LTN

LTN.1 Zeolite framework type code and topology

The designation of the FTC refers to **L**inde **T**ype **N**, a synthetic aluminosilicate with the composition $Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 518.4H_2O$, first synthesized by [68Aca1] and described in [82Fäl1]. The framework structure (Fig. LTN.1.1) can be described by a close packing of *can* ($4^6 6^3 6^2$), *grc* ($4^{12}6^8 8^6$), *hpr* ($4^6 6^2$), *ltn* ($4^2 4^2 4^2 4^1 6^4 6^2 6^2 8^1$), and *toc* ($4^6 6^8$) units as shown in Fig. LTN.1.2. One can view the framework of LTN-type as an intimate intergrowth of KFI and SOD frameworks. This can best be seen in Figs. LTN.1.2a, b, e, g and i, where one can recognize the connections of the *grc* units (KFI) to the *toc* units *via* the *ltn* units in the **a** and **b** directions, and by implication in the **c** direction. The *grc* units are arranged in a diamond-type pattern, analogous to the *toc* units in FAU. They are connected to each other *via* double six-rings (*hpr* units), again as in FAU. Because the *grc* units (called alpha cages in the older literature) are larger than the truncated cuboctahedral *toc* cages, the unit cell constant of the LTN framework is by about 50% larger than for the FAU-type (the space group is the same). However in LTN the space between the large cavities is not empty as in FAU, but is filled completely with parts of the SOD-type framework. The cancrinite type cages (*can* units) and the *ltn* units connect the SOD framework to the *grc* framework, which on its own corresponds to one half of the KFI framework.

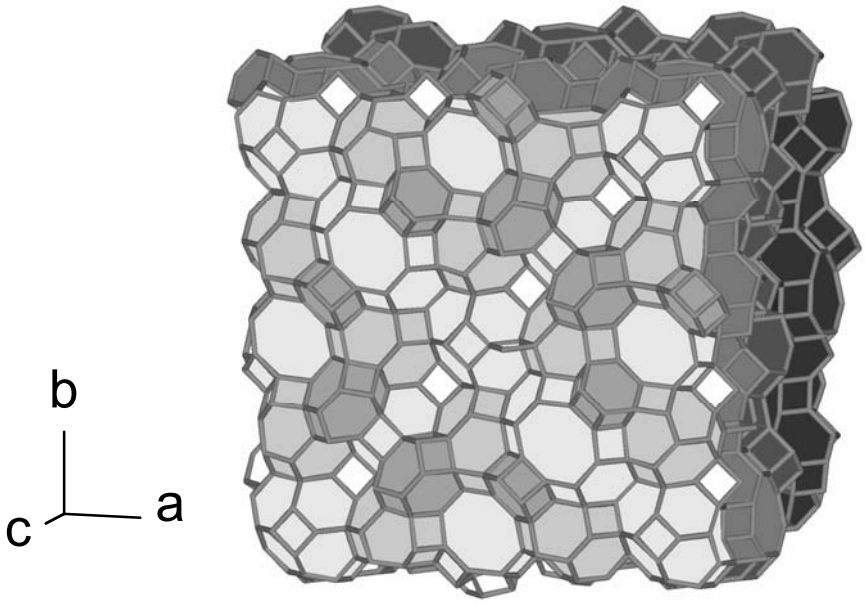
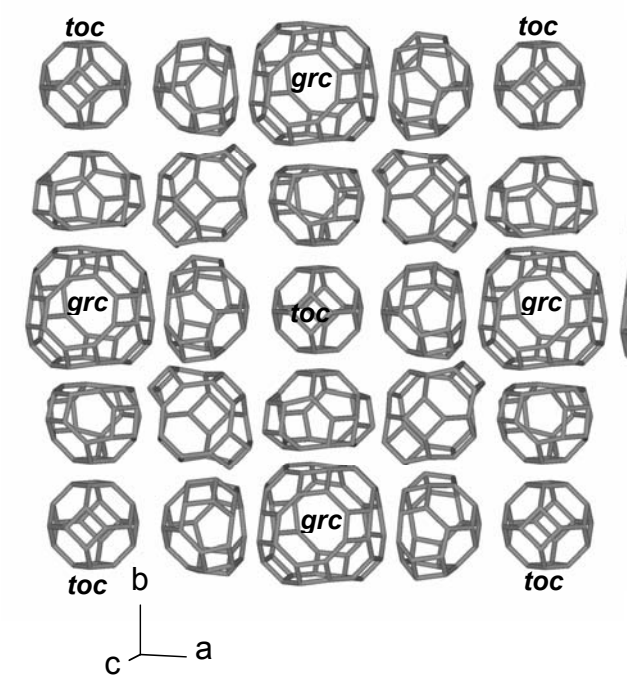
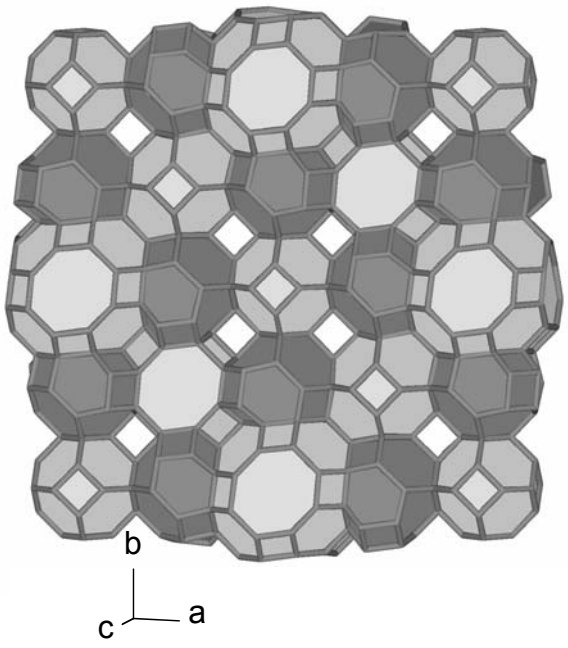


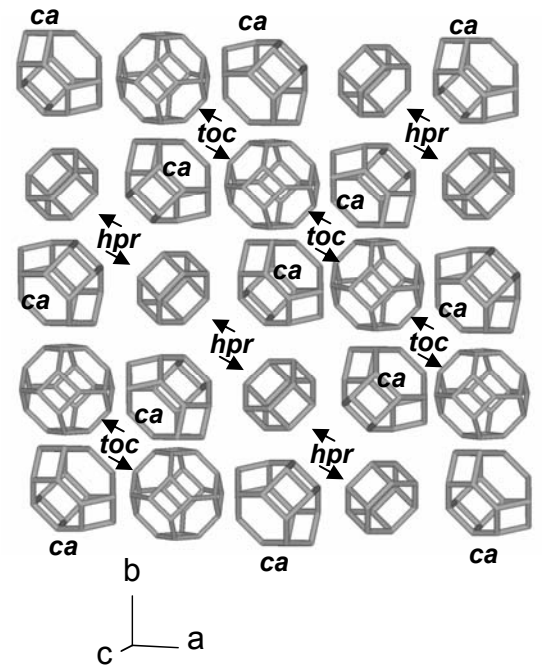
Fig. LTN.1.1. The framework structure of LTN-type compounds in the highest possible topological symmetry $F\,d\,\bar{3}\,m$. View parallel **c** rotated by 10° about **a** and 20° about **b**.



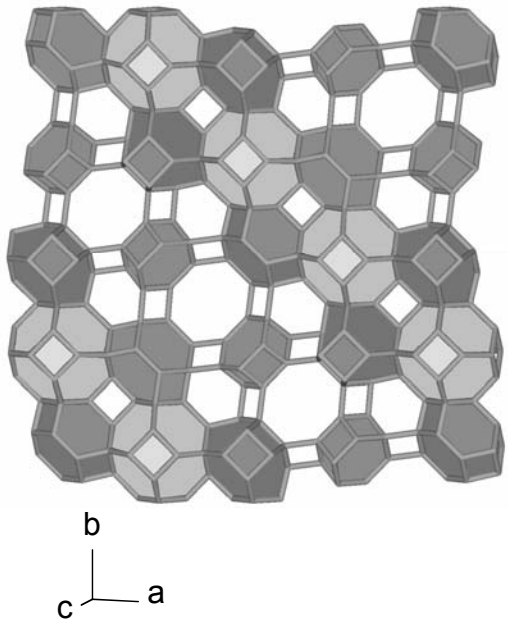
a Linkage of *grc*, *toc*, and *ltn* units in the *xy*-layer at z = 1/8. Units not labeled are *ltn* units.



b The assemblage shown in a) with solid units.

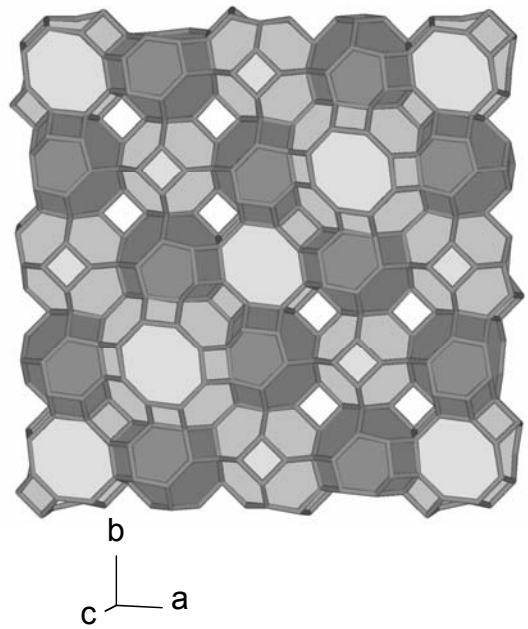


c Linkage of *can*, *toc*, and *hpr* units in the *xy*-layer at z = 2/8.

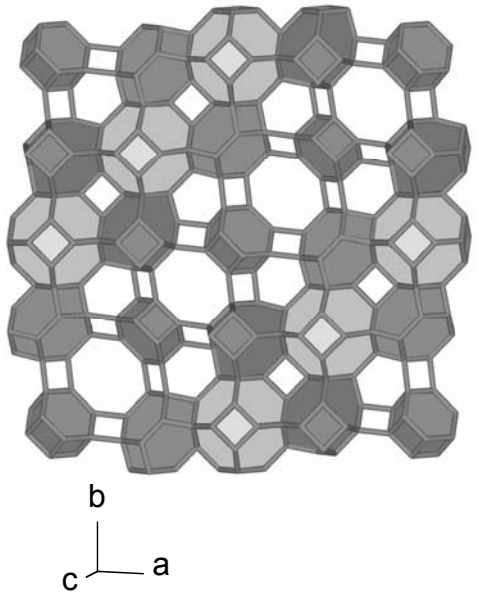


d The assemblage shown in c) with solid units.

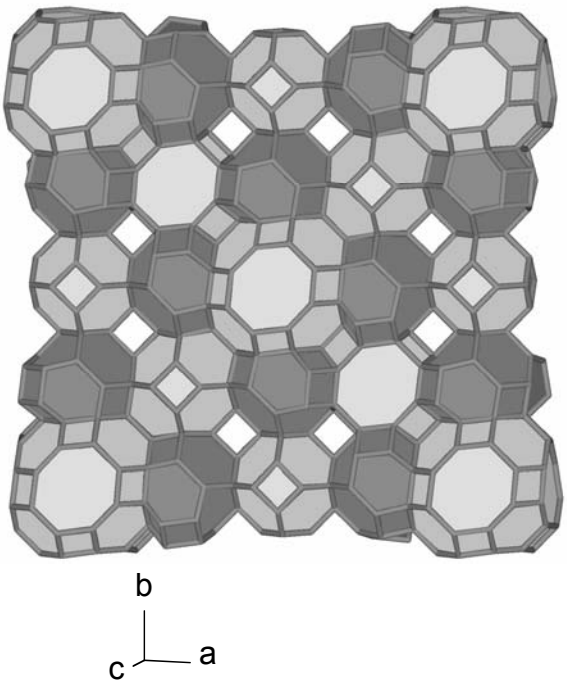
Fig. LTN.1.2. Building scheme of the LTN-type framework. View parallel **c** rotated by 5° about **a** and 10° about **b**.



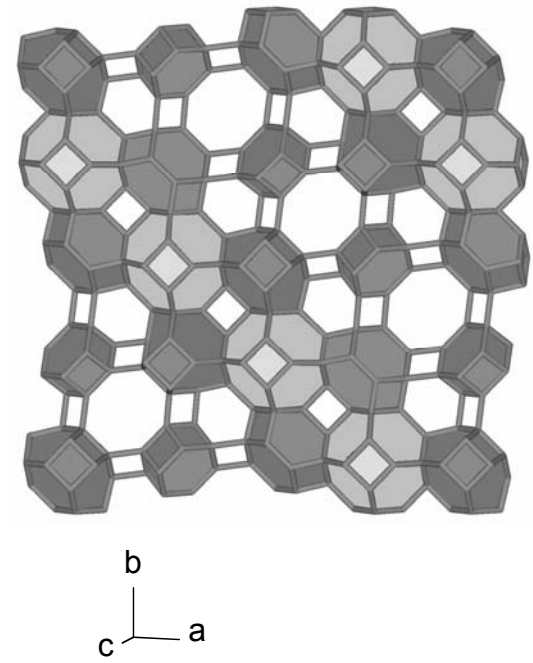
e Linkage of *grc*, *toc*, and *ltn* units in the *xy*-layer at z = 3/8.



f Linkage of *can*, *toc*, and *hpr* units in the *xy*-layer at z = 4/8.

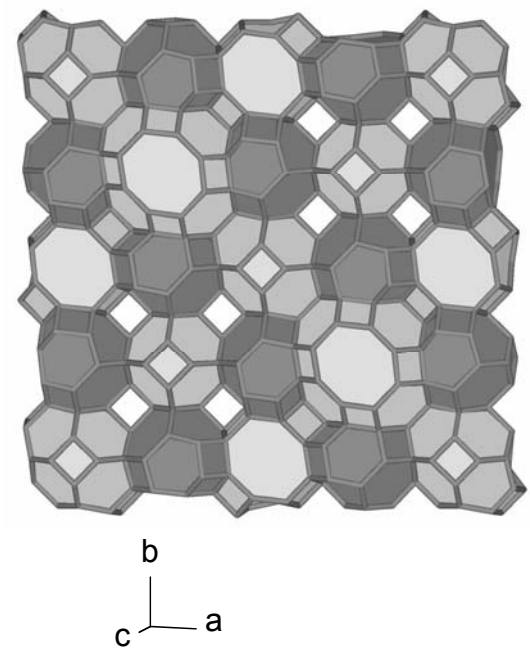


g Linkage of *grc*, *toc*, and *ltn* units in the *xy*-layer at z = 5/8.

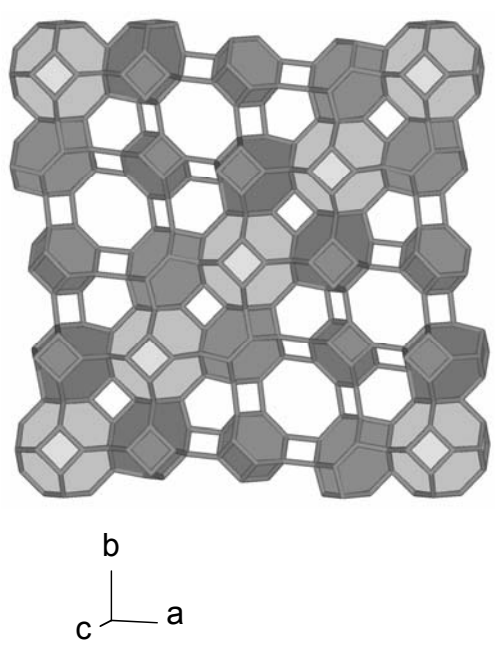


h Linkage of *can*, *toc*, and *hpr* units in the *xy*-layer at z = 6/8.

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



i Linkage of *grc*, *toc*, and *ltn* units in the *xy*-layer at z = 7/8.



j Linkage of *can*, *toc*, and *hpr* units in the *xy*-layer at z = 8/8.

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

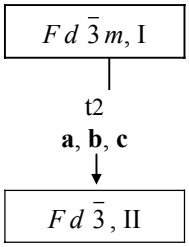


Fig. LTN.1.3 The Bärnighausen tree illustrating the symmetry relationship of the LTN types.

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

LTN-I	LTN-II	LTN-I	LTN-II
$Fd\bar{3}m$	$Fd\bar{3}$	$Fd\bar{3}m$	$Fd\bar{3}$
T1 [192(i), 1]	→ T11 [96(g), 1] → T12 [96(g), 1]	T2 [192(i), 1]	→ T21 [96(g), 1] → T22 [96(g), 1]
T3 [192(i), 1]	→ T31 [96(g), 1] → T32 [96(g), 1]	T4 [192(i), 1]	→ T41 [96(g), 1] → T42 [96(g), 1]

Table LTN.1.1 (continued).

LTN-I $Fd\bar{3}m$		LTN-II $Fd\bar{3}$	LTN-I $Fd\bar{3}m$		LTN-II $Fd\bar{3}$	
O1	[192(i), 1]	→ O1_1 [96(g), 1] → O1_2 [96(g), 1]	O2	→	O21 O22	[96(g), 1] [96(g), 1]
O3	[192(i), 1]	→ O31 [96(g), 1] → O32 [96(g), 1]	O4	→	O4	[96(g), 1]
O5	[96(h), ..2]	→ O5 [96(g), 1]	O6	→	O6	[96(g), 1]
O7	[96(g), ..m]	→ O7 [96(g), 1]	O8	→	O8	[96(g), 1]
O9	[96(g), ..m]	→ O9 [96(g), 1]	O10	→	O10	[96(g), 1]
O11	[96(g), ..m]	→ O11 [96(g), 1]	O12	→	O12	[96(g), 1]
O13	[96(g), ..m]	→ O13 [96(g), 1]				

LTN.2 Compounds and crystal data

Table LTN.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]

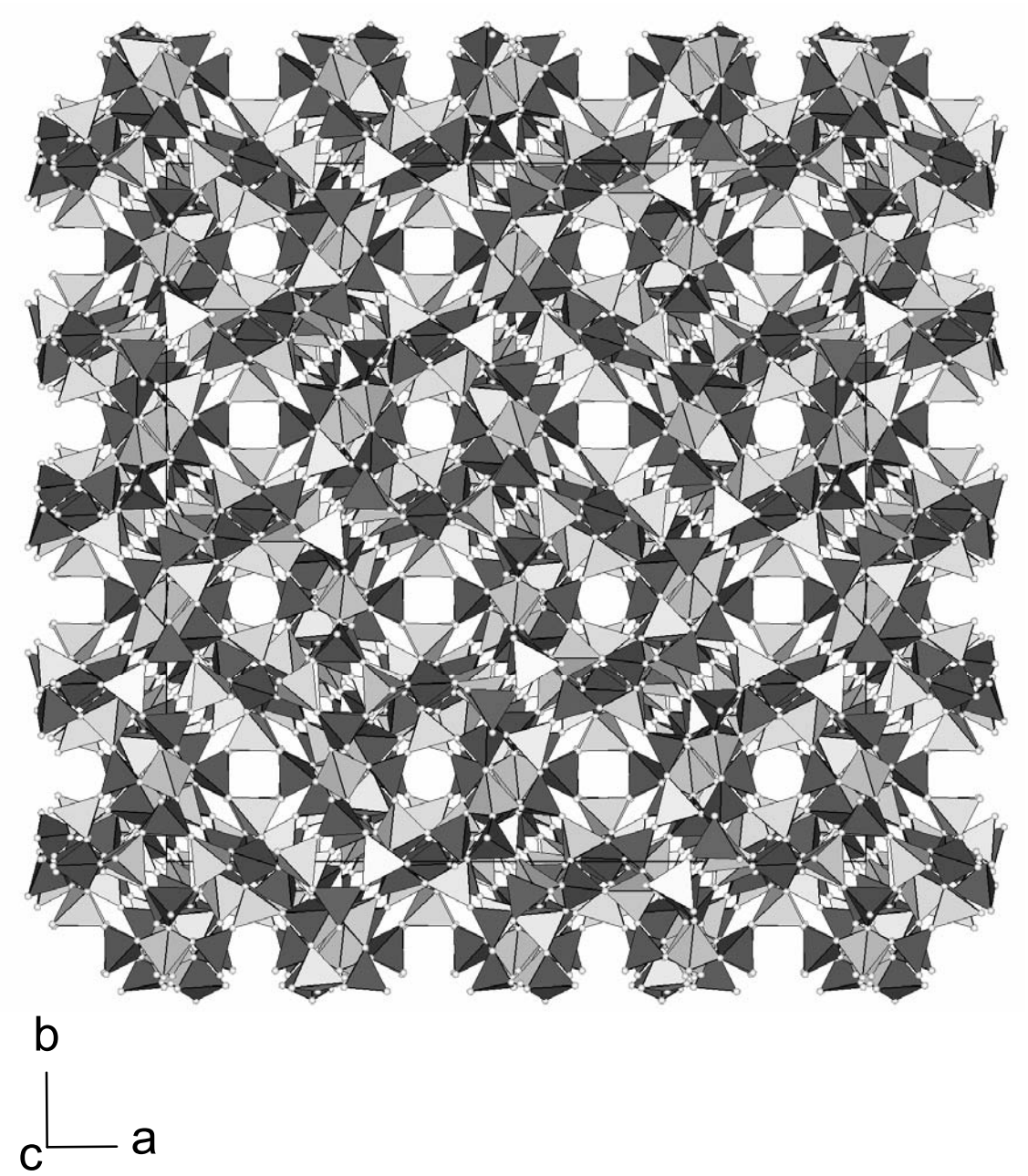
code	chemical composition	compound name	FD	SM	CE	SR	TT	T	REF
LTN-II $Fd\bar{3}$									
LTN1982a01	$Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 518.4H_2O$	N	15.2	S	-	H_2O	-	-	82Fäl1
LTN1983a01	$Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 422.4H_2O$	NaZ-21	15.2	S	-	H_2O	-	-	83She1
LTN1983a02	$Na_{384} \cdot Al_{384}Si_{384}O_{1536}$	NaZ-21	15.2	S	-	-	D	723	83She1

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

code	a [Å]	shift	matrix	coord. trans.	V [Å^3]	T [K]	reference
LTN-II $Fd\bar{3}$							
LTN1982a01	36.93(1)	1/8, 1/8, 1/8	**a**, **b**, **c**	x-1/8, y-1/8, z-1/8	50366	n.s.	82Fäl1
LTN1983a01	36.95(1)	0, 0, ½	**a**, **b**, **c**	x, y, z-½	50448	n.s.	83She1
LTN1983a02	36.95(1)[1])	0, 0, ½	**a**, **b**, **c**	x, y, z-½	50448	n.s.	83She1

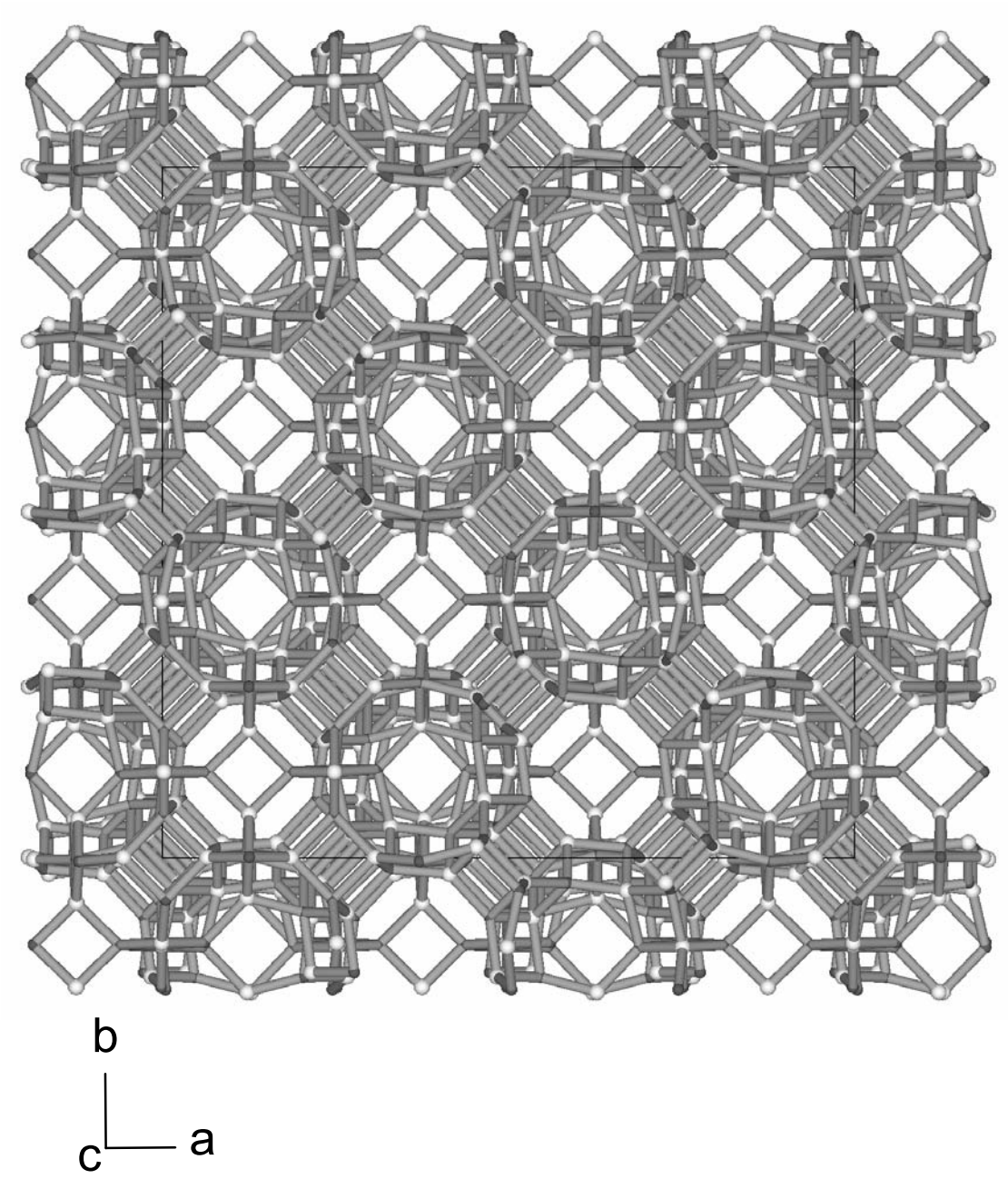
[1]) Lattice constant from LTN1983a01.

LTN.3 Framework structure of the LTN-II compound ($Fd\bar{3}$, IT #203)



a Polyhedral representation. SiO_4-tetrahedra are dark grey, AlO_4-tetrahedra are light grey.

Fig. LTN.3.1 Projections of the LTN-II crystal structure of zeolite NaZ-21, $Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 422.4H_2O$ (LTN1983a01, 83She1). View parallel **c**.



b Ball and stick model corresponding to a).

Fig. LTN.3.1 (continued) Projections of the LTN-II crystal structure of zeolite NaZ-21, $Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 422.4H_2O$ (LTN1983a01, 83She1). View parallel **c**.

Table LTN.3.1 Atomic coordinates and site definitions for LTA-II, (LTN1983a01, 83She1).

atom	*x*	*y*	*z*	*B* [Å^2]	site sym.	Wyck. pos.	no. of atoms
Si11	0.2481(1)	0.0633(1)	0.1252(1)	0.4(1)	1	96(g)	96
Al12	0.0641(1)	0.2484(1)	0.1251(1)	0.5(1)	1	96(g)	96
Si21	0.3103(1)	0.1213(1)	0.2456(1)	0.5(1)	1	96(g)	96
Al22	0.1221(1)	0.3066(1)	0.2484(1)	0.5(1)	1	96(g)	96
Si31	0.1717(1)	0.0154(1)	0.4540(1)	0.4(1)	1	96(g)	96
Al32	0.0164(1)	0.1706(1)	0.4535(1)	0.4(1)	1	96(g)	96
Si41	0.2230(1)	0.0852(1)	0.7858(1)	0.7(1)	1	96(g)	96
Al42	0.0853(1)	0.2273(1)	0.7850(1)	0.7(1)	1	96(g)	96
O11	0.1135(2)	0.0417(2)	0.9616(2)	1.4(3)	1	96(g)	96
O12	0.0417(2)	0.1126(2)	0.9654(2)	1.4(3)	1	96(g)	96
O21	0.3261(2)	0.0877(2)	0.0060(2)	1.8(3)	1	96(g)	96
O22	0.0844(2)	0.3233(2)	0.0046(2)	1.9(3)	1	96(g)	96
O31	0.2160(2)	0.1228(2)	0.4583(2)	1.7(3)	1	96(g)	96
O32	0.1193(2)	0.2197(2)	0.4564(2)	1.7(3)	1	96(g)	96
O4	0.0029(2)	0.3444(2)	0.1556(2)	1.4(3)	1	96(g)	96
O5	0.0037(2)	0.0709(2)	0.4302(2)	1.9(3)	1	96(g)	96
O6	0.4651(2)	0.4635(2)	0.8645(2)	1.6(3)	1	96(g)	96
O7	0.4113(2)	0.4083(2)	0.9857(2)	1.0(3)	1	96(g)	96
O8	0.0308(2)	0.0360(2)	0.8857(2)	1.7(3)	1	96(g)	96
O9	0.0866(2)	0.0894(2)	0.2580(2)	1.3(3)	1	96(g)	96
O10	0.4482(2)	0.4505(2)	0.2083(2)	1.6(3)	1	96(g)	96
O11	0.2639(2)	0.2652(2)	0.6814(2)	1.8(3)	1	96(g)	96
O12	0.0018(2)	0.0067(2)	0.5777(2)	2.0(3)	1	96(g)	96
O13	0.0653(2)	0.0648(2)	0.4661(2)	1.8(3)	1	96(g)	96
Na1	0.042(2)	0.042(2)	-0.458(2)	3.0(1)	. 3 *m*	32(e)	32
Na2	0.2132(2)	0.2132(2)	-0.2868(2)	0.8(2)	. 3 *m*	32(e)	17.9(6)
Na3	0.2337(3)	0.2337(3)	-0.2663(3)	3.0(4)	. 3 *m*	32(e)	8.3(6)
Na4	0.6964(3)	0.6964(3)	0.1964(3)	2.4(1)	. 3 *m*	32(e)	24.6(6)
Na5	0.4184(3)	0.4184(3)	-0.0816(3)	3.0(2)	. 3 *m*	32(e)	17(1)
Na6	0.4322(4)	0.4322(4)	-0.0678(4)	3.5(2)	. 3 *m*	32(e)	7(1)
Na7	0.456(1)	0.456(1)	-0.044(1)	3(1)	. 3 *m*	32(e)	3(1)
Na8	0.1770(2)	0.0742(2)	0.3278(2)	2.1(1)	1	96(g)	44(1)
Na9	0.1895(4)	0.0621(4)	0.3156(4)	2.4(3)	1	96(g)	23(1)
Na10	0.2006(4)	0.0501(4)	0.2983(4)	2.6(3)	1	96(g)	22(2)
Na11	0.1805(1)	0.0705(1)	-0.0677(1)	2.7(1)	1	96(g)	96(2)
Na12	0.2723(2)	0.1111(2)	-0.1379(2)	2.8(1)	1	96(g)	58(2)
Na13	0.2541(6)	0.1110(6)	-0.1385(6)	0.9(2)	1	96(g)	24(1)
Na14	0.2311(2)	0.1084(2)	-0.1360(2)	3.0(5)	1	96(g)	14(2)
OW1	0.2685(6)	0.2685(6)	-0.2315(6)	7.3(5)	. 3 *m*	32(e)	28(2)
OW2	0.370(1)	0.067(1)	-0.334(1)	2.6(7)	1	96(g)	16(2)
OW3	0.3693(8)	0.0758(8)	-0.3252(8)	3.8(7)	1	96(g)	60(2)
OW4	0.3679(4)	0.0911(3)	-0.3172(3)	2.3(4)	1	96(g)	19(2)
OW5	0.0754(7)	0.0754(7)	-0.4246(7)	6(1)	. 3 *m*	32(e)	13(2)
OW6	0.3268(4)	1/8	1/8	5.5(3)	2. .	48(f)	41(1)
OW7	0.1558(5)	0.0849(5)	0.3880(5)	5.4(3)	1	96(g)	58(3)
OW8	0.1471(7)	0.1066(7)	0.3896(7)	4.6(5)	1	96(g)	35(2)
OW9	0.3553(5)	0.0276(5)	-0.1088(5)	6.3(6)	1	96(g)	36(3)
OW10	0.350(3)	0.047(3)	-0.101(3)	3.4(2)	1	96(g)	59(2)
OW11	0.2063(8)	0.0449(9)	-0.3957(8)	3.8(5)	1	96(g)	28(2)

[1]) y-coordinate of Al 12 in [83She1] corrected from 0.0016 to -0.0016

Table LTN.3.2 Selected interatomic distances and angles for LTA-II, NaZ-21, $Na_{384} \cdot Al_{384}Si_{384}O_{1536} \cdot 422.4H_2O$ (LTN1983a01, 83She1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O7	1.608(8)	144.5(5)	Al 12 - O6	1.726(8)	150.7(5)
Si11 - O6	1.620(8)	150.7(5)	Al 12 - O9	1.739(8)	145.9(5)
Si11 - O9	1.620(8)	145.9(5)	Al 12 - O1 1	1.746(8)	141.4(5)
Si11 - O1 2	1.631(8)	138.9(5)	Al 12 - O7	1.746(8)	144.5(5)
mean	1.620	145.0	mean	1.739	145.6
Si21 - O8	1.601(8)	151.8(5)	Al 22 - O8	1.709(8)	151.8(5)
Si21 - O4	1.606(8)	164.2(5)	Al 22 - O2 2	1.725(8)	146.3(5)
Si21 - O1 1	1.624(8)	141.4(5)	Al 22 - O1 2	1.726(8)	138.9(5)
Si21 - O2 1	1.625(8)	145.6(5)	Al 22 - O4	1.740(8)	164.2(5)
mean	1.614	150.8	mean	1.725	150.3
Si31 - O10	1.604(8)	163.4(5)	Al 32 - O10	1.721(8)	163.4(5)
Si31 - O2 2	1.610(8)	146.3(5)	Al 32 - O11	1.724(8)	153.7(5)
Si31 - O11	1.611(8)	153.7(5)	Al 32 - O2 1	1.737(8)	145.6(5)
Si31 - O3 2	1.614(8)	149.8(5)	Al 32 - O3 1	1.740(8)	148.6(5)
mean	1.610	153.3	mean	1.731	152.8
Si41 - O3 1	1.588(8)	148.6(5)	Al 42 - O13	1.723(8)	143.3(5)
Si41 - O12	1.603(8)	140.2(5)	Al 42 - O3 2	1.730(8)	149.8(5)
Si41 - O13	1.605(8)	143.3(5)	Al 42 - O5	1.743(8)	143.5(5)
Si41 - O5	1.612(8)	143.5(5)	Al 42 - O12	1.746(8)	140.2(5)
mean	1.602	143.9	mean	1.736	144.2

LTN.4 Chemical composition

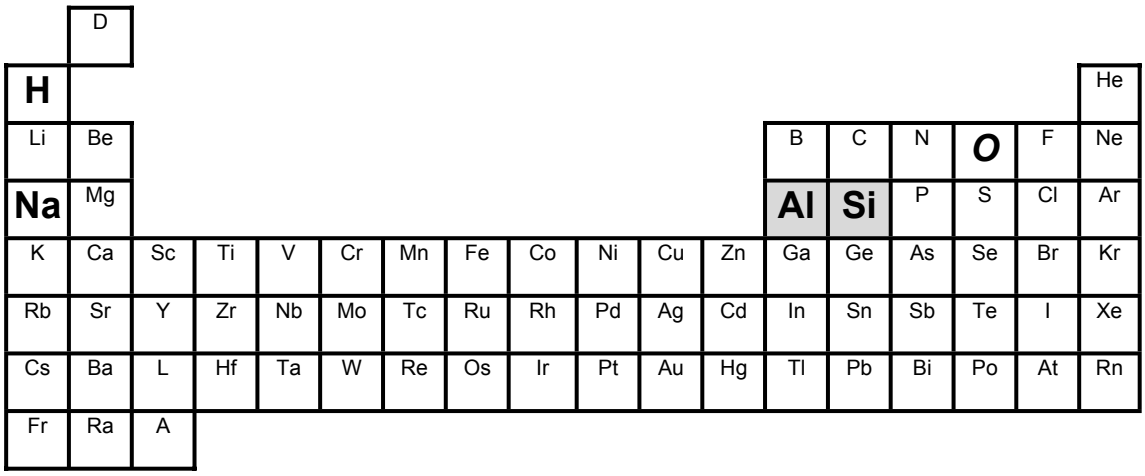


Fig. LTN.4.1 Chemical elements (highlighted) occurring in LTN-type compounds. Framework cations are in grey fields.

LTN.5 Flexibility and apertures

There is insufficient information about LTN to speak about its flexibility.

The eight rings in the *grc* units are effectively blocked by the six rings in the adjoining *ltn* units. Thus, despite its openness, the LTN framework is not easily accessible.

LTN.6 Other Information

Nothing has been reported about useful properties of the LTN-type.

LTN.7 References

68Aca1 Acara, N.A., Kenmore, N.Y.: U.S. Patent 3,414,602 (1968).

82Fäl1 Fälth, L., Andersson, S.: Z. Krist. **160** (1982) 313.

83She1 Shepelev, Yu. F., Butikova, I.K., Smolin, Yu. I., Tarasov, V.I.: Sov. Phys. Dokl. **28** (1983) 826.

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