d The assemblage shown in a) with solid *toc* and *cub* units.

Fig. LTA.1.2. Building scheme of the LTA-type framework corresponding to the models shown in Fig. LTA.1.1. View parallel **c** rotated by 8° about **a** and 12° about **b**.

The simplest way to visualize the crystal structure of LTA-type compounds is to view the *toc* unit (truncated octahedron) as its 'atom' of composition $T_{24}O_{36}O_{24/2}$. Then LTA can be seen as a metastructure of the NaCl-net [99Sch1]. The $T_{24}O_{36}O_{24/2}$ units are arranged in a simple cubic packing and joined by the *cub* units at the cube faces of the truncated octahedron. The space group of the simple cubic packing is preserved in the aristotype of LTA ($Pm\bar{3}m$).

Partial ordering of Na atoms in the aluminosilicate causes further reduction of the symmetry from $Fm\bar{3}c$ to $R\bar{3}c$ [83Ben1], a space group also adopted by an aluminophosphate (LTA1998e01, 98Sch1). Similarly, ordering of K atoms in K loaded LTA-type zeolites yields a symmetry reduction from $Pm\bar{3}m$ *to* $Fm\bar{3}m$ by doubling the lattice constant recognized by the occurrence of superstructure reflections [94Arm1, 94Arm2]. Refinements in other space groups than those given in the Bärnighausen tree in Fig. LTA.1.3 are of dubious significance. A crystal structure described in space group $F432$ [75Thöl] can only be interpreted when we assume that the origin is on the 4_2-axis, in the nonstandard setting ¼, ¼, ¼ from the standard origin in 4 3 2, and when we invert the *x*-values of O32, Ca11, and Ca21 to their negative values. Crystal structure refinements in space group $F\,3\,2$ [2000Ike1] yielded T-O distances ranging from 1.53 Å to 1.88 Å indicating a wrong symmetry assignment. Likewise, a Rietveld X-ray refinement of a K-LTA in space group $F\,3\,2$ [2004Ike1] yielded T-O distances ranging from 1.47 Å to 2.06 Å indicating a wrong choice. Space group $F\,3\,2$ is a subgroup of $F\bar{4}3c$, which itself has not been shown to be likely for an LTA-type crystal structure. A crystal structure described in space group $F\bar{4}3c$ is mentioned by [2000Por1] as a hypothetical model and is also not considered here. The Rietveld X-ray refinement of a K-LTA in space group $F\bar{4}3c$ (2004Ike1) does not appear to be convincing. The corresponding centrosymmetric space group $Fm\bar{3}c$ cannot be excluded.

There do exist numerous cation exchanged forms and compounds with various adsorbed species. Those which have been structurally characterized are listed in Table LTA.2.1. It is assumed that some elements, as e.g. Ag, form metal clusters or charged complexes in the zeolite cavities and, consequently, the sum of the ionic charges of nonframework atoms does not necessarily match the total charge of the anionic framework in some cases. It is difficult to estimate the total charge of such complexes and therefore some chemical compositions given in Table LTA.2.1 might by approximate only.

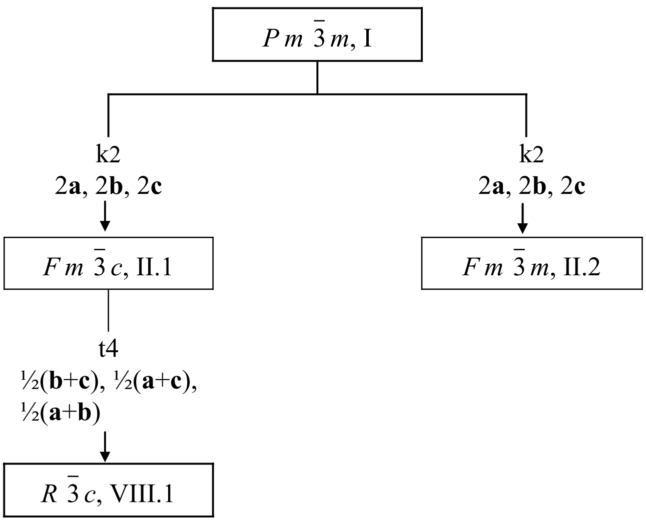


Fig. LTA.1.3 The Bärnighausen tree illustrating the symmetry relationship of the LTA types.

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

LTA-I $Pm\bar{3}m$		LTA-II.1 $Fm\bar{3}c$		LTA-VIII.1 $R\bar{3}c$
T1 [24(k), *m* . .]	→	T11 [96(i), *m* . .]	→	T11a [12(f), 1]
			→	T11b [12(f), 1]
	→	T12 [96(i), *m* . .]	→	T12a [12(f), 1]
			→	T12b [12(f), 1]
O1 [24(m), . . *m*]	→	O1 [192(j), 1]	→	O11 [12(f), 1]
			→	O12 [12(f), 1]
			→	O13 [12(f), 1]
			→	O14 [12(f), 1]
O2 [12(i), *m* . *m*2]	→	O2 [96(i), *m* . .]	→	O21 [12(f), 1]
			→	O22 [12(f), 1]
O3 [12(h), *m m*2 ..]	→	O3 [96(i), *m* . .]	→	O31 [12(f), 1]
			→	O32 [12(f), 1]

LTA-I $Pm\bar{3}m$		LTA-II.2 $Fm\bar{3}m$
T1 [24(k), *m* . .]	→	T1 [192(l), 1]
O1 [24(m), . . *m*]	→	O11 [96(k), . . *m*]
	→	O12 [96(k), . . *m*]
O2 [12(i), *m* . *m*2]	→	O2 [96(k), . . *m*]
O3 [12(h), *m m*2 ..]	→	O3 [96(j), *m* . .]

LTA.2 Compounds and crystal data

Table LTA.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
LTA-I $\boldsymbol{Pm\bar{3}m}$								
LTA1956a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	-	-	D	n.s.	56Ree1
LTA1956a02	$Na_{2.4}Tl_{9.6} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Tl	-	D	n.s.	56Ree1
LTA1956a03	$Na_{4.0}Li_{8.0} \cdot Al_{12}Si_{12}O_{48}$	13.8	S	Li	-	D	n.s.	56Ree1
LTA1958a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	-	-	D	623	58Bar1
LTA1960a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	-	-	D	n.s.	60How1

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1960b01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot nH_2O$	12.9	S	-	H_2O	-	-	60Bro1
LTA1960b02	$Na_4Ca_4 \cdot Al_{12}Si_{12}O_{48} \cdot nH_2O$	12.9	S	-	H_2O	-	-	60Bro1
LTA1966a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 6Br_2$	12.9	S	-	Br_2	D	n.s.	66Mei1
LTA1967a01	$Ca_4Na_4 \cdot Al_{12}Si_{12}O_{48}$	12.5	S	Ca	-	D	723	67Sef1
LTA1967a02	$Ca_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 5.65I_2$	12.9	S	Ca	I_2	D	>573	67Sef1
LTA1968a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	-	-	D	673	68Smi1
LTA1968a02	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	-	-	D	673	68Smi1
LTA1971a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 27H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1971a02	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 27H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1972a01	$Tl_{11} \cdot Al_{11}Si_{13}O_{48}$	13.3	S	Tl	-	D	623	72Ril1
LTA1972a02	$Tl_{11} \cdot Al_{11}Si_{13}O_{48} \cdot nH_2O$	12.8	S	Tl	H_2O	-	-	72Ril1
LTA1972b01	$Na_{11} \cdot Al_{11}Si_{13}O_{48} \cdot 32NH_3$	12.9	S	-	NH_3	D	623	72Yan1
LTA1972c01	$Na_{11} \cdot Al_{11}Si_{13}O_{48} \cdot 16S$	12.9	S	-	S	D	623	72Sef1
LTA1973a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 8NH_3$	12.9	S	-	NH_3	D	623	73Yan1
LTA1973b01	$Na_{11} \cdot Al_{11}Si_{13}O_{48}$	13.0	S	-	-	D	623	73Yan2
LTA1973c01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 6C_2H_2$	13.0	S	-	acetylene	D	623	73Ama1
LTA1973d01	$Mn_{4.5}Na_3 \cdot Al_{12}Si_{12}O_{48} \cdot 4.5C_2H_2$	13.2	S	Mn	acetylene	D	623	73Ril1
LTA1974a01	$Mn_{4.5}Na_3 \cdot Al_{12}Si_{12}O_{48} \cdot 30H_2O$	13.0	S	Mn	H_2O	-	-	74Yan1
LTA1974a02	$Mn_{4.5}Na_3 \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Mn	-	D	623	74Yan1
LTA1974b01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48}$	13.6	S	Co	-	D	623	74Ril1
LTA1974b02	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4CO$	13.6	S	Co	CO	D	623	74Ril1
LTA1975a01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 35H_2O$	13.0	S	Co	H_2O	-	-	75Ril1
LTA1975b01	$K_{12} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	K	-	D	573	75Leu1
LTA1975b02	$K_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 20H_2O$	12.9	S	K	H_2O	-	-	75Leu1
LTA1975c01	$Cs_7Na_5 \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Cs	-	D	623	75Van1
LTA1975c02	$Cs_7Na_5 \cdot Al_{12}Si_{12}O_{48} \cdot 27\ H_2O$	12.8	S	Cs	H_2O	-	-	75Van1
LTA1975d01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_4$	13.4	S	Co	ethylene	D	673	75Ril2
LTA1975e01	$Mn_{4.5}Na_3 \cdot Al_{12}Si_{12}O_{48} \cdot 4.5C_2H_2$	13.2	S	Mn	acetylene	D	623	75Ril3
LTA1975e02	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_2$	13.3	S	Co	acetylene	D	673	75Ril3
LTA1975f01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 9.3NaNO_3\ 6.7H_2O$	12.6	S	Na	$NaNO_3$, H_2O	D	603	75Bar1
LTA1975g01	$Tl_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 18H_2O$	12.7	S	Tl	H_2O	-	-	75Thö1
LTA1975g02	$Ca_6 \cdot Al_{12}Si_{12}O_{48} \cdot 28H_2O$	13.1	S	Ca	H_2O	-	-	75Thö1
LTA1975g07	$Ag_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 23H_2O$	12.9	S	Ag	H_2O	-	-	75Thö1
LTA1976a01	$Zn_5K_2 \cdot Al_{12}Si_{12}O_{48} \cdot 3.5H_2O$	13.6	S	Zn	H_2O	D	673	76Rag1
LTA1977a01	$Rb_{11}Na \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb	-	D	623	77Fir1
LTA1977a02	$Rb_{11}Na \cdot Al_{12}Si_{12}O_{48} \cdot nH_2O$	12.8	S	Rb	H_2O	-	-	77Fir1
LTA1977b01	$Tl_{12} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Tl	-	D	623	77Fir2
LTA1977b02	$Tl_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 9H_2O\ TlOH$	12.6	S	Tl	H_2O, TlOH	-	-	77Fir2
LTA1977c01	$Cs_7K_5 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	K	-	D	623	77Fir3
LTA1977d01	$Ag_{10} \cdot Al_{12}Si_{12}O_{47} \cdot 2Ag$	12.9	S	Ag	Ag-metal	C	673	77Kim1
LTA1977d02	$Ag_{8.5} \cdot Al_{12}Si_{12}O_{46.25} \cdot 3.5Ag$	12.9	S	Ag	Ag-metal	C	698	77Kim1
LTA1977e01	$Ag_{10} \cdot Al_{12}Si_{12}O_{47} \cdot 3N_3H_5\ 4N_3H_3\ 4NH_3\ 2NH_4\ 2Ag$	13.2	S	Ag	[1])	C	673	77Kim2

[1]) triazane, cyclotriazane, ammonia, ammonium, silver metal.

Table LTA.2.1 (LTA-I, $P m \bar{3} m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1977f01	$Eu_6 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Eu	-	D	623	77Fir4
LTA1977g01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	-	-	D	623	77Sub1
LTA1978a01	$Ag_{11} \cdot Al_{12}Si_{12}O_{46} \cdot 0.5Ag$	12.9	S	Ag	Ag-metal	C	673	78Kim1
LTA1978b01	$Ag_{9.8} \cdot Al_{12}Si_{12}O_{46} \cdot 6Br_2$	13.0	S	Ag	Br_2	D	673	78Kim2
LTA1978c01	$Ag_{12} \cdot Al_{12}Si_{12}O_{46} \cdot nH_2O$	13.2	S	Ag	H_2O	D	623	78Kim3
LTA1978c02	$Ag_{12} \cdot Al_{12}Si_{12}O_{46} \cdot nH_2O$	12.9	S	Ag	H_2O	-	-	78Kim3
LTA1978d01	$Ag_{6.5}Tl_{5.5} \cdot Al_{12}Si_{12}O_{46}$	13.1	S	Ag, Tl	-	D	713	78Kim4
LTA1978e01	$Na_6Ni_3 \cdot Al_{12}Si_{12}O_{48} \cdot 30H_2O$ 9OH	13.0	S	Ni	H_2O	-	-	78Fir1
LTA1978e02	$Fe_{2.7}Na_{6.6} \cdot Al_{12}Si_{12}O_{48} \cdot 15H_2O$	13.1	S	Fe	H_2O	-	-	78Fir1
LTA1978f01	$Ag_9 \cdot Al_{12}Si_{12}O_{46} \cdot 3.8C_2H_4$ 3Ag	13.2	S	Ag	ethylene, Ag-metal	D	673	78Kim5
LTA1978g01	$Eu_{4.5}Na_3 \cdot Al_{12}Si_{12}O_{48} \cdot 2.75O$	13.1	S	Eu	O	D	673	78Fir2
LTA1978h01	$Eu_{5.5}Na \cdot Al_{12}Si_{12}O_{48} \cdot 4Cl$	13.1	S	Eu	Cl	D	673	78Fir3
LTA1978i01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4Cl_2$	13.5	S	Co	Cl2	D	623	78Sub1
LTA1978j01	$Ca_6 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ca	-	D	623	78Fir4
LTA1978j02	$Sr_6 \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Sr	-	D	623	78Fir4
LTA1978k01	$H_{2.25}Ag_{12}Cl_{2.25} \cdot Al_{12}Si_{12}O_{48} \cdot 6Cl_2$	13.1	S	Ag	Cl2	D	673	78Kim6
LTA1978l01	$Cd_{9.5} \cdot Al_{12}Si_{12}O_{48} \cdot 4Cl$ 3OH	13.0	S	Cd	-	D	773	78McC1
LTA1978l02	$Cd_{9.5} \cdot Al_{12}Si_{12}O_{48} \cdot 4Cl$ 3OH nH_2O	13.2	S	Cd	H_2O	-	-	78McC1
LTA1978m01	$Ag_{5.6}H_{2n} \cdot Al_{12}Si_{12}O_{44.8+n} \cdot 1.2Ag$	13.0	S	Ag	Ag	C	673	78Kim7
LTA1978m02	$Ag_{10.3}H_{2n} \cdot Al_{12}Si_{12}O_{47.2+n} \cdot 1.6Ag$	12.8	S	Ag	Ag	C	668	78Kim7
LTA1978m03	$Ag_{10}H_{2n} \cdot Al_{12}Si_{12}O_{47+n} \cdot 2Ag$	12.9	S	Ag	Ag	C	673	78Kim7
LTA1978m04	$Ag_{8.5}H_{1.5} \cdot Al_{12}Si_{12}O_{47} \cdot 3.5Ag$	12.9	S	Ag	Ag	C	698	78Kim7
LTA1978m05	$Ag_8H_2 \cdot Al_{12}Si_{12}O_{47} \cdot 4Ag$	12.9	S	Ag	Ag	C	723	78Kim7
LTA1978m06	$Ag_{6.8}H_{2n} \cdot Al_{12}Si_{12}O_{45.4+n} \cdot 2.4Ag$	13.4	S	Ag	Ag	C	748	78Kim7
LTA1978n01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_3H_6$	13.4	S	Co	cyclo-propane	D	623	78Cru1
LTA1978n02	$Mn_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_3H_6$	13.4	S	Mn	cyclo-propane	D	623	78Cru1
LTA1978o01	$Eu_5Na_2 \cdot Al_{12}Si_{12}O_{48} \cdot 21H_2O$	12.9	S	Eu	H_2O	-	-	78Fir5
LTA1979a01	$Cd_{7.5} \cdot Al_{12}Si_{12}O_{48} \cdot 3H_2O$	12.9	S	Cd	H_2O	D	773	79McC1
LTA1979a02	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 3H_2O$	13.1	S	Cd	H_2O	D	773	79McC1
LTA1979b01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 3NO$	13.3	S	Co	NO	D	623	79Cru1
LTA1979b02	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 2NO_2$	13.4	S	Co	NO_2	D	623	79Cru1
LTA1979c01	$Cs_9Tl_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Cs	-	D	623	79Sub1
LTA1979d01	$K_{11.5} \cdot Al_{11.8}Si_{12.2}O_{48}$	12.8	S	K	-	D	573	79Plu1
LTA1979d02	$K_{11.5} \cdot Al_{11.8}Si_{12.2}O_{48}$	12.9	S	K	-	D	573	79Plu1
LTA1980a01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 3SCH_3$	13.2	S	Co	DMDS	D	573	80Sub1
LTA1980b01	$Na_{12.5} \cdot Al_{11.8}Si_{12.2}O_{48}$	13.0	S	-	-	D	623	80Plu1
LTA1980c01	$Ba_6 \cdot Al_{12}Si_{12}O_{48} \cdot 12H_2O$	12.9	S	Ba	H_2O	-	-	80Kim1
LTA1980c02	$Ba_6 \cdot Al_{12}Si_{12}O_{48} \cdot 6H_2O$	13.3	S	Ba	H_2O	D	323	80Kim1

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1980c03	$Ba_{3.5}Na_5 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ba	-	D	373	80Kim1
LTA1980c04	$BaNa_{10} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ba	-	D	673	80Kim1
LTA1980d01	$Zn_5Na_2 \cdot Al_{12}Si_{12}O_{48} \cdot 24H_2O$	13.2	S	Zn	H_2O	-	-	80Kim2
LTA1980e01	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot O_2$	13.0	S	Cd	O_2	D	873	80McC1
LTA1980e02	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot O_2$	13.1	S	Cd	O_2	D	973	80McC1
LTA1980f01	$Ca_{5.1}Cs_{1.7} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ca, Cs	-	D	623	80Sub2
LTA1980f02	$Ca_4Cs_4 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Ca, Cs	-	D	623	80Sub2
LTA1980f03	$Ca_{3.4}Cs_{5.2} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ca, Cs	-	D	623	80Sub2
LTA1980f04	$Ca_3Cs_6 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ca, Cs	-	D	623	80Sub2
LTA1980f05	$Ca_{2.8}Cs_{6.4} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ca, Cs	-	D	623	80Sub2
LTA1980g01	$Ca_{5.8}Na_{0.4} \cdot Al_{12.6}Si_{11.4}O_{48} \cdot 26H_2O$	13.0	S	Ca	H_2O	-	-	80DeR1
LTA1980g02	$Ca_{5.8}Na_{0.4} \cdot Al_{12.6}Si_{11.4}O_{48} \cdot 18.5H_2O$	13.2	S	Ca	H_2O	D	353	80DeR1
LTA1980g03	$Ca_{5.8}Na_{0.4} \cdot Al_{12.6}Si_{11.4}O_{48} \cdot 5H_2O$	12.9	S	Ca	H_2O	D	423	80DeR1
LTA1981a01	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 31H_2O$	13.1	S	Cd	H_2O	-	-	81McC1
LTA1981a02	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 5H_2O$	13.1	S	Cd	H_2O	D	298	81McC1
LTA1981b01	$Cu_8 \cdot Al_{12}Si_{12}O_{48} \cdot OH\ nH_2O$	13.4	S	Cu	OH, H_2O	D	623	81Lee1
LTA1981b02	$Cu_8 \cdot Al_{12}Si_{12}O_{48} \cdot 4OH\ nH_2O$	13.3	S	Cu	OH, H_2O	D	623	81Lee1
LTA1981b03	$Cu_8 \cdot Al_{12}Si_{12}O_{48} \cdot 0.5OH\ nH_2O$	13.2	S	Cu	OH, H_2O	D	723	81Lee1
LTA1981b04	$Cu_6 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cu	-	D	773	81Lee1
LTA1981c01	$Zn_6 \cdot Al_{12}Si_{12}O_{48} \cdot 29H_2O$	13.3	S	Zn	H_2O	-	-	81McC2
LTA1981c02	$Zn_6 \cdot Al_{12}Si_{12}O_{48} \cdot 2H_2O$	13.7	S	Zn	H_2O	D	873	81McC2
LTA1981e01	$Ag_{6.5}Na_{5.5} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	-	-	D	563	81Gel1
LTA1981f01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 10NaNO_3\ 6.6H_2O$	12.9	S	Na	$NaNO_3$, H_2O	-	-	81Pet1
LTA1981f02	$Li_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 9.8LiNO_3\ 9.3H_2O$	13.6	S	Li	$LiNO_3$, H_2O	-	-	81Pet1
LTA1982a03	$Sr_{5.7} \cdot Al_{11.6}Si_{12.4}O_{48} \cdot 0.05Al(OH)_4$	12.8	S	Sr	$Al(OH)_4$	D	623	82Plu1
LTA1982a04	$Sr_{5.8} \cdot Al_{11.6}Si_{12.4}O_{48} \cdot 0.18Al(OH)_4$	12.8	S	Sr	$Al(OH)_4$	D	773	82Plu1
LTA1982b02	$Na_{11.5} \cdot Al_{11.5}Si_{12.5}O_{48}$	12.9	S	-	-	D	573	82Ada1
LTA1982c01	$Cu_2(NH_4)_{10} \cdot Al_{12}Si_{12}O_{48} \cdot 2OH$	13.0	S	Cu	NH_4	-	-	82Lee1
LTA1982c02	$Cu_2(NH_4)_{10} \cdot Al_{12}Si_{12}O_{48} \cdot 2OH\ 15H_2O\ 6NH_3$	12.7	S	Cu	NH_4, NH_3	D	RT	82Lee1
LTA1983e02	$Ca_{5.3}Na_{0.4} \cdot Al_{11}Si_{13}O_{48} \cdot 0.3AlO_2(OH)_2$	13.1	S	Ca	$AlO_2(OH)_2$	D	623	83Plu1
LTA1983g01	$Ag_3Mg_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Ag, Mg	-	D	653	83Sch1

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1983g02	$Ag_3Ca_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag, Ca	-	D	653	83Sch1
LTA1983g03	$Ag_3Ba_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag, Ba	-	D	653	83Sch1
LTA1983g04	$Ag_3Na_{6.6}Zn_{1.2} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ag, Zn	-	D	653	83Sch1
LTA1983g05	$Ag_3Na_9 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	653	83Sch1
LTA1983g06	$Ag_3Mg_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ag, Mg		D	653	83Sch1
LTA1983g07	$Ag_3Ca_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag, Ca	-	D	653	83Sch1
LTA1983g08	$Ag_3Ba_{1.2}Na_{6.6} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag, Ba	-	D	653	83Sch1
LTA1983g09	$Ag_3Na_{6.6}Zn_{1.2} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ag, Zn	-	D	653	83Sch1
LTA1983g10	$Ag_3Na_9 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	653	83Sch1
LTA1983h01	$Li_{9.7}Na_{2.3} \cdot Al_{12}Si_{12}O_{48}$	13.9	S	Li	-	D	623	83Jir1
LTA1983h02	$Li_9Na_3 \cdot Al_{12}Si_{12}O_{48}$	14.0	S	Li	-	D	673	83Jir1
LTA1983i01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 9CH_3OH$	12.9	S	-	methanol	D	623	83Che2
LTA1983i02	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot nCH_3CN$	12.9	S	-	acetoni-trile	D	623	83Che2
LTA1983j01	$Ba_{0.6}K_{0.2}Na_{0.4}Rb_{9.9} \cdot Al_{11.4}Si_{12.6}O_{48}$	12.9	S	Rb	-	D	623	83Plu2
LTA1983j02	$Ba_{0.6}K_{0.2}Na_{0.4}Rb_{9.8} \cdot Al_{11.4}Si_{12.6}O_{48}$	13.0	S	Rb	-	D	623	83Plu2
LTA1983j03	$NaRb_{11.0} \cdot Al_{12.0}\,Si_{12.0}O_{48}$	13.0	S	Rb	-	D	623	83Plu2
LTA1984a01	$Ag_{4.7}Cs_{7.3} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	633	84Kim1
LTA1984b01	$Ag_6Na_6 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ag	-	D	623	84Kim2
LTA1984c02	$Ca_5Na_2 \cdot Al_{12}Si_{12}O_{48}$	12.8	S	-	-	D	598	84Ada1
LTA1985a01	$Ag_{4.6}Na_{7.4} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Ag	-	D	623	85Kim1
LTA1985b01	$Ag_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 9.5AgNO_3\ 5.9H_2O$	12.9	S	Ag	$AgNO_3$, H_2O	-	-	85Dim1
LTA1985c01	$Pb_6 \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Pb	-	D	623	85Ron1
LTA1985c02	$Pb_9 \cdot Al_{12}Si_{12}O_{48} \cdot 3H_2O\ 8OH$	13.1	S	Pb	OH, H_2O	D	723	85Ron1
LTA1986a01	$Ag_{7.6}Na_{4.4} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	86Kim1
LTA1986b01	$Al_{0.5}Na_3Ni_{3.5} \cdot Al_{12}Si_{12}O_{48} \cdot 31H_2O\ 9OH$	13.5	S	Ni	OH, H_2O	-	348	86Heo1
LTA1986c01	$Na_9 \cdot Al_9Si_{15}O_{48}$	13.3	S	-	-	D	823	86Edd1
LTA1986c02	$Na_9 \cdot Al_9Si_{15}O_{48}$	13.2	S	-	-	D	823	86Edd1
LTA1987b01	$Ca_4Na_{4.0} \cdot Al_{12}Si_{12}O_{48} \cdot 32H_2O$	13.0	S	Ca	H_2O	-	-	87Sie1
LTA1987b02	$Ca_4Na_{4.0} \cdot Al_{12}Si_{12}O_{48} \cdot 10H_2O$	13.1	S	Ca	H_2O	D	293	87Sie1
LTA1987b03	$Ca_4Na_{4.0} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ca	-	D	380	87Sie1
LTA1987b04	$Ca_4Na_{4.0} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	D	673	87Sie1
LTA1987b05	$Ca_4Na_{4.0} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	D	673	87Sie1
LTA1987b06	$Ca_4\,Na_{4.0} \cdot Al_{12}Si_{12}O_{48} \cdot 40H_2O$	12.9	S	Ca	H_2O	R	673	87Sie1
LTA1987c01	$Cs_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Cs	-	C	1273	87Heo1
LTA1987c02	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5Cs$	13.0	S	Cs	Cs-metal	C	623	87Heo1

Table LTA.2.1 (LTA-I, $P\,m\,\bar{3}\,m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1987d01	$Ag_{4.6}Na_{7.4} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Ag	-	D	623	87Kim1
LTA1987e01	$Ag_{7.6}Na_{4.4} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	87Kim2
LTA1987f01	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5Cs$	13.0	S	Cs	Cs	D	623	87Heo2
LTA1987f02	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot CsOH$	12.9	S	Cs	CsOH	D	297	87Heo2
LTA1987g01	$Cs_{8.5}Na_{3.5} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5Cs$	13.0	S	Cs	Cs-metal	D	623	87Heo3
LTA1987g02	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5Cs$	13.0	S	Cs	Cs-metal	D	623	87Heo3
LTA1987g03	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5Cs$	13.0	S	Cs	Cs-metal	D	723	87Heo3
LTA1987h01	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Ca	-	D	673	87Sie2
LTA1987h02	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48} \cdot 25.5H_2O$	12.8	S	Ca	H_2O	R	673	87Sie2
LTA1987h03	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	C	873	87Sie2
LTA1987h04	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48} \cdot 23.4H_2O$	12.8	S	Ca	H_2O	R	873	87Sie2
LTA1987h05	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	C	453	87Sie2
LTA1987h06	$Ca_{3.72}Na_{4.28} \cdot Al_{12}Si_{12}O_{48} \cdot 20.7H_2O$	12.9	S	Ca	H_2O	R	453	87Sie2
LTA1987i01	$Ag_9\,Cs_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	87Kim3
LTA1987i02	$Ag_9\,Cs_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	87Kim3
LTA1987k01	$Si_{24}O_{48}$	14.2	T	-	-	-	-	87van1
LTA1988b01	$Ag_9Cs_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	88Kim1
LTA1988b02	$Ag_9Cs_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	88Kim1
LTA1988c01	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot Cs_{0.75}$	13.0	S	Cs	Cs-metal	D	623	88Heo1
LTA1988d01	$Ag_{10}Tl_2 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	623	88Kim2
LTA1988d02	$Ag_9Tl_3 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ag	-	D	623	88Kim2
LTA1988d03	$Ag_8Tl_4 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	623	88Kim2
LTA1988d04	$Ag_7Tl_5 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	623	88Kim2
LTA1988e01	$Si_{24}O_{48}$	14.2	T	-	-	-	-	88van1
LTA1988f01	$Ag_{10.7}K_{1.3} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	88Kim3
LTA1988f02	$Ag_{9.3}K_{2.7} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	643	88Kim3
LTA1988g01	$Ag_3Co_{4.5} \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Ag	-	D	643	88Son1
LTA1988g02	$Ag_6Co_3 \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Ag	-	D	643	88Son1
LTA1989a01	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot CsOH$	12.9	S	Cs	CsOH	D	RT	89Dej1
LTA1989a02	$Cs_{12} \cdot Al_{12}Si_{12}O_{48} \cdot CsOH\ 10H_2O$	12.7	S	Cs	CsOH, H_2O	-	-	89Dej1
LTA1989b01	$Ag_9 \cdot Al_{12}Si_{12}O_{48} \cdot 3.6CO$	13.5	S	Ag	CO	D	643	89Kim1
LTA1989c01	$Ag_{3.2}Cs_{8.8} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Cs	-	D	633	89Kim2
LTA1989d01	$Ag_2Cs_{10} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Cs	-	D	633	89Kim3
LTA1989d02	$Ag_2Ca_5 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	D	633	89Kim3
LTA1989e01	$Co_{3.5}Na_5 \cdot Al_{12}Si_{12}O_{48} \cdot 2.5I_2$	13.3	S	Co	I_2	D	633	89Kim4
LTA1989e02	$Co_{3.5}Na_5 \cdot Al_{12}Si_{12}O_{48} \cdot 5I_2$	13.4	S	Co	I_2	D	633	89Kim4
LTA1989f01	$Ag_{10}Rb_2 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	643	89Kim5
LTA1989f02	$Ag_9Rb_3 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ag	-	D	643	89Kim5
LTA1989g01	$Mg_{2.5}Na_7 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Mg	-	D	633	89Kim6
LTA1989g02	$Mg_{1.5}Na_9 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Mg	-	D	633	89Kim6

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1989h01	$Ag_7Ca_{2.5} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	633	89Son1
LTA1989h02	$Ag_2Ca_5 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ag	-	D	633	89Son1
LTA1989i01	$Sr_{1.6}Tl_{8.8} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Tl	-	D	633	89Yan1
LTA1989i02	$Sr_{5.45}Tl_{1.1} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Tl	-	D	633	89Yan1
LTA1989j01	$Si_{24}O_{48}$	14.2	T	-	-	-	-	89Uyt1
LTA1990a01	$Ag_2Ca_5 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Ca	-	D	633	90Kim1
LTA1990a02	$Ag_2Cs_{10} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Cs	-	D	633	90Kim1
LTA1990b01	$Ni_2(NH_4)_{10} \cdot Al_{12}Si_{12}O_{48} \cdot$ 2OH $3H_20$	12.9	S	Ni, NH_4	H_2O	D	296	90Pat1
LTA1990b02	$Ni_{1.75}(NH_4)_{10} \cdot Al_{12}Si_{12}O_{48} \cdot$ mOH nH_20	12.9	S	Ni, NH_4	H_2O	-	-	90Pat1
LTA1990c01	$Tl_{3.4}Zn_{4.3} \cdot Al_{12}Si_{12}O_{48}$	13.5	S	Tl	-	D	723	90Jeo1
LTA1990c02	$Tl_{5.5}Zn_{3.25} \cdot Al_{12}Si_{12}O_{48}$	13.6	S	Tl	-	D	723	90Jeo1
LTA1990d01	$Cd_{4.0}Rb_{4.0} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cd	-	D	723	90Son1
LTA1990d02	$Cd_{5.0}Rb_{2.0} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cd	-	D	723	90Son1
LTA1990d03	$Cd_{6.0}Rb_{0.1} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Cd	-	D	723	90Son1
LTA1991a01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 2Br_2$ 12Br	13.5	S	Co	Br	D	633	91Kim1
LTA1991a02	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 2Br_2$ 12Br	13.5	S	Co	Br	D	633	91Kim1
LTA1991b01	$Ag_3Rb_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb	-	D	623	91Son1
LTA1991b02	$Ag_3Rb_{12} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb	-	D	623	91Son1
LTA1991b03	$Ag_7Rb_{12} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Rb	-	D	623	91Son1
LTA1991c01	$Cd_6 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Cd	-	D	723	91Koh1
LTA1991c02	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_4$	13.2	S	Cd	ethylene	D	723	91Koh1
LTA1991d01	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_2$	13.2	S	Cd	acetylene	D	723	91Koh2
LTA1991e01	$Ag_{2.8}Zn_{4.6} \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Zn	-	D	673	91Jeo1
LTA1991e02	$Ag_{2.8}Zn_{4.6} \cdot Al_{12}Si_{12}O_{48} \cdot 5.6C_2H_4$	13.5	S	Zn	ethylene	D	673	91Jeo1
LTA1991f01	$Ca_6 \cdot Al_{12}Si_{12}O_{48} \cdot 6Br_2$	13.2	S	Co	Br_2	D	633	91Jan1
LTA1992a01	$Ca_3Cs_6 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Cs, Ca	-	D	623	92Heo1
LTA1992a02	$Ca_{0.5}Cs_{11} \cdot Al_{12}Si_{12}O_{48}$ 0.5Cs	13.2	S	Cs, Ca	Cs-metal	D	623	92Heo1
LTA1992a03	$Cs_{12} \cdot Al_{12}Si_{12}O_{48}$ 0.5Cs	13.1	S	Cs, Ca	Cs-metal	D	623	92Heo1
LTA1992b01	$Ca_6 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_4$	13.0	S	Ca	ethylene	D	733	92Jan1
LTA1992b02	$Ca_6 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_2H_2$	13.1	S	Ca	acetylene	D	733	92Jan1
LTA1992c01	$Rb_{12.6} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Rb	-	D	633	92Son1
LTA1992c02	$Rb_{13.2} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Rb	-	D	633	92Son1
LTA1992c03	$Rb_{13.5} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Rb	-	D	633	92Son1
LTA1992c04	$Rb_{13.4} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb	-	D	633	92Son1
LTA1993b01	$Pb_6 \cdot Al_{12}Si_{12}O_{48} \cdot Pb_3O(OH)_4$	12.9	S	Pb	$Pb_3O(OH)_4$	D	299	93Ron1
LTA1993c01	$Ag_{5.6}K_{6.4} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	K	-	D	633	93Jeo1
LTA1993c02	$Ag_{4.5}Cs_{13} \cdot Al_{12}Si_{12}O_{48}$	12.7	S	Cs	-	D	633	93Jeo1
LTA1993c03	$Ag_{4.5}Cs_{13.5} \cdot Al_{12}Si_{12}O_{48}$	12.7	S	Cs	-	D	633	93Jeo1
LTA1993d01	$K_{15} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	K	-	D	673	93Sun1

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1993e01	$Ag_{3.3}Ca_{4.35} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Ca, Ag	-	D	633	93Jan1
LTA1993e02	$Ag_{3.3}Ca_{4.35} \cdot Al_{12}Si_{12}O_{48} \cdot 6.65C_2H_4$	13.0	S	Ca, Ag	ethylene	D	633	93Jan1
LTA1993f01	$Ag_{5.6}K_{6.4} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	K, Ag	-	D	633	93Kim1
LTA1993f02	$Ag_{4.5}Cs_{13} \cdot Al_{12}Si_{12}O_{48}$	12.7	S	Cs, Ag	-	D	633	93Kim1
LTA1993f03	$Ag_{4.5}Cs_{13.5} \cdot Al_{12}Si_{12}O_{48}$	12.7	S	Cs, Ag	-	D	633	93Kim1
LTA1993f04	$Ag_{3.4}Rb_{11} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb, Ag	-	D	633	93Kim1
LTA1993g01	$Rb_{12} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Rb	-	D	633	93Son1
LTA1993g02	$Rb_{13} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Rb	-	D	633	93Son1
LTA1993h01	$Ca_{5.6}Tl_{0.8} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ca, Tl	-	D	633	93Kim2
LTA1993h02	$Ca_{1.4}Tl_{9.2} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Tl, Ca	-	D	633	93Kim2
LTA1993i01	$Cd_6 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cd	-	D	1023	93Jan2
LTA1993i02	$Cs_{12.7} \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cs	-	D	1023	93Jan2
LTA1994a01	$K_{12} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	K	-	D	723	94Arm1
LTA1994a02	$K_{13} . Al_{12}Si_{12}O_{48}$	12.9	S	K	-	D	723	94Arm1
LTA1994a03	$K_{13} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	K	-	D	723	94Arm1
LTA1994b01	$(CH_3NH_3)_{10}Na_2 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	MMA	MMA	-	373	94Jeo1
LTA1994c01	$Cd_6 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cd	-	D	1023	94Jan1
LTA1994c02	$Rb_{13.5} \cdot Al_{12}Si_{12}O_{48}$	13.3	S	Rb	-	D	1023	94Jan1
LTA1994d01	$Cs_3Na_9 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Cs	-	D	623	94Cho1
LTA1994d02	$Cs_3Na_9 \cdot Al_{12}Si_{12}O_{48} \cdot 20H_2O$	13.0	S	Cs	H_2O	-	-	94Cho1
LTA1994d03	$Cs_3Na_8H \cdot Al_{12}Si_{12}O_{48} \cdot 24H_2O$	12.9	S	Cs	H_2O	-	-	94Cho1
LTA1994g01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 4CS_2$	13.4	S	Co	Cs_2	D	633	94Jan2
LTA1994h01	$Cd_6 \cdot Al_{12}Si_{12}O_{48}$	13.2	S	Cd	-	D	1023	94Jan3
LTA1994h02	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 5Cd$	13.5	S	Cd	Cd-metal	D	1023	94Jan3
LTA1994i01	$Cs_{11}Na_3 \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Cs	-	D	723	94Arm3
LTA1994j01	$K_{12.5} \cdot Al_{12}Si_{12}O_{48}$	13.1	S	K	-	D	673	94Sun1
LTA1994k01	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Cs	-	D	623	94Heo1
LTA1994k02	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 5Kr$	13.0	S	Cs	Kr	D	673	94Heo1
LTA1994l01	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Cs	-	D	623	94Heo2
LTA1994l02	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 5Kr$	13.0	S	Cs	Kr	D	673	94Heo2
LTA1994m01	$Ag_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 3.5C_2H_4$ $1.25C_2H_4B$	13.3	S	Ag	ethylene, 1,2-dibro-moethane	D	673	94Jeo2
LTA1994n01	$Ag_{2.2}Rb_{12.1} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb, Ag	-	D	653	94Lee1
LTA1994n02	$Ag_{3.6}Rb_{11.4} \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb, Ag	-	D	653	94Lee1
LTA1994n03	$Ag_{4.8}Rb_{11.8} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Rb, Ag	-	D	653	94Lee1
LTA1994o01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 6.5CH_3OH$	13.3	S	Co	methanol	D	633	94Jan4
LTA1994p01	$Ag_{4.3}Cs_{12.7} \cdot Al_{12}Si_{12}O_{48}$	12.8	S	Cs, Ag	-	D	623	94Son1
LTA1994p02	$Ag_{4.1}Cs_{12.4} \cdot Al_{12}Si_{12}O_{48}$	12.9	S	Cs, Ag	-	D	623	94Son1
LTA1995a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48}$	12.9	T	-	-	-	-	95Kim1
LTA1995b01	$Na_8Rb_3H \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Rb		D	623	95Par1

Table LTA.2.1 (LTA-I, $Pm\bar{3}m$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1995b02	$Na_9Rb_3 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	Rb		D	623	95Par1
LTA1995b03	$Na_8K_3H \cdot Al_{12}Si_{12}O_{48}$	13.0	S	K		D	623	95Par1
LTA1995b04	$Na_9K_3 \cdot Al_{12}Si_{12}O_{48}$	13.0	S	K		D	623	95Par1
LTA1995c01	$Ca_4Na_4 \cdot Al_{12}Si_{12}O_{48}$	13.1	S	Ca		D	633	95Jan1
LTA1995c02	$Ca_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 6Br_2$	13.2	S	Ca	Br_2	D	633	95Jan1
LTA1995d01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 2S_8$	13.7	S	Co	S_8	D	653	95Yeo1
LTA1996a01	$Co_4Na_4 \cdot Al_{12}Si_{12}O_{48} \cdot 11H_2S$	13.4	S	Co	H_2S	D	653	96Yeo1
LTA1996b01	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 5Ar$	13.0	S	Ar	Ar	D	673	96Heo1
LTA1996b02	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 6Ar$	13.0	S	Ar	Ar	D	673	96Heo1
LTA1996c01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 12H_2S$	12.9	S	-	H_2S	D	653	96Yeo2
LTA1997a01	$Tl_{12} \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Tl	-	D	623	97Heo1
LTA1997a02	$In_{10} \cdot Al_{12}Si_{12}O_{48} \cdot In$	13.6	S	In	In	D	623	97Heo1
LTA1997b01	$Tl_{12} \cdot Al_{12}Si_{12}O_{48}$	13.4	S	Tl	-	D	623	97Heo2
LTA1997b02	$In_{10} \cdot Al_{12}Si_{12}O_{48} \cdot In$	13.6	S	Tl	In	D	623	97Heo2
LTA1998a01	$In_8 \cdot Al_{12}Si_{12}O_{48} \cdot In_{0.75}S_2$	13.6	S	In	In, S_2	D	623	98Heo1
LTA1998b01	$Al_{12}Si_{12}O_{48}$	13.0	S	T	-	-	-	98Lee1
LTA1999a01	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 2.5Xe$	13.1	S	Cs	Xe	D	673	99Heo1
LTA1999a02	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 4.5Xe$	13.0	S	Cs	Xe	D	673	99Heo1
LTA1999a03	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 5.25Xe$	13.1	S	Cs	Xe	D	673	99Heo1
LTA1999b01	$H_{12}Al_{12}Si_{12}O_{48}$	13.0	T	-	-	-	-	99Lee1
LTA1999b02	$H_{12}Al_{12}Si_{12}O_{48}$	13.0	T	-	-	-	-	99Lee1
LTA1999c01	$Na_{12}Al_{12}Si_{12}O_{48}$	13.0	T	-	-	-	-	99Lee2
LTA2000a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 7Xe$	13.1	S	-	Xe	D	673	2000Lim1
LTA2000c01	$Zn_6 \cdot Al_{12}Si_{12}O_{48} \cdot Zn_{2.75}O_{2.7}$	14.2	S	Zn	Zn	D	773	2000Rea1
LTA2000e01	$Cd_6 \cdot Al_{12}Si_{12}O_{48} \cdot 4C_3H_6$	13.1	S	Cd	cyclo-propane	D	733	2000Cho1
LTA2001a01	$Na_{12} \cdot Al_{12}Si_{12}O_{48} \cdot 3.7PbI_2$	13.2	S	-	PbI_2	D	n.s.	2001Tog1
LTA2001b01	$Cs_3HNa_8 \cdot Al_{12}Si_{12}O_{48} \cdot 6Kr$	13.1	S	Cs	Kr	D	673	2001Lim1
LTA2002a01	$In_{9.5}H_{0.5} \cdot Al_{12}Si_{12}O_{48} \cdot 0.5InSH$ $2.5H_2S$	13.6	S	Cs	InSH, H_2S	D	623	2002Heo1
LTA2002a02	$In_{8.4}H_{1.2} \cdot Al_{12}Si_{12}O_{48} \cdot 0.6InSH$ $2H_2S$	13.6	S	In	InSH, H_2S	D	623	2002Heo1
LTA2002a03	$In_{9.8}H_{0.4} \cdot Al_{12}Si_{12}O_{48} \cdot 0.4InSH$ H_2S	13.6	S	In	InSH, H_2S	D	623	2002Heo1
LTA2002a04	$In_{10.2} \cdot Al_{12}Si_{12}O_{48} \cdot 0.8H_2S$	13.6	S	In	H_2S	D	623	2002Heo1
LTA2003a02	$K_{9.1}H_{0.4} \cdot Al_{9.5}Si_{14.5}O_{48}$	13.4	S	K	-	D	773	2003Ike1
LTA2003a03	$K_{7.0}H_{1..3} \cdot Al_{8..3}Si_{15.7}O_{48}$	13.7	S	K	-	D	773	2003Ike1
LTA2003a04	$K_{4.90}H_{1..6} \cdot Al_{6.5}Si_{17.4}O_{48}$	13.9	S	K	-	D	773	2003Ike1
LTA2004a01	$K_9 \cdot Al_{12}Si_{12}O_{48} \cdot Ag_2I_3K_4$	12.9	S	K,I, Ag	-	D	294	2004Heo1
LTA2004c01	$Ge_{7.4}Si_{16.6}O_{48}$	13.8	S	-	-	C	973	2004Cor1
LTA2004c02	$Si_{24}O_{48}$	14.4	S	-	-	C	973	2004Cor1
LTA2005a01	$K_{13}Br \cdot Al_{12}Si_{12}O_{48} \cdot Ag_3Br_3$	12.9	S	K,Ag,Br	-	D	294.	2005Lim1
LTA-II.1								
Fm $\bar{3}$ ***c***								
LTA1971a03	$Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1971a04	$Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1971a05	$Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1971a06	$Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$	12.9	S	-	H_2O	-	-	71Gra1
LTA1979d03	$K_{92} \cdot Al_{94.4}Si_{97.6}O_{384}$	12.9	S	K	-	D	573	79Plu1

Table LTA.2.1 (LTA-II.1, $Fm\bar{3}c$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA1980b02	$Na_{92} \cdot Al_{94.4}Si_{97.6}O_{384}$	13.0	S	-	-	D	623	80Plu1
LTA1981d01	$95NH_4 \cdot Al_{96.4}Si_{96.6}O_{384}$	12.9	S	NH_4	NH_4	D	298	81McC3
LTA1982a01	$Sr_{45} \cdot Al_{92.4}Si_{99.6}O_{384} \cdot 0.44Al(OH)_4$	12.8	S	Sr	$Al(OH)_4$	D	623	82Plu1
LTA1982a02	$Sr_{47} \cdot Al_{92.4}Si_{99.6}O_{384} \cdot 1.5Al(OH)_4$	12.8	S	Sr	$Al(OH)_4$	D	773	82Plu1
LTA1982b01	$Na_{92} \cdot Al_{92}Si_{100}O_{384}$	12.9	S	-	-	D	573	82Ada1
LTA1982d01	$Na_{20}Tl_{46} \cdot Al_{91}Si_{101}O_{384}$	12.9	S	Tl	-	D	n.s.	82Che1
LTA1983a01	$Na_{20}Tl_{46} \cdot Al_{91}Si_{101}O_{384}$	12.9	S	Tl	-	D	n.s.	83Che1
LTA1983b01	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben1
LTA1983b02	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben1
LTA1983b03	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben1
LTA1983c01	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben2
LTA1983c02	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben2
LTA1983c03	$Na_{93} \cdot Al_{93}Si_{99}O_{384}$	12.9	S	-	-	D	573	83Ben2
LTA1983d01	$Ag_{70}H_{26} \cdot Al_{96}Si_{96}O_{384}$	13.0	S	Ag	-	D	683	83Gel1
LTA1983e01	$Ca_{42.4}Na_{3.2}Al_{88}Si_{104}O_{384} \cdot 2.4AlO_2(OH)_2$	13.1	S	Ca	$AlO_2(OH)_2$	D	623	83Plu1
LTA1983f01	$K_{60}Na_{35} \cdot Al_{95}Si_{97}O_{384}$	12.9	S	K	-	D	623	83Ada1
LTA1983j04	$Ba_{4.8}K_{1.6}Na_{3.2}Rb_{79}Al_{91}Si_{101}O_{384}$	12.9	S	Rb	-	D	623	83Plu2
LTA1983j05	$Ba_{4.8}K_{1.6}Na_{3.2}Rb_{78}Al_{91}Si_{101}O_{384}$	13.0	S	Rb	-	D	623	83Plu2
LTA1984c01	$Ca_{40}Na_{16} \cdot Al_{96}Si_{96}O_{384}$	12.8	S	-	-	D	598	84Ada1
LTA1984d01	$Co_{42}Na_{12} \cdot Al_{96}Si_{96}O_{384} \cdot 12CO$ $6Al(OH)_4$	13.6	S	Co	Co, $Al(OH)_4$	D	593	84Ada2
LTA1986d01	$Mg_{16}Na_{64} \cdot Al_{96}Si_{96}O_{384} \cdot 5.9H_2O$	13.2	S	Mg		D	603	86Ada1
LTA1987a01	$Ca_{40}Na_{16} \cdot Al_{96}Si_{96}O_{384} \cdot 40CO$ $6.2AlO(OH)_3$	12.8	S	-	Co, $AlO(OH)_3$	D	600	87Ada1
LTA1987a02	$Ca_{40}Na_{16} \cdot Al_{96}Si_{96}O_{384} \cdot 40CO$ $6.2AlO(OH)_3$	12.8	S	-	Co, $AlO(OH)_3$	D	600	87Ada1
LTA1988a01	$Na_{96} \cdot Al_{96}Si_{96}O_{384}$	13.0	T	-	-	-	-	88Dem1
LTA1988a02	$Na_{96} \cdot Al_{96}Si_{96}O_{384}$	13.0	T	-	-	-	-	88Dem1
LTA1988a03	$Na_{96} \cdot Al_{96}Si_{96}O_{384}$	13.0	T	-	-	-	-	88Dem1
LTA1988a04	$Na_{96} \cdot Al_{96}Si_{96}O_{384}$	13.0	T	-	-	-	-	88Dem1
LTA1992d01	$Ga_{96}P_{96}O_{384} \cdot F_{24} \cdot 24C_6H_{14}NH_2 \cdot 48H_2O$	13.8	S	-	DPA	-	-	92Sim1
LTA1993a01	$Ga_{96}P_{96}O_{384} \cdot F_{24} \cdot 24C_6H_{14}NH_2 \cdot 48H_2O$	13.8	S	-	DPA	-	-	93Sim1
LTA1996d01	$Na_{83.2}Ni_{3.8} \cdot Al_{92.8}Si_{99.2}O_{384} \cdot 120H_2O$	13.0	S	Ni	H_2O	-	-	96Hor1
LTA1997a03	$In_{80} \cdot Al_{96}Si_{96}O_{384} \cdot In_8$	13.6	S	In	In	D	623	97Heo1
LTA1998c01	$Na_{95} \cdot Al_{95}Si_{97}O_{384} \cdot 7H_2O$	13.0	S	-	H_2O	D	623	98Ike1
LTA1998c02	$Na_{95} \cdot Al_{95}Si_{97}O_{384} \cdot 44H_2O$	12.9	S	-	H_2O	D	623	98Ike1
LTA1998c03	$Na_{95} \cdot Al_{95}Si_{97}O_{384} . 248H_2O$	12.9	S	-	H_2O	-	-	98Ike1
LTA1998d01	$Li_{96} \cdot Al_{96}Si_{96}O_{384}$	14.1	S	Li	-	D	723	98Por1
LTA1998d02	$Li_{96} \cdot Al_{96}Si_{96}O_{384}$	14.1	S	Li	-	D	723	98Por1
LTA1999d01	$Na_{95} \cdot Al_{96}Si_{96}O_{384} \cdot 39H_2O$	13.0	S	-	H_2O	-	-	99Has1
LTA2000d01	$Ca_{48} \cdot Al_{96}Si_{96}O_{384}$	13.1	S	Ca	-	D	723	2000Por1
LTA2000d02	$Ca_{48} \cdot Al_{96}Si_{96}O_{384}$	13.1	S	Ca	-	D	723	2000Por1

Table LTA.2.1 (LTA-II.1, $F m \bar{3} c$ continued).

code	chemical composition	FD	SM	CE	SR	TT	T	REF
LTA2000d03	$Ca_{48} \cdot Al_{96}Si_{96}O_{384}$	13.1	S	Ca	-	D	723	2000Por1
LTA2001c01	$(C_{18}N_2O_6H_{38})_8 \cdot Al_{76.8}Zn_{19.2}P_{96}O_{384}$	13.9	S	-	-	-	-	2001Map1
LTA2003a01	$K_{98..8} \cdot Al_{95.04}Si_{96.96}O_{384}$	13.1	S	K	-	D	773	2003Ike1
LTA-VIII.1 $R \bar{3} c$								
LTA1983b04	$Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$	12.9	S	-	-	D	573	83Ben1
LTA1983b05	$Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$	13.0	S	-	-	D	573	83Ben1
LTA1983c04	$Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$	12.9	S	-	-	D	573	83Ben2
LTA1983c05	$Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$	13.0	S	-	-	D	573	83Ben2
LTA1998e01	$Al_{72}P_{72}O_{288} \cdot F_{18}$ $6N(CH_3)_4$ $6C_{18}N_2O_6H_{38}$	14.2	S	-	F, TMA, Krypto-fix 222	-	-	98Sch1
LTA-II.2 $F m \bar{3} m$								
LTA1994a04	$K_{120} \cdot Al_{96}Si_{96}O_{384}$	12.9	S	K	-	D	723	94Arm1
LTA1994a05	$K_{136} \cdot Al_{96}Si_{96}O_{384}$	12.8	S	K	-	D	723	94Arm1
LTA1994f01	$K_{136} \cdot Al_{96}Si_{96}O_{384}$	12.8	S	K	-	D	n.s.	94Arm2

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

code	a [Å]	V [Å^3]	T [K]	reference
LTA-I $P m \bar{3} m$				
LTA1956a01	12.32	1870	n.s.	56Ree1
LTA1956a02	12.33	1875	n.s.	56Ree1
LTA1956a03	12.04	1745	n.s.	56Ree1
LTA1958a01	12.273(3)	1849	n.s.	58Bar1
LTA1960a01	12.28	1852	n.s.	60How1
LTA1960b01	12.30(1)	1861	n.s.	60Bro1
LTA1960b02	12.31(1)	1865	n.s.	60Bro1
LTA1966a01	12.30(4)	1861	n.s.	66Mei1
LTA1967a01	12.42(1)	1916	RT	67Sef1
LTA1967a02	12.29(7)	1856	RT	67Sef1
LTA1968a01	12.28	1852	n.s.	68Smi1
LTA1968a02	12.28	1852	n.s.	68Smi1
LTA1971a01	12.305(5)	1863	n.s.	71Gra1
LTA1971a02	12.305(5)	1863	n.s.	71Gra1
LTA1972a01	12.17(1)	1802	293	72Ril1
LTA1972a02	12.33(1)	1875	296	72Ril1
LTA1972b01	12.29(1)	1856	294	72Yan1
LTA1972c01	12.289(2)	1856	293	72Sef1
LTA1973a01	12.289(5)	1856	n.s.	73Yan1
LTA1973b01	12.263(2)	1844	292.5	73Yan2
LTA1973c01	12.260(5)	1843	293	73Ama1
LTA1973d01	12.205(7)	1818	293	73Ril1
LTA1974a01	12.268(4)	1846	293	74Yan1
LTA1974a02	12.175(3)	1805	292	74Yan1
LTA1974b01	12.087(5)	1766	293	74Ril1
LTA1974b02	12.093(4)	1768	293	74Ril1

Table LTA.2.2 (LTA-I, $Pm\bar{3}m$ continued).

code	a [Å]	V [Å³]	T [K]	reference
LTA-I $Pm\bar{3}m$				
LTA1975a01	12.267(5)	1846	292	75Ril1
LTA1975b01	12.309(2)	1865	293	75Leu1
LTA1975b02	12.301(2)	1861	293	75Leu1
LTA1975c01	12.158(2)	1797	n.s.	75Van1
LTA1975c02	12.320(2)	1870	n.s.	75Van1
LTA1975d01	12.135(3)	1787	294	75Ril2
LTA1975e01	12.205(7)	1818	293	75Ril3
LTA1975e02	12.171(6)	1803	293	75Ril3
LTA1975f01	12.39(2)	1902	n.s.	75Bar1
LTA1975g01	12.35(1)	1884	n.s.	75Thö1
LTA1975g02	12.240(5)	1834	n.s.	75Thö1
LTA1975g07	12.30(1)	1861	n.s.	75Thö1
LTA1976a01	12.075(2)	1761	n.s.	76Rag1
LTA1977a01	12.261(2)	1843	296	77Fir1
LTA1977a02	12.321(3)	1870	296	77Fir1
LTA1977b01	12.180(2)	1807	296	77Fir2
LTA1977b02	12.380(2)	1897	296	77Fir2
LTA1977c01	12.266(2)	1845	n.s.	77Fir3
LTA1977d01	12.295(2)	1859	n.s.	77Kim1
LTA1977d02	12.295(2)	1859	n.s.	77Kim1
LTA1977e01	12.211(2) [1]	1821	n.s.	77Kim2
LTA1977f01	12.296(2)	1859	n.s.	77Fir4
LTA1977g01	12.292(2)	1857	299	77Sub1
LTA1978a01	12.305(1)	1863	297	78Kim1
LTA1978b01	12.259(2)	1842	n.s.	78Kim2
LTA1978c01	12.206(2)	1819	297	78Kim3
LTA1978c02	12.288(3)	1855	297	78Kim3
LTA1978d01	12.245(1)	1836	297	78Kim4
LTA1978e01	12.263(2)	1844	n.s.	78Fir1
LTA1978e02	12.238(2)	1833	n.s.	78Fir1
LTA1978f01	12.212(1)	1821	296	78Kim5
LTA1978g01	12.238(2)	1833	296	78Fir2
LTA1978h01	12.251(2)	1839	296	78Fir3
LTA1978i01	12.103(2)	1773	297	78Sub1
LTA1978j01	12.278(2)	1851	n.s.	78Fir4
LTA1978j02	12.316(2)	1868	n.s.	78Fir4
LTA1978k01	12.244(1)	1836	296	78Kim6
LTA1978l01	12.269(1)	1847	300	78McC1
LTA1978l02	12.219(2)	1824	298	78McC1
LTA1978m01	12.279(3)	1851	297	78Kim7
LTA1978m02	12.333(2)	1876	297	78Kim7
LTA1978m03	12.296(1)	1859	297	78Kim7
LTA1978m04	12.295(1)	1859	297	78Kim7
LTA1978m05	12.284(1) [2]	1854	297	78Kim7
LTA1978m06	12.148(2)	1793	297	78Kim7
LTA1978n01	12.147(2)	1792	299	78Cru1
LTA1978n02	12.146(4)	1792	299	78Cru1
LTA1978o01	12.290(2)	1856	296	78Fir5
LTA1979a01	12.291(1)	1857	298	79McC1
LTA1979a02	12.242(2)	1835	298	79McC1
LTA1979b01	12.187(4)	1810	297	79Cru1
LTA1979b02	12.143(2)	1791	297	79Cru1
LTA1979c01	12.312(3)	1866	n.s.	79Sub1
LTA1979d01	12.317(3)	1869	n.s.	79Plu1
LTA1979d02	12.300(3)	1861	n.s.	79Plu1
LTA1980a01	12.198(2)	1815	297	80Sub1
LTA1980b01	12.277(1)	1851	n.s.	80Plu1
LTA1980c01	12.288(1)	1855	297	80Kim1
LTA1980c02	12.189(2)	1811	297	80Kim1
LTA1980c03	12.267(2)	1846	297	80Kim1

[1]) From personal communiation [2]) Corrected to 12.284 from 12.248

Table LTA.2.2 (LTA-I, $P m \bar{3} m$ continued).

code	a [Å]	V [Å³]	T [K]	reference	code	a [Å]	V [Å³]	T [K]	reference
LTA1980c04	12.262(3)	1844	297	80Kim1	LTA1983g05	12.268(4)	1846	653	83Sch1
LTA1980d01	12.196(2)	1814	297	80Kim2	LTA1983g06	12.245(3)	1836	293	83Sch1
LTA1980e01	12.258(2)	1842	297	80McC1	LTA1983g07	12.301(6)	1861	293	83Sch1
LTA1980e02	12.237(2)	1832	297.	80McC1	LTA1983g08	12.310(3)	1865	293	83Sch1
LTA1980f01	12.277(2)	1850	297	80Sub2	LTA1983g09	12.241(2)	1834	293	83Sch1
LTA1980f02	12.199(2)	1815	297	80Sub2	LTA1983g10	12.302(6)	1862	293	83Sch1
LTA1980f03	12.226(1)	1827	297	80Sub2	LTA1983h01	11.99	1724	n.s.	83Jir1
LTA1980f04	12.225(2)	1827	297	80Sub2	LTA1983h02	11.956(2)	1709	n.s.	83Jir1
LTA1980f05	12.242(2)	1835	297	80Sub2	LTA1983i01	12.298(2)	1860	296	83Che2
LTA1980g01	12.253(3)	1840	RT	80DeR1	LTA1983i02	12.293(2)	1858	296	83Che2
LTA1980g02	12.190(2)	1811	n.s.	80DeR1	LTA1983j01	12.284(1)	1854	n.s.	83Plu2
LTA1980g03	12.310(3)	1865	n.s.	80DeR1	LTA1983j02	12.282(1)	1853	n.s.	83Plu2
LTA1981a01	12.230(1)	1829	299	81McC1	LTA1983j03	12.261(2)	1843	n.s.	83Plu2
LTA1981a02	12.240(1)	1834	300	81McC1	LTA1984a01	12.282(1)	1853	297	84Kim1
LTA1981b01	12.146(5)	1792	n.s.	81Lee1	LTA1984b01	12.221(2)	1825	297	84Kim2
LTA1981b02	12.176(4)	1805	n.s.	81Lee1	LTA1984c02	12.3252(4)	1872	300	84Ada1
LTA1981b03	12.192(2)	1812	n.s.	81Lee1	LTA1985a01	12.208(2)	1819	297	85Kim1
LTA1981b04	12.21(2)	1819	n.s.	81Lee1	LTA1985b01	12.313(1)	1867	297	85Dim1
LTA1981c01	12.163(1)	1799	298	81McC2	LTA1985c01	12.162(2)	1799	297	85Ron1
LTA1981c02	12.049(1)	1749	298	81McC2	LTA1985c02	12.225(3)	1827	297	85Ron1
LTA1981e01	12.32	1870	n.s.	81Gel1	LTA1986a01	12.311(1)	1866	297	86Kim1
LTA1981f01	12.295(1)	1859	n.s.	81Pet1	LTA1986b01	12.124(2)	1782	296	86Heo1
LTA1981f02	12.075(1)	1761	n.s.	81Pet1	LTA1986c01	12.1714(8)	1803	5	86Edd1
LTA1982a03	12.3370(5)	1878	n.s.	82Plu1	LTA1986c02	12.1907(8)	1812	5	86Edd1
LTA1982a04	12.3435(5)	1881	n.s.	82Plu1	LTA1987b01	12.263(1)	1844	293	87Sie1
LTA1982b02	12.2960(1)	1859	300	82Ada1	LTA1987b02	12.230(1)	1829	293	87Sie1
LTA1982c01	12.280(2)	1852	n.s.	82Lee1	LTA1987b03	12.273(1)	1849	380	87Sie1
LTA1982c02	12.369(2)	1892	n.s.	82Lee1	LTA1987b04	12.291(1)	1857	673	87Sie1
LTA1983e02	12.221(1)	1825	n.s.	83Plu1	LTA1987b05	12.285(1)	1854	293	87Sie1
LTA1983g01	12.193(2)	1813	653	83Sch1	LTA1987b06	12.313(1)	1867	298	87Sie1
LTA1983g02	12.280(2)	1852	653	83Sch1	LTA1987c01	12.258	1842	n.s.	87Heo1
LTA1983g03	12.281(2)	1852	653	83Sch1	LTA1987c02	12.279	1851	n.s.	87Heo1
LTA1983g04	12.234(2)	1831	653	83Sch1	LTA1987d01	12.208(2)	1819	297	87Kim1

Table LTA.2.2 (LTA-I, $Pm\bar{3}m$ continued).

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference	code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
LTA1987e01	12.311(1)	1866	297	87Kim2	LTA1989e01	12.173(1)	1804	294	89Kim4
LTA1987f01	12.279(1)	1851	n.s.	87Heo2	LTA1989e02	12.130(1)	1785	294	89Kim4
LTA1987f02	12.291(5)	1857	n.s.	87Heo2	LTA1989f01	12.286(2)	1855	294	89Kim5
LTA1987g01	12.252(1)	1839	297	87Heo3	LTA1989f02	12.278(2)	1851	294	89Kim5
LTA1987g02	12.279(1)	1851	297	87Heo3	LTA1989g01	12.251(1)	1839	294	89Kim6
LTA1987g03	12.276(1)	1850	297	87Heo3	LTA1989g02	12.214(1)	1822	294	89Kim6
LTA1987h01	12.325(1)	1872	RT	87Sie2	LTA1989h01	12.310(1)	1865	294	89Son1
LTA1987h02	12.326(1)	1873	RT	87Sie2	LTA1989h02	12.287(2)	1855	294	89Son1
LTA1987h03	12.299(1)	1860	RT	87Sie2	LTA1989i01	12.214(2)	1822	294	89Yan1
LTA1987h04	12.325(1)	1872	RT	87Sie2	LTA1989i02	12.291(2)	1857	294	89Yan1
LTA1987h05	12.297(1)	1860	RT	87Sie2	LTA1989j01	11.91	1689	-	89Uyt1
LTA1987h06	12.297(1)	1860	RT	87Sie2	LTA1990a01	12.294(1)	1858	294	90Kim1
LTA1987i01	12.288(1)	1855	297	87Kim3	LTA1990a02	12.166(1)	1801	294	90Kim1
LTA1987i02	12.291(2)	1857	297	87Kim3	LTA1990b01	12.289(1)	1856	298	90Pat1
LTA1987k01	11.91	1689	-	87van1	LTA1990b02	12.289(1)	1856	298	90Pat1
LTA1988b01	12.288(1)	1855	297	88Kim1	LTA1990c01	12.100(2)	1772	294	90Jeo1
LTA1988b02	12.291(2)	1857	297	88Kim1	LTA1990c02	12.092(2)	1768	294	90Jeo1
LTA1988c01	12.283(1)	1853	n.s.	88Heo1	LTA1990d01	12.204(3)	1818	294	90Son1
LTA1988d01	12.300(2)	1861	294	88Kim2	LTA1990d02	12.202(1)	1817	294	90Son1
LTA1988d02	12.243(2)	1835	294	88Kim2	LTA1990d03	12.250(2)	1838	294	90Son1
LTA1988d03	12.281(1)	1852	294	88Kim2	LTA1991a01	12.118(1)	1779	294	91Kim1
LTA1988d04	12.263(1)	1844	294	88Kim2	LTA1991a02	12.111(2)	1776	294	91Kim1
LTA1988e01	11.91	1689	-	88van1	LTA1991b01	12.271(1)	1848	294	91Son1
LTA1988f01	12.287(2)	1855	297	88Kim3	LTA1991b02	12.255(1)	1841	294	91Son1
LTA1988f02	12.282(2)	1853	297	88Kim3	LTA1991b03	12.339(1)	1879	294	91Son1
LTA1988g01	12.145(1)	1791	294	88Son1	LTA1991c01	12.225(2)	1827	294	91Koh1
LTA1988g02	12.131(5)	1785	294	88Son1	LTA1991c02	12.219(2)	1824	294	91Koh1
LTA1989a01	12.291(5)	1857	294	89Dej1	LTA1991d01	12.202(3)	1817	294	91Koh2
LTA1989a02	12.357(4)	1887	294	89Dej1	LTA1991e01	12.137(2)	1788	296	91Jeo1
LTA1989b01	12.116(2)	1779	296	89Kim1	LTA1991e02	12.106(2)	1774	296	91Jeo1
LTA1989c01	12.262(2)	1844	294	89Kim2	LTA1991f01	12.211(2)	1821	294	91Jan1
LTA1989d01	12.166(1)	1801	294	89Kim3	LTA1992a01	12.240(2)	1834	297	92Heo1
LTA1989d02	12.294(1)	1858	294	89Kim3	LTA1992a02	12.207(2)	1819	297	92Heo1

Table LTA.2.2 (LTA-I, $P m \bar{3} m$ continued).

code	a [Å]	V [Å^3]	T [K]	reference	code	a [Å]	V [Å^3]	T [K]	reference
LTA1992a03	12.241(1)	1834	297	92Heo1	LTA1994g01	12.145(2)	1791	294	94Jan2
LTA1992b01	12.272(2)	1848	294	92Jan1	LTA1994h01	12.216(1)	1823	294	94Jan3
LTA1992b02	12.245(2)	1836	294	92Jan1	LTA1994h02	12.127(1)	1783	294	94Jan3
LTA1992c01	12.236(3)	1832	295	92Son1	LTA1994i01	12.30979(6)	1865	298	94Arm3
LTA1992c02	12.246(3)	1836	295	92Son1	LTA1994j01	12.248(2)	1837	297	94Sun1
LTA1992c03	12.246(2)	1836	295	92Son1	LTA1994k01	12.256(1)	1841	294	94Heo1
LTA1992c04	12.254(3)	1840	295	92Son1	LTA1994k02	12.260(3)	1843	294	94Heo1
LTA1993b01	12.31(1)	1865	297	93Ron1	LTA1994l01	12.256(1)	1841	294	94Heo2
LTA1993c01	12.255(1)	1841	294	93Jeo1	LTA1994l02	12.260(3)	1843	294	94Heo2
LTA1993c02	12.367(1)	1891	294	93Jeo1	LTA1994m01	12.180(2)	1807	295	94Jeo2
LTA1993c03	12.350(1)	1884	294	93Jeo1	LTA1994n01	12.264(4)	1845	295	94Lee1
LTA1993d01	12.298(2)	1860	297	93Sun1	LTA1994n02	12.269(1)	1847	295	94Lee1
LTA1993e01	12.256(2)	1841	294	93Jan1	LTA1994n03	12.332(3)	1875	295	94Lee1
LTA1993e02	12.259(2)	1842	294	93Jan1	LTA1994o01	12.169(1)	1802	294	94Jan4
LTA1993f01	12.255(1)	1841	294	93Kim1	LTA1994p01	12.344(2)	1881	294	94Son1
LTA1993f02	12.367(1)	1891	294	93Kim1	LTA1994p02	12.304(2)	1863	294	94Son1
LTA1993f03	12.350(1)	1884	294	93Kim1	LTA1995a01	12.298	1860	-	95Kim1
LTA1993f04	12.263(1)	1844	294	93Kim1	LTA1995b01	12.228(1)	1828	294	95Par1
LTA1993g01	12.160(2)	1798	295	93Son1	LTA1995b02	12.258(3)	1842	294	95Par1
LTA1993g02	12.166(2)	1801	295	93Son1	LTA1995b03	12.257(3)	1841	294	95Par1
LTA1993h01	12.242(2)	1835	294	93Kim2	LTA1995b04	12.257(3)	1841	294	95Par1
LTA1993h02	12.191(1)	1812	294	93Kim2	LTA1995c01	12.243(1)	1835	294	95Jan1
LTA1993i01	12.204(1)	1818	294	93Jan2	LTA1995c02	12.214(1)	1822	294	95Jan1
LTA1993i02	12.279(1)	1818	294	93Jan2	LTA1995d01	12.058(2)	1753	294	95Yeo1
LTA1994a01	12.2962(4)	1859	295	94Arm1	LTA1996a01	12.149(2)	1793	294	96Yeo1
LTA1994a02	12.3061(1)	1864	295	94Arm1	LTA1996b01	12.253(2)	1840	294	96Heo1
LTA1994a03	12.2952(1)	1859	4	94Arm1	LTA1996b02	12.253(2)	1840	294	96Heo1
LTA1994b01	12.280(2)	1852	295	94Jeo1	LTA1996c01	12.289(8)	1856	294	96Yeo2
LTA1994c01	12.216(1)	1823	294	94Jan1	LTA1997a01	12.153(4)	1795	294	97Heo1
LTA1994c02	12.187(1)	1810	294	94Jan1	LTA1997a02	12.098(2)	1771	294	97Heo1
LTA1994d01	12.265(1)	1845	294	94Cho1	LTA1997b01	12.153(4)	1795	294	97Heo2
LTA1994d02	12.273(1)	1849	294	94Cho1	LTA1997b02	12.098(1)	1771	294	97Heo2
LTA1994d03	12.286(1)	1855	294	94Cho1	LTA1998a01	12.090(2)	1767	294	98Heo1

Table LTA.2.2 (LTA-I, $P m \bar{3} m$ continued).

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
LTA1998b01	12.2775	1851	-	98Lee1
LTA1999a01	12.245(2)	1836	294	99Heo1
LTA1999a02	12.258(2)	1842	294	99Heo1
LTA1999a03	12.236(2)	1832	294	99Heo1
LTA1999b01	12.2775	1851	-	99Lee1
LTA1999b02	12.2775	1851	-	99Lee1
LTA1999c01	12.2775	1851	-	99Lee2
LTA2000a01	12.249(1)	1838	294	2000Lim1
LTA2000c01	11.9061(1)	1688	RT	2000Rea1
LTA2000e01	12.221(2)	1825	294	2000Cho1
LTA2001a01	12.207(3)	1819	n.s.	2001Tog1
LTA2001b01	12.247(2)	1837	294	2001Lim1
LTA2002a01	12.083(3)	1764	294	2002Heo1
LTA2002a02	12.076(2)	1761	294	2002Heo1
LTA2002a03	12.094(2)	1769	294	2002Heo1
LTA2002a04	12.094(2)	1769	294	2002Heo1
LTA2003a02	12.147(3)	1792	RT	2003Ike1
LTA2003a03	12.06180(13)	1755	RT	2003Ike1
LTA2003a04	12.0077(2)	1731	RT	2003Ike1
LTA2004a01	12.290(1)	1856	294	2004Heo1
LTA2004c01	12.0157(4)	1735	n.s.	2004Cor1
LTA2004c02	11.8671(4)	1671	n.s.	2004Cor1
LTA2005a01	12.186(1)	1810	294	2005Lim1

LTA-II.1 $F m \bar{3} c$

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
LTA1971a03	24.61(1)	14905	n.s.	71Gra1
LTA1971a04	24.61(1)	14905	n.s.	71Gra1
LTA1971a05	24.61(1)	14905	n.s.	71Gra1
LTA1971a06	24.61(1)	14905	n.s.	71Gra1
LTA1979d03	24.600(6)	14887	n.s.	79Plu1
LTA1980b02	24.555(2)	14805	n.s.	80Plu1
LTA1981d01	24.568(2)	14829	296	81McC3
LTA1982a01	24.674(1)	15022	n.s.	82Plu1
LTA1982a02	24.687(1)	15045	n.s.	82Plu1
LTA1982b01	24.5920(2)	14872	300	82Ada1
LTA1982d01	24.373	14887	RT	82Che1
LTA1983a01	24.373 [1])	14887	n.s.	83Che1
LTA1983b01	24.5693(5)	14831	603	83Ben1
LTA1983b02	24.5692(5)	14831	603	83Ben1
LTA1983b03	24.623(1)	14928	367	83Ben1
LTA1983c01	24.5693(5)	14831	603	83Ben2
LTA1983c02	24.5692(5)	14831	603	83Ben2
LTA1983c03	24.623(1)	14928	367	83Ben2
LTA1983d01	24.548(3)	14793	n.s.	83Gel1
LTA1983e01	24.443(2)	14604	n.s.	83Plu1
LTA1983f01	24.6	14887	n.s.	83Ada1
LTA1983j04	24.569(1)	14831	n.s.	83Plu2
LTA1983j05	24.564(2)	14822	n.s.	83Plu2
LTA1984c01	24.6497(8)	14977	300	84Ada1
LTA1984d01	24.156(1)	14095	n.s.	84Ada2
LTA1986d01	24.424(1)	14570	298	86Ada1
LTA1987a01	24.6558(2)	14988	n.s.	87Ada1
LTA1987a02	24.6558(2)	14988	n.s.	87Ada1
LTA1988a01	24.555	14805	n.s.	88Dem1
LTA1988a02	24.555	14805	n.s.	88Dem1
LTA1988a03	24.555	14805	n.s.	88Dem1
LTA1988a04	24.555	14805	n.s.	88Dem1
LTA1992d01	24.035(3)	13885	293	92Sim1
LTA1993a01	24.035(3)	13885	293	93Sim1
LTA1996d01	24.556(1)	14807	n.s.	96Hor1
LTA1997a03	24.188(3)	14151	294	97Heo1
LTA1998c01	24.5335(2)	14767	RT	98Ike1
LTA1998c02	24.5693(3)	14831	RT	98Ike1

[1]) Lattice constant from 82Che1.

Table LTA.2.2 (LTA-II.1, $Fm\bar{3}c$ continued).

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
LTA1998c03	24.6077(8)	14901	RT	98Ike1
LTA1998d01	23.895(2)	13643	293	98Por1
LTA1998d02	23.895(2)	13643	293	98Por1
LTA1999d01	24.5528(2)	14801	RT	99Has1
LTA2000d01	24.47(1)	14652	RT	2000Por1
LTA2000d02	24.47(1)	14652	RT	2000Por1
LTA2000d03	24.47(1)	14652	RT	2000Por1
LTA2001c01	23.990(8)	13807	150	2001Map1
LTA2003a01	24.4848(4)	14679	RT	2003Ike1

code	*a* [Å]	*α* [°]	*V* [Å^3]	*T* [K]	reference
LTA-VIII.1 $R\bar{3}c$					
LTA1983b04 1)	17.451(1)	59.652(7)	3728	296	83Ben1
LTA1983b05 1)	17.413(1)	59.652(7)	3704	4.5	83Ben1
LTA1983c04 1)	17.451(1)	59.652(7)	3728	296	83Ben2
LTA1983c05 1)	17.413(1)	59.652(7)	3704	4.5	83Ben2
LTA1998e01 2)	17.1236(9)	57.972(7)	3385	RT	98Sch1

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
LTA-II.2 $Fm\bar{3}m$				
LTA1994a04 3)	24.6054(1)	14897	295	94Arm1
LTA1994a05 3)	24.6324(2)	14946	295	94Arm1
LTA1994f01 3)	24.6324(2)	14946	RT	94Arm2

transformations: origin shift; unit cell transformation; coordinate transformation
1) 0, 0, 0; ½(**b**+**c**), ½(**a**+**c**), ½(**a**+**b**); *-x+y+z*, *x-y+z*, *x+y-z*
2) 0,0, 0; ⅔**a**+⅓**b**+⅓**c**, -⅓**a**+⅓**b**+⅓**c**, -⅓**a**-⅔**b**+⅓**c**; *x+z*, *-x+y+z*, *-y+z* 3) ¼, ¼, ¼; **a**, **b**, **c**; *x*-¼, *y*-¼, *z*-¼

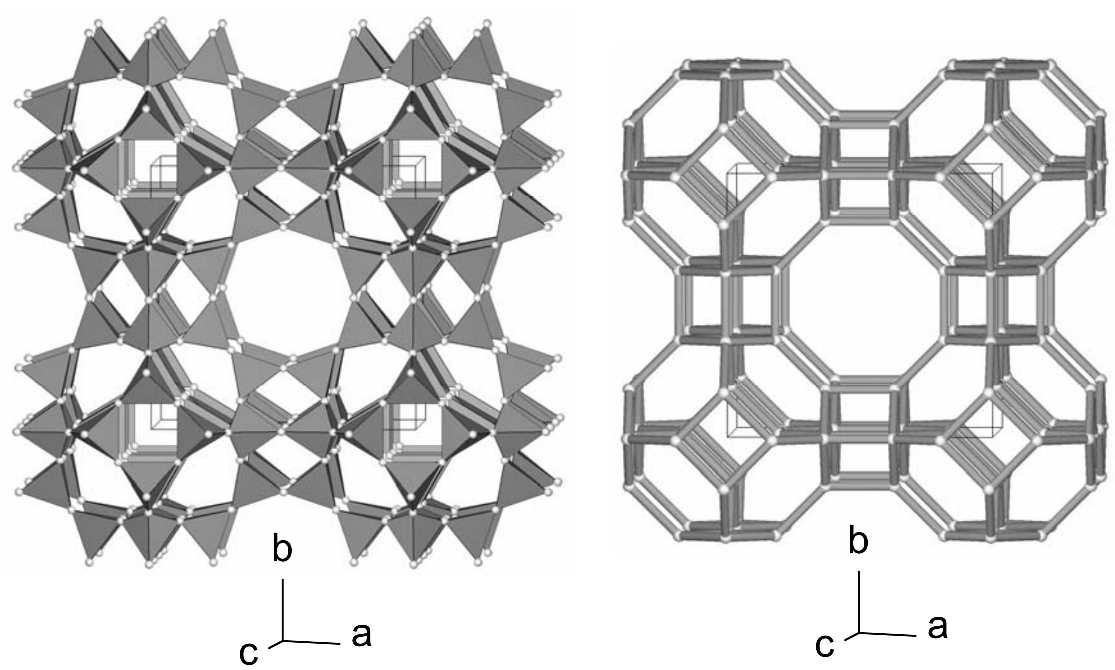
LTA.3 Framework structures

LTA.3.1 LTA-I compound ($Pm\bar{3}m$, IT #221)

Several of the LTA-type crystal structures originally refined in space group $Pm\bar{3}m$ have subsequently been successfully refined in $Fm\bar{3}c$. It might be necessary in certain cases to view the details of the results obtained in space group $Pm\bar{3}m$ with caution.

Table LTA.3.1.1 Atomic coordinates and site definitions for $Na_{12} \cdot Al_{12}Si_{12}O_{48}$ (LTA1968a02, 68Smi1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0	0.182(1)	0.3701(9)	0.0(3)	*m* . .	24(k)	12 / 12
O1	0.112(1)	*x*	0.340(2)	1.5(6)	. . *m*	24(m)	24
O2	0	0.302(2)	*y*	1(1)	*m* . *m* 2	12(i)	12
O3	0.234(3)	½	0	2(1)	*mm* 2 . .	12(h)	12
Na1	0.212(1)	*x*	*x*	1.4(8)	. 3 *m*	8(g)	8
Na2	½	0.438(5)	0.043(7)	1(3)	*m* . .	24(l)	4



a polyhedral representation. **b** Ball and stick model corresponding to a).

Fig. LTA.3.1.1 Projections of the LTA-I crystal structure of zeolite A, $Na_{12} \cdot Al_{12}Si_{12}O_{48}$ (LTA1968a02,68Smi1). View parallel **c** rotated by 2° about **a** and **b**.

Table LTA.3.1.2 Selected interatomic distances and angles for $Na_{12} \cdot Al_{12}Si_{12}O_{48}$ (LTA1968a02,68Smi1).

	T - O [Å]	T - O - T [°]
(Si,Al)1 - O1	1.66(2)	144(1)
(Si,Al)1 - O1	1.66(2)	144(1)
(Si,Al)1 - O2	1.69(2)	150(1)
(Si,Al)1 - O3	1.72(2)	136(2)
Mean	1.68	144

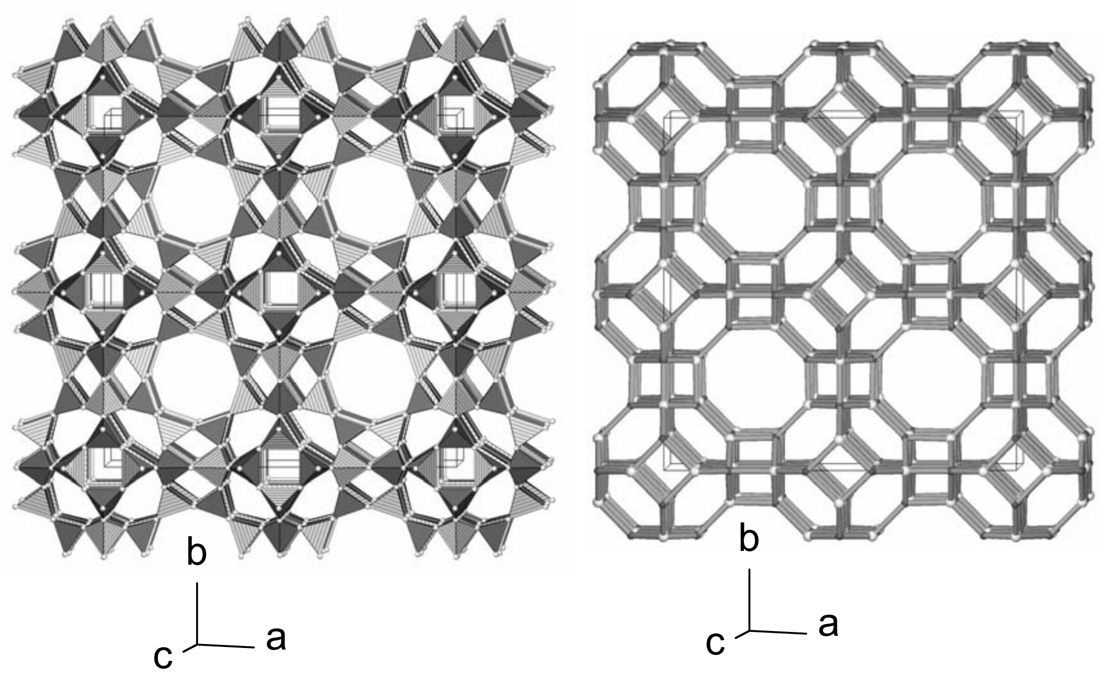
LTA.3.2 LTA-II.1 compound ($Fm\bar{3}c$, IT #226)

Table LTA.3.2.2 Selected interatomic distances and angles for LTA-II, $Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$ (LTA1971a06, 71Gra1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O2	1.60(2)	159.5(14)	Al 12 - O3	1.72(3)	145.6(5)
Si11 - O1	1.61(1)	144.3(7)	Al 12 - O2	1.72(2)	159.5(14)
Si11 - O1	1.61(1)	144.3(7)	Al 12 - O1	1.74(1)	144.3(7)
Si11 - O3	1.62(3)	145.6(5)	Al 12 - O1	1.74(1)	144.3(7)
mean	1.61	139.3	mean	1.73	139.3

Table LTA.3.2.1 Atomic coordinates and site definitions for LTA-II.1, $Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$ (LTA1971a06,71Gra1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0	0.0929(4)	0.1844(4)	1.16	*m* . .	96(i)	96
Al 12	0	0.1864(4)	0.0902(4)	1.00	*m* . .	96(i)	96
O1	0.0538(5)	0.0583(5)	0.1704(2)	2.45	1	192(j)	192
O2	0	0.1463(8)	0.1476(8)	2.08	*m* . .	96(i)	96
O3	0.1116(2)	0.247(1)	0	2.55	*m* . .	96(i)	96
Na1	0.1064(2)	*x*	*x*	7.74	. 3 .	64(g)	64
OW11	0.02(1)	0.03(1)	0.064(3)	25.0	1	192(j)	22
OW12	0.03(1)	0.02(1)	0.064(3)	25.0	1	192(j)	22
OW2	0.1598(4)	*x*	*x*	18.2	. 3 .	64(g)	58.2
OW31	0.1155(8)	0.167(1)	0.262(7)	33.4	1	192(j)	62.4
OW32	0.167(1)	0.1155(8)	0.262(7)	33.4	1	192(j)	62.4
OW41	0.041(1)	0.210(2)	0.235(5)	34.7	1	192(j)	42.2
OW42	0.210(2)	0.041(1)	0.235(5)	34.7	1	192(j)	42.2
OW5	¼	¼	¼	61.6	4 3 2	8(a)	15.0



a polyhedral representation. **b** Ball and stick model corresponding to a).

Fig. LTA.3.2.1 Projections of the LTA-II.1 crystal structure of zeolite A, $Na_{96} \cdot Al_{96}Si_{96}O_{384} \cdot 216H_2O$ (LTA1971a06, 71Gra1). View parallel **c** rotated by 1° about **a** and **b**.

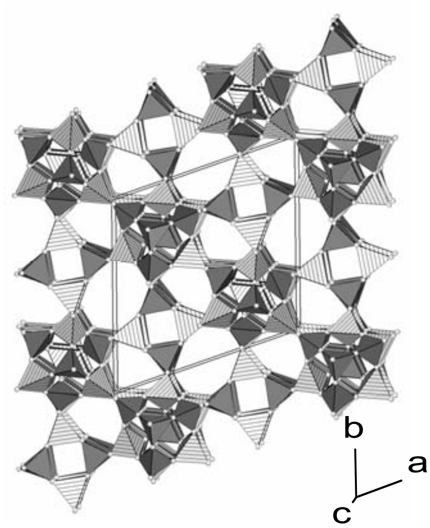
LTA.3.3 LTA-VIII.1 compound ($R\bar{3}c$, IT #167)

Table LTA.3.3.1 Atomic coordinates and site definitions for LTA-VIII.1, $Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$ (LTA1983c04, 83Ben2).

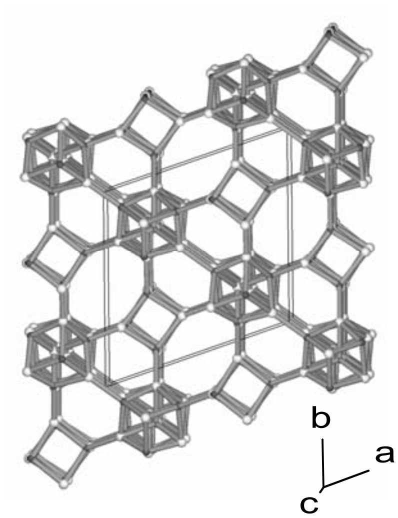
atom	*x*	*y*	*z*	B_{iso} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11a	0.274(2)	0.102(2)	0.898(2)	0.4(4)	1	12(f)	12
Si11b	0.102(2)	0.274(2)	0.726(2)	0.4(4)	1	12(f)	12
Al 12a	0.276(2)	-0.085(2)	0.085(2)	0.4(4)	1	12(f)	12
Al 12b	-0.085(2)	0.276(2)	0.724(2)	0.4(4)	1	12(f)	12
O11	0.173(1)	0.170(1)	-0.060(1)	0.7(2)	1	12(f)	12
O12	0.170(1)	0.173(1)	0.718(1)	0.7(2)	1	12(f)	12
O13	0.940(1)	-0.282(1)	0.173(1)	0.7(2)	1	12(f)	12
O14	0.718(1)	-0.060(1)	0.170(1)	0.7(2)	1	12(f)	12
O21	0.2938(8)	0.0162(8)	-0.0162(8)	0.7(2)	1	12(f)	12
O22	0.0162(8)	0.2938(8)	0.7062(8)	0.7(2)	1	12(f)	12
O31	0.364(2)	0.140(2)	0.860(2)	0.7(2)	1	12(f)	12
O32	0.140(2)	0.364(2)	0.636(2)	0.7(2)	1	12(f)	12
Na11	0.101(1)	*x*	*x*	2.0(8)	3 .	4(c)	3.8(6)
Na12	0.698(1)	0.101(1)	0.101(1)	2.0(8)	1	12(f)	9.8(7)
Na21	0.459(2)	0.000(2)	0.000(2)	2.0(8)	1	12(f)	6.1(4)
Na31	0.125(2)	0.250(2)	0.250(2)	2.0(8)	1	12(f)	0.5(6)
Na32	0.375(2)	-*x*+½	¼	2.0(8)	. 2	6(e)	1.4(2)
Na33	0.125(2)	-*x*+½	¼	2.0(8)	. 2	6(e)	1.44

Table LTA.3.3.2 Selected interatomic distances and angles for LTA-VIII.1, $Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$ (LTA1983c04, 83Ben2).

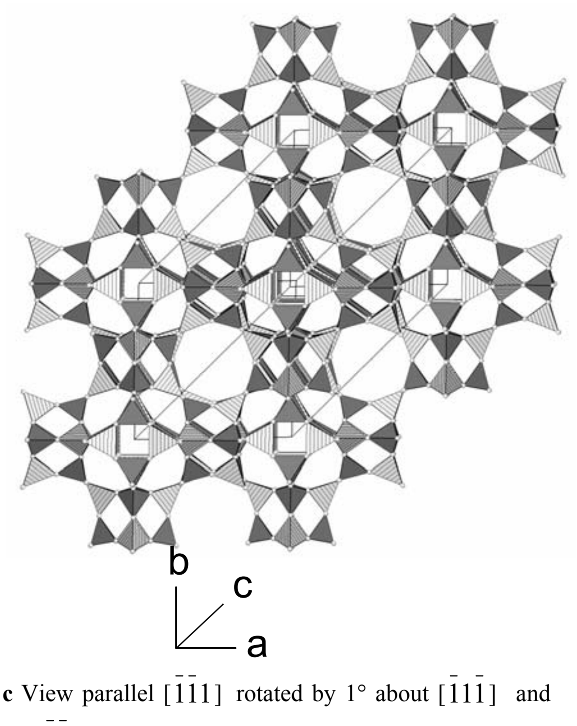
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11a - O21	1.53(4)	157(2)	Al 12a - O32	1.71(6)	144(2)
Si11a - O11	1.58(3)	146(2)	Al 12a - O11	1.72(6)	146(2)
Si11a - O14	1.59(3)	146(2)	Al 12a - O13	1.73(6)	146(2)
Si11a - O31	1.70(5)	144(2)	Al 12a - O21	1.79(4)	157(2)
mean	1.60	148	mean	1.74	148
Si11b - O22	1.54(4)	157(2)	Al 12b - O31	1.71(6)	144(2)
Si11b - O12	1.59(3)	146(2)	Al 12b - O12	1.72(6)	146(2)
Si11b - O13	1.59(3)	146(2)	Al 12b - O14	1.73(6)	146(2)
Si11b - O32	1.70(5)	144(2)	Al 12b - O22	1.79(4)	157(2)
mean	1.60	148	mean	1.74	148



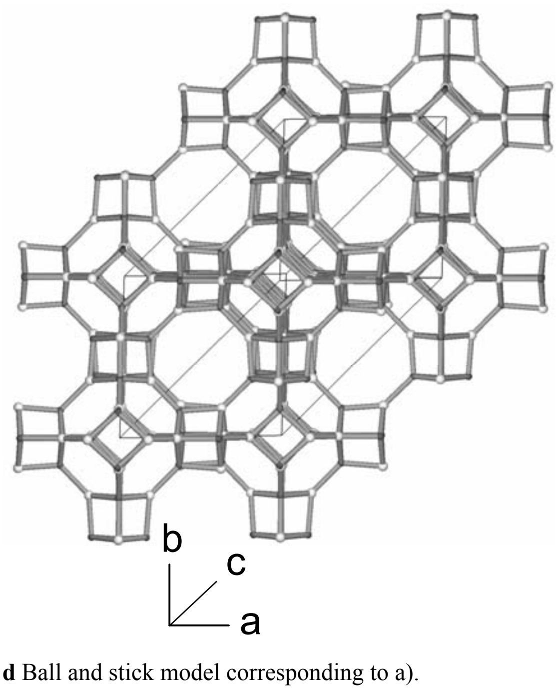
a View parallel [001] rotated by 1° about **b**×**c**.



b Ball and stick model corresponding to a).



c View parallel $[\bar{1}\bar{1}1]$ rotated by 1° about $[\bar{1}1\bar{1}]$ and $[1\bar{1}\bar{1}]$ corresponding to the view parallel [001] of the cubic compounds.



d Ball and stick model corresponding to a).

Fig. LTA.3.3.1 Projections of the LTA-VIII.1 crystal structure of zeolite A, $Na_{23.5} \cdot Al_{23.25}Si_{24.75}O_{96}$ (LTA1983c04, 83Ben2).

LTA.3.4 LTA-II.2 compound ($F m\bar{3} m$, IT #225)

Table LTA.3.4.1 Atomic coordinates and site definitions for LTA-II.2, $K_{120} \cdot Al_{96}Si_{96}O_{384}$ (LTA1994a04, 94Arm1).

atom	*x*	*y*	*z*	B_{iso} / B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0	0.0933(4)	0.1885(1)	0.93	1	192(l)	104 / 88
O11	0.0556(1)	*x*	0.1770(2)	0.97	. . *m*	96(k)	96
O12	0.5573(2)	*x*	0.6827(2)	2.57	. . *m*	96(k)	96
O2	-0.0042(2)	0.1422(1)	*y*	1.20	. . *m*	96(k)	96
O3	0.1225(1)	¼	0.0049(2)	1.53	*m* . .	96(j)	96
K1	0.6164(3)	*x*	*x*	3.20	. 3 *m*	32(f)	26.56
K2	¾	¾	½	2.90	4*m* . *m*	24(e)	14.88
K3	0.0662(2)	*x*	*x*	0.40	. 3 *m*	32(f)	17.60
K4	¼	0.1218(3)	0.1218(3)	1.47	*m*. *m* 2	48(i)	34.08
K5	0.1164(3)[1)]	*x*	*x*	3.20	. 3 *m*	32(f)	9.28
K6	0.5662(2)[2)]	*x*	*x*	0.40	. 3 *m*	32(f)	5.44

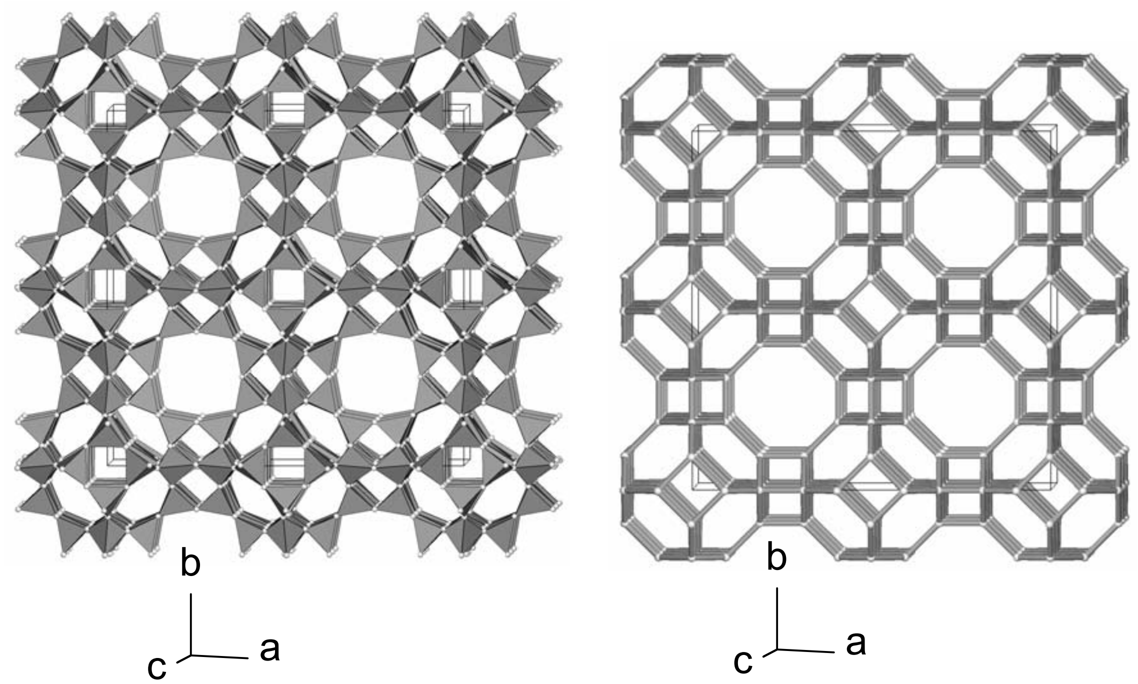
[1)] constrained to *x*(K1)-½
[2)] constrained to *x*(K3)+½
Nonstandard setting with origin in ¼, ¼, ¼ from center $m\bar{3}m$
Symmetry operators:

x, *y*, *z*	*x*, -*y*-½, -*z*-½	-*x*-½, *y*, -*z*-½	-*x*-½, -*y*-½, *z*	*y*, *z*, *x*	-*y*-½, -*z*-½, *x*
y, -*z*-½, -*x*-½	-*y*-½, *z*, -*x*-½	*z*, *x*, *y*	-*z*-½, *x*, -*y*-½	-*z*-½, -*x*-½, *y*	*z*, -*x*-½, -*y*-½
y, *x*, *z*	-*y*-½, *x*, -*z*-½	*y*, -*x*-½, -*z*-½	-*y*-½, -*x*-½, *z*	*z*, *y*, *x*	-*z*-½, -*y*-½, *x*
-*z*-½, *y*, -*x*-½	*z*, -*y*-½, -*x*-½	*x*, *z*, *y*	*x*, -*z*-½, -*y*-½	-*x*-½, -*z*-½, *y*	-*x*-½, *z*, -*y*-½
-*x*-½, -*y*-½, -*z*-½	-*x*-½, *y*, *z*	*x*, -*y*-½, *z*	*x*, *y*, -*z*-½	-*y*-½, -*z*-½, -*x*-½	*y*, *z*, -*x*-½
-*y*-½, *z*, *x*	*y*, -*z*-½, *x*	-*z*-½, -*x*-½, -*y*-½	*z*, -*x*-½, *y*	*z*, *x*, -*y*-½	-*z*-½, *x*, *y*
-*y*-½, -*x*-½, -*z*-½	*y*, -*x*-½, *z*	-*y*-½, *x*, *z*	*y*, *x*, -*z*-½	-*z*-½, -*y*-½, -*x*-½	*z*, *y*, -*x*-½
z, -*y*-½, *x*	-*z*-½, *y*, *x*	-*x*-½, -*z*-½, -*y*-½	-*x*-½, *z*, *y*	*x*, *z*, -*y*-½	*x*, -*z*-½, *y*

and equivalent positions related by F-centering (½, ½, 0)+, (½, 0, ½)+, (0, ½, ½)+

Table LTA.3.4.2 Selected interatomic distances and angles for LTA-II.2, $K_{120} \cdot Al_{96}Si_{96}O_{384}$ (LTA1994a04, 94Arm1).

	T - O [Å]	T - O - T [°]
(Si,Al)1 - O2	1.660(8)	172.2(5)
(Si,Al)1 - O12	1.671(7)	152.5(4)
(Si,Al)1 - O11	1.677(6)	150.9(5)
(Si,Al)1 - O3	1.679(5)	128.6(42)
mean	1.672	151.1



a polyhedral representation.

b Ball and stick model corresponding to a).

Fig. LTA.3.4.1 Projections of the LTA-II.2 crystal structure, $K_{120} \cdot Al_{96}Si_{96}O_{384}$ (LTA1994a04, 94Arm1).

LTA.4 Chemical composition

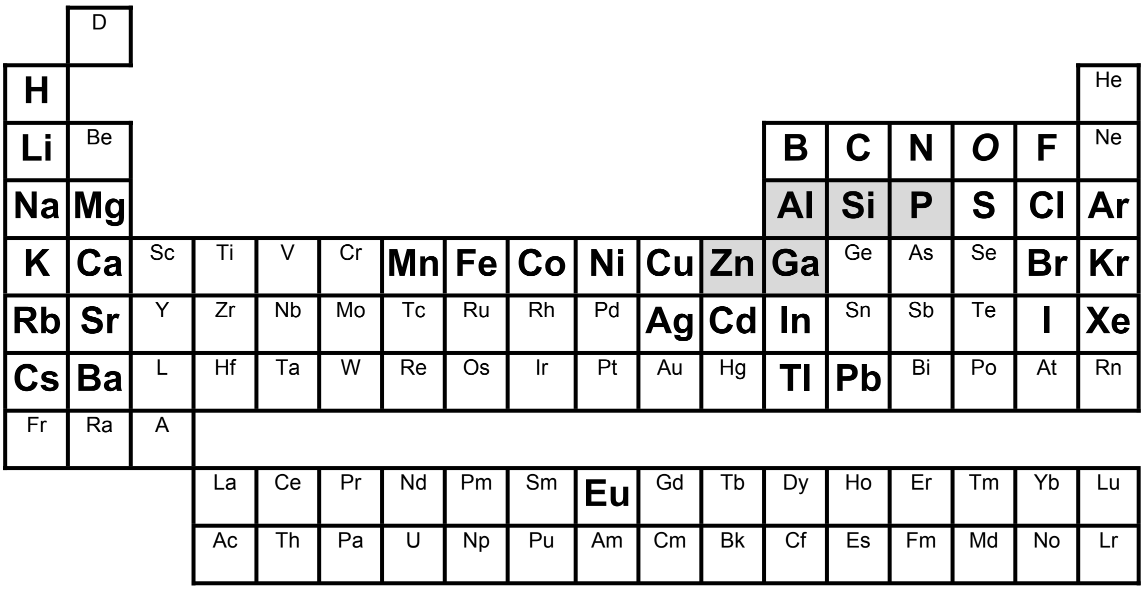


Fig. LTA.4.1 Chemical elements (highlighted) occurring in LTA-type compounds. Framework cations are in grey fields.

LTA.5 Flexibility and apertures

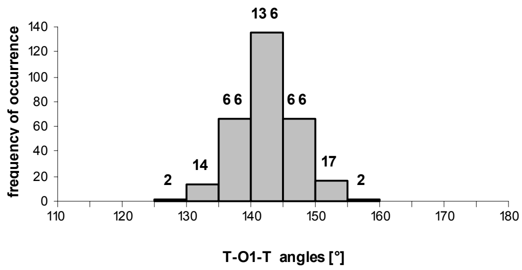


Fig. LTA.5.1 Individual T-O1-T angles from 303 experimental crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space groups $Pm\bar{3}m$ and $Fm\bar{3}c$. The individual values of the angles range from 128° to 157°, with a mean value of 143°.

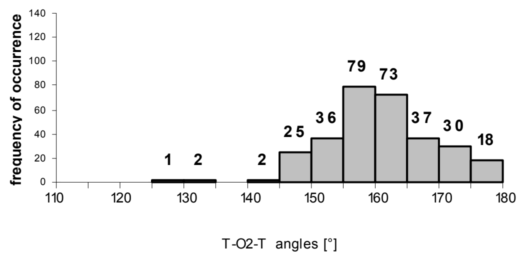


Fig. LTA.5.2 Individual T-O2-T angles from 303 experimental crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space groups $Pm\bar{3}m$ and $Fm\bar{3}c$. The individual values of the angles range from 129° to 179°, with a mean value of 161°.

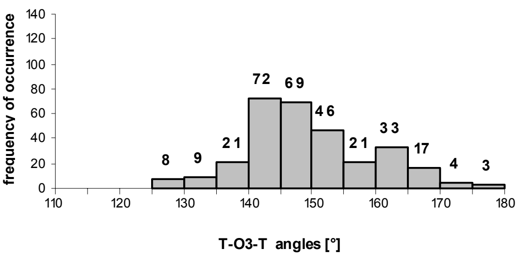


Fig. LTA.5.3 Individual T-O3-T angles from 303 experimental crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space groups $Pm\bar{3}m$ and $Fm\bar{3}c$. The individual values of the angles range from 125° to 178°, with a mean value of 149°.

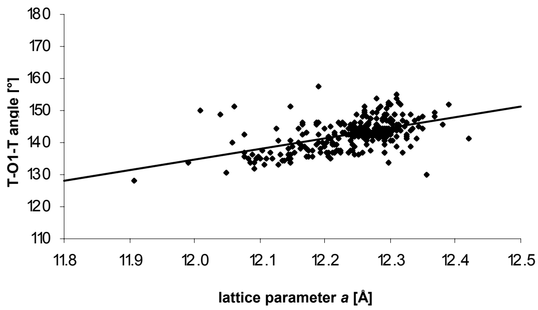


Fig. LTA.5.4 Individual T-O1-T angles from 278 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Pm\bar{3}m$ plotted against the unit cell constants. The plot shows 278 pairs of experimental values. The individual values of the cell constants range from 11.91 Å to 12.42 Å, the values of the angles from 128° to 157°. The line is a least-squares fit to all points.

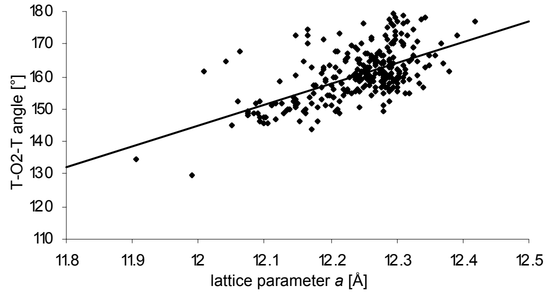


Fig. LTA.5.5 Individual T-O2-T angles from 278 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Pm\bar{3}m$ plotted against the unit cell constants. The plot shows 278 pairs of experimental values. The individual values of the cell constants range from 11.91 Å to 12.42 Å, the values of the angles from 129° to 179°. The line is a least-squares fit to all points.

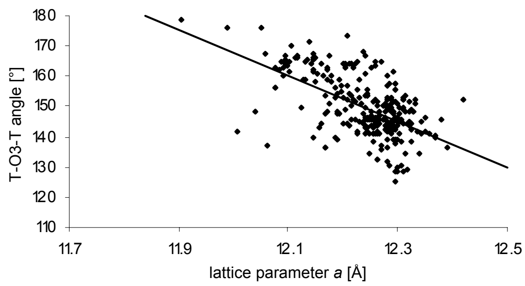


Fig. LTA.5.6 Individual T-O3-T angles from 278 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Pm\bar{3}m$ plotted against the unit cell constants. The plot shows 278 pairs of experimental values. The individual values of the cell constants range from 11.91 Å to 12.42 Å, the values of the angles from 125° to 178°. The line is a least-squares fit to all points.

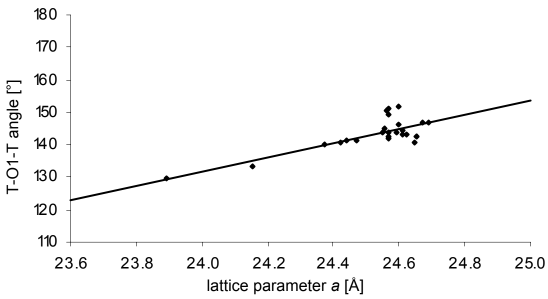


Fig. LTA.5.7 Individual T-O1-T angles from 25 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Fm\bar{3}c$ plotted against the unit cell constants. The plot shows 25 pairs of experimental values. The individual values of the cell constants range from 23.90 Å to 24.69 Å, the values of the angles from 129° to 147°. The line is a least-squares fit to all points.

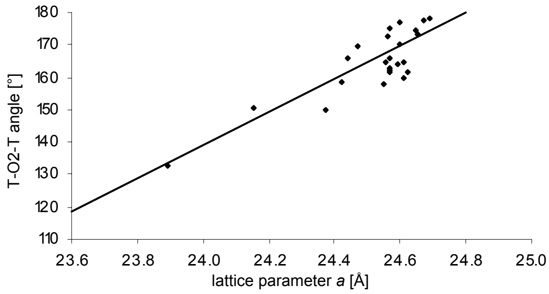


Fig. LTA.5.8 Individual T-O2-T angles from 25 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Fm\bar{3}c$ plotted against the unit cell constants. The plot shows 25 pairs of experimental values. The individual values of the cell constants range from 23.90 Å to 24.69 Å, the values of the angles from 133° to 178°. The line is a least-squares fit to all points

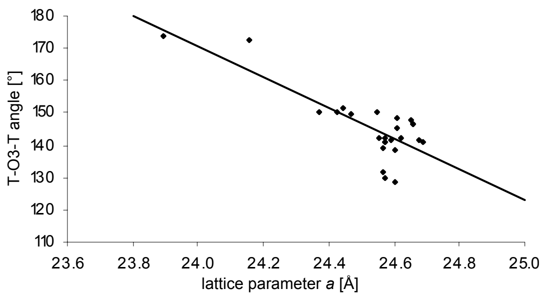


Fig. LTA.5.9 Individual T-O3-T angles from 25 crystal structure determinations of LTA-type compounds with silicoaluminate frameworks crystallizing in space group $Fm\bar{3}c$ plotted against the unit cell constants. The plot shows 25 pairs of experimental values. The individual values of the cell constants range from 23.90 Å to 24.69 Å, the values of the angles from 141° to 174°. The line is a least-squares fit to all points.

The unit cell constants of LTA-type silicoaluminate compounds in space group $Fm\bar{3}c$ vary from 23.90 Å to 24.69 Å, or by 3.3%. For those crystallizing in space group $Pm\bar{3}m$ the range is from 11.91 Å to 12.42 Å, for a difference of 2.8%. 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]. It is the more surprising to see such stable values of the cell constants when one observes that T-O-T angles in LTA-type structures vary from 125° to 179° (Figs. LTA.5.1, LTA.5.2 and LTA.5.3), or by almost the full range of values displayed by numerous zeolite frameworks of different types (115° to 180° observed in a sample of 2436 T-O-T values [95Bau1]). Less than 10% of the angles T-O1-T, T-O2-T and T-O3-T fall outside ±15° of their mean values. Conversely for a given constant value of the unit cell constant each of the three crystallographically and topologically distinct angles T-O-T can assume values which can differ by about 30°. These observations were made previously [92Bau1] on a smaller dataset of LTA-type structures and are confirmed here on the basis of 303 structures (be aware that the labeling of the oxygen atoms here and in [92Bau1] is different: the labels of O1 and O3 have been exchanged). FAU-type structures [see the FAU chapter], display an analogous behavior: we observe a large flexibility of the individual T-O-T angles coupled with a limited range of observed values of the unit cell constants. When one views the tetrahedral framework of a zeolite as an assembly of rigid coordination tetrahedra connected by flexible hinges (the oxygen bridges between the tetrahedra) then this observation is explained by the antirotation of the angles T-O-T concomitant to volume changes: that is, while one type of angle T-O-T opens up, another angle T-O-T gets smaller. This can be seen by comparing the plots of T-O-T *vs. a* (Figs. LTA.5.4, LTA.5.5, LTA.5.6 on one hand and LTA.5.7, LTA.5.8, LTA.5.9 on the other hand). Angle T-O3-T is antirotating to the other two T-O-T angles, that is the unit cell constant unexpectedly and counterintuitively increases while the T-O3-T angles becomes smaller. The other two angles (T-O1-T and T-O2-T) behave normally, as they increase, the cell constant increases. Frameworks with antirotating hinges are noncollapsible, frameworks with corotating hinges (where the angles T-O-T open and close in concert upon volume change) are collapsible [92Bau1]. A good example of a collapsible framework is the NAT-type with its pronounced changes in unit cell constants with chemically different pore fillings and with changes in temperature [95Bau1].

The framework density of LTA-type compounds is similar to the framework density of FAU-type compounds. However, the largest ring in the LTA net is only an 8-ring with a free diameter of slightly in excess of 4 Å. This value should be taken only as an approximation and a lower bound. In view of the remarkable flexibility of this framework it is entirely feasible for slightly larger molecules to enter the pores of LTA-type frameworks.

LTA.6 Other information

After FAU (723 crystal structures published so far) and SOD (635 structures) the LTA framework is the most studied with 375 entries listed in Tables LTA.2.1 and LTA.2.2. This is out of a total of more than 4,000 crystal structure determinations on which these volumes are based. Inasmuch as LTA-type compounds are not important as catalysts the general literature about them is much less voluminous than about FAU-type compounds. Nevertheless, there were at one time or another heated discussions about the properties of LTA-type silicoaluminates as detailed below.

LTA.6.1 Uses

The first publication in which zeolite A is announced [56Bre2] already mentions its cation exchange properties and that its adsorption of molecules depends on which cations are present in the pores. The ability of Na-zeolite A for cation exchange is the basis of its most widely used application, the softening of water, that is the removal from it of Ca and Mg ions. For this purpose it is added to household detergents. The annual production of Na-zeolite A for this application alone exceeds one million metric tons [2005Fla1]. Dehydrated Na-zeolite A is used as a desiccant. In this form it is added in some countries to non-dairy creamers in powdered form (to keep the powder dry). Thus it possibly is the only zeolite that has become part of the human diet [85Bau1]. Zeolite A in its Ca-form is being used to separate O_2 and N_2 from air and to remove straight hydrocarbon molecules from gasoline thus suppressing knocking [89Ker1]. A more recent application is the use of zeolite A for stanching blood on fresh wounds [2005Fla1]. The applications mentioned here are just examples, for additional uses see [99She1, 79Bre1, 2005Fla1].

LTA.6.2 The space groups of LTA-type compounds

The original crystal structure determination of LTA-type zeolite A was based on powder diffraction data and described the structure in space group $Pm\bar{3}m$ [56Ree1]. The same was true of the subsequent determinations in the 1950's and 1960's [58Bar1, 60How1, 60Bro1, 66Mei1, 67Sef1]. The exception was the dehydrated Na form of zeolite A which was studied [68Smi1] using very small single crystals (cubes with an edge length of 23 µm). It was described in space group $Pm\bar{3}m$. Barrer and Meier [58Bar1] observed two superstructure lines in the powder pattern of Na-zeolite A investigated by them. This necessitated a doubling of the unit cell constant. The paucity of data did not allow a refinement in the larger cell, but they recognized that the refinement in space group $Pm\bar{3}m$ corresponded to a pseudosymmetric description. With one exception all the crystal structure determinations of silicoaluminate LTA-type frameworks have been performed on samples with an Si:Al ratio of close to 1:1. The only clear exception is a ratio Si:Al of 15:9 [86Edd1], otherwise the ratio is at the utmost 13:11 [83Plu1]. This constancy of the Si/Al ratio was used in [58Bar1] as an argument for the ordering and alternating of the Si and Al atoms within the framework and for a proper description in the larger unit cell.

In 1971 relatively large crystals of zeolite A grown by Charnell using his gel growth method [71Cha1] became available. Gramlich and Meier [71Gra1] used a cube of hydrated Na-zeolite A with an edge length of 70 µm (or 27 times the volume of the crystal employed in [68Smi1]). They recorded 298 symmetrically independent so called "a" diffractions due to the pseudosymmetric small unit cell and 90 "b" type diffractions due to the large cell. They refined the crystal structure in space group $Fm\bar{3}c$, with a doubled unit cell constant, and showed in a careful study that the Si and Al atoms of the framework were ordered in such a way that each Si coordination tetrahedron was surrounded by four Al tetrahedra and vice versa.

Nevertheless, most crystal structure determinations of zeolite A type crystal structures continue to be described in the higher symmetry space group $Pm\bar{3}m$. So far 297 crystal structure refinements in space group $Pm\bar{3}m$ have been published and 39 in space group $Fm\bar{3}c$. Almost all of the latter are based either on laboratory X-ray diffraction using Cu-Kα radiation, or on experiments performed with synchrotron X-rays or else on neutron powder diffraction. All these types of measurements allow the weak "b" reflections to be measured more precisely relative to the strong "a" reflections. In a number of cases additional "b" type reflections have been recorded which violate the c-glide plane condition of space group $Fm\bar{3}c$. This might mean that the actual symmetry of these samples is even lower. In any event space group $Fm\bar{3}c$ is a better approximation to the actual structures of these compounds than the more highly symmetric space group $Pm\bar{3}m$. Conversely, most crystal structure refinements by single crystal methods in space group $Pm\bar{3}m$ were performed using Mo-Kα radiation, which means that the chances of detecting "b" type reflections were much impaired. It is to be suspected that numerous refinements based on space group $Pm\bar{3}m$ should actually have been performed in $Fm\bar{3}c$. If this is true, then many of the published details about the pore contents of these structures are of questionable value.

In 1980 a paper was published [80Eng1] in which the validity of the crystal structure determination of Na-zeolite A and its space group assignment to $Fm\bar{3}c$ by Gramlich and Meier [71Gra1] was questioned in a fundamental way on the basis of the then new method of high-resolution ^{29}Si NMR spectroscopy. By comparing the high-resolution magic angle spinning ^{29}Si nuclear magnetic resonance (MAS-NMR) spectra of several zeolites with those of zeolite A it was concluded that in zeolite A each Si coordination tetrahedron was surrounded by three Al tetrahedra and one Si tetrahedron. Therefore space group $Fm\bar{3}c$ could not be the proper description for the zeolite A structure and in addition the general assumption that in zeolite A the Si and Al atoms were alternating regularly in three dimensions had to be wrong. This paper was followed by several contributions reiterating and deepening the discussion, including evidence from electron diffraction which was interpreted as ruling out space group $Fm\bar{3}c$ [80Bur1, 80Lod1, 81Bur1, 81Kli1, 81Lip1, 81Tho1]. Space groups $Fm\bar{3}$, $Pm\bar{3}$, and $R\bar{3}$ were considered, but it was not possible to get reasonable refinements of diffraction data in any of them.

It was immediately pointed out by several crystallographers that certainly the new data were not compatible with the crystallographic evidence, but that meant only that the new evidence was not convincing [81Smi1, 82Gra1, 82Ada2, 82Mel1, 83Plu3]: the peak of NMR absorption at -89.1 p.p.m. had been wrongly assigned to an environment of three Al and one Si around each Si atom. At first this was not accepted [81Bur2], but finally agreement was reached that indeed space group $Fm\bar{3}c$ explains most of the available data for zeolite A and that within the framework of zeolite A each Si coordination tetrahedron is surrounded by four Al tetrahedra and vice versa. [82Che2].

LTA.6.3 Absence of zero coordination

In a series of publications from 1975 to 1978 either "zero-coordinated" or "near zero-coordinated" cations were described as existing in the pores of zeolite A. Zero coordination was assumed to exist when the shortest distance from the cation in question to an oxygen atom of the framework was longer by 1.0 Å than the sum of the radii of the ions involved. Near zero-coordination was postulated when the cation-oxygen distances exceeded the sum of the radii by about 0.5 Å. Such results were specifically reported, for dehydrated zeolites with K^+ [75Leu1, 77Fir3], Tl^+ [77Fir2], Rb^+ [76Fir1, 77Fir1], Na^+ [77Sub1], Ag^+ [78Kim1], Eu^{2+} [77Fir1], Ca^{2+} [78Fir1], Sr^{2+} [78Fir1], Cd^{2+} [78McC1]. All these structures were refined in space group $Pm\bar{3}m$. This was an extraordinary claim inasmuch as it disagreed with a large amount of empirical evidence collected over the years which pointed to a relative constancy of measured cation-oxygen distances. That "cations float in space without bonding" [80Smi1] to neighboring anions had previously not been observed. Some of the dehydrated zeolite A crystal structures with zero-coordinated cations were subsequently reinvestigated: Na-zeolite A [80Plu1], K-exchanged zeolite A [79Plu1], Sr-exchanged zeolite A [82Plu1], Ca-exchanged zeolite A [83Plu1], and Rb-exchanged zeolite A [83Plu2]. All of these were described in space group $Fm\bar{3}c$, that is in terms of the superstructure with doubled unit cell constants, as well as in the pseudosymmetric space group $Pm\bar{3}m$. In none of these cases was zero-coordination or near zero-coordination confirmed. The supposed zero-coordinate cations were only artifacts of flawed experiments. The respective cations had unusual coordinations, as can be expected in dehydrated zeolites, but none of the ions were floating without bonding in the pores of the zeolite. In one case (Na) the atom was close to the position described as near zero-coordinated in [77Sub1], but the distances from Na to O were clearly shorter, while in all other cases the alleged zero-coordinated positions of the cations were not found to be occupied at all by electron density in these new refinements. This was true of the new refinements in both, the pseudocells and in the superstructures. The main difference between the old and the new determinations was that by the use of Cu-Kα radiation more significant measurements of diffraction data had been made possible.

Finally it was accepted that zero coordination or near zero coordination does not exist in zeolite A compounds [80Sef1] and that it is only an artifact of the use of incorrect methods. In addition it is clear that in the five cases of the reinvestigated crystal structures space group $Fm\bar{3}c$ is the correct space group for describing these zeolites while in $Pm\bar{3}m$ we get only a pseudosymmetric approximation. The other numerous LTA-type structures published in $Pm\bar{3}m$ await further study.

LTA.6.4 The chemical compositions of silicoaluminate LTA-type compounds

In the early work on silicoaluminate LTA-type crystal structures it was assumed that the ratio of Si/Al in the framework was 1. Later a chemical analysis [72Ril1, 73Yan2]] of small single crystals prepared by the Charnell method [71Cha1] yielded a value of 1.12 which was assumed to be due to the imprecision of the analysis and replaced by the idealized value of 1. That value was used in many subsequent studies. Electron microprobe analyses on six different zeolite A single crystal samples resulted in the conclusion that the ratio Si/Al was at least 1.03, that is there should be 12.2 Si and 11.8 Al in the primitive small unit cell [79Plu1]. Later it was argued [84Sef1] that such deviations from unity were within the limits of experimental error and that therefore the ratio Si/Al was exactly 1. This was supported by a reference to the evidence for strict alternation of Si and Al atoms as shown by the crystallization of zeolite A in space group $Fm\bar{3}c$ and by the fact that ^{29}Si NMR investigations did not indicate the presence of excess silicon [84Sef1]. A new study of single crystals of zeolite A by ^{29}Si NMR yielded a value of the Si/Al ratio of 1.03(1) [85Bla1]. An investigation of the Si/Al ratio by proton inelastic scattering resulted in a value of 1.04(1) [87Han1]. Thus the results of three independent experimental methods indicate that the question of the Si/Al ratios is settled. There is a slight excess of Si in single crystals of zeolite A and a small part of the Al sites must contain Si. This has a consequence for the study of the matter inside of the pores. When there is an excess of Si in the framework the crystals do not have to contain quite as many ions compensating for the charge of the framework. Once one makes the assumption that the ratio of Si/Al is unity, while in fact it is not, one has to find in the pores additional matter, which simply is not there.

Another unresolved problem concerning the chemical compositions of the zeolites A studied so far is that most of the single crystal studies explore the pore filling materials without the benefit of chemical analyses. The chemical compositions are usually deduced from the crystal structure refinements (for one of many examples, see [94Jeo1]). Inasmuch as in the case of X-ray studies the only thing which is really being measured are electron densities, this is a risky undertaking. This was shown in the case of Rb-exchanged zeolite A where a Na-zeolite was exchanged for Rb [83Plu2]. An electron microprobe analysis and the crystal structure refinement showed that the resulting compound had the composition $Ba_{0.6}K_{0.2}Na_{0.4}Rb_{9.9} \cdot Al_{11.4}Si_{12.6}O_{48}$. This means for one that the sodium was not completely exchanged and that secondly potassium and barium impurities were introduced during the cation exchange.

All the discussions of the chemistry of zeolite A presented here relate to single crystal samples. Zeolite A in powder form can be prepared with Si/Al ratios ranging from 1 to 3 [85Jar1, 88Dut1].

LTA.6.5 A warning

The questions regarding the space groups and the chemical compositions of many of the published zeolite A data are experimentally unresolved. Before a user of this chapter accepts all the results presented in tables LTA.2.1 and LTA.2.2 of this chapter he or she should consult the original literature and make up her or his mind about the reliability of the data.

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