NES

NES.1 Zeolite framework type and topology

The designation of the FTC refers to the type material NU-87 (**N**ew (ICI, Imperial Chemical Industries) with sequence number **E**ighty-**S**even), first synthesized by [90Cas1]. The crystal structure was solved by [91Sha1] in space group $P\,2_1/c$. The natural counterpart of NU-87, the zeolite mineral gottardiite, was found in the Jurassic dolerites of Mt. Adamson (Victoria Land, Antarctica) and first described by [96Gal1] and [96Alb1]. The framework structure (Fig. NES.1.1) can be described as being built from *bb37* ($5^8 5^8 5^4 5^4 6^8 10^4$) units forming the 10-ring channels (Fig. NES.1.3) parallel **b**. The *bb37* units are linked parallel **c** by chains of alternating *eun* ($5^4 6^2$) and *kdw* (5^4) units, and parallel **a** by pairs of *non* ($4^1 5^4 5^2 5^2$) units as shown in Fig. NES.1.2. In the **a** direction there is another, sinuous, channel limited also by 10-rings, but widening to 12-rings.

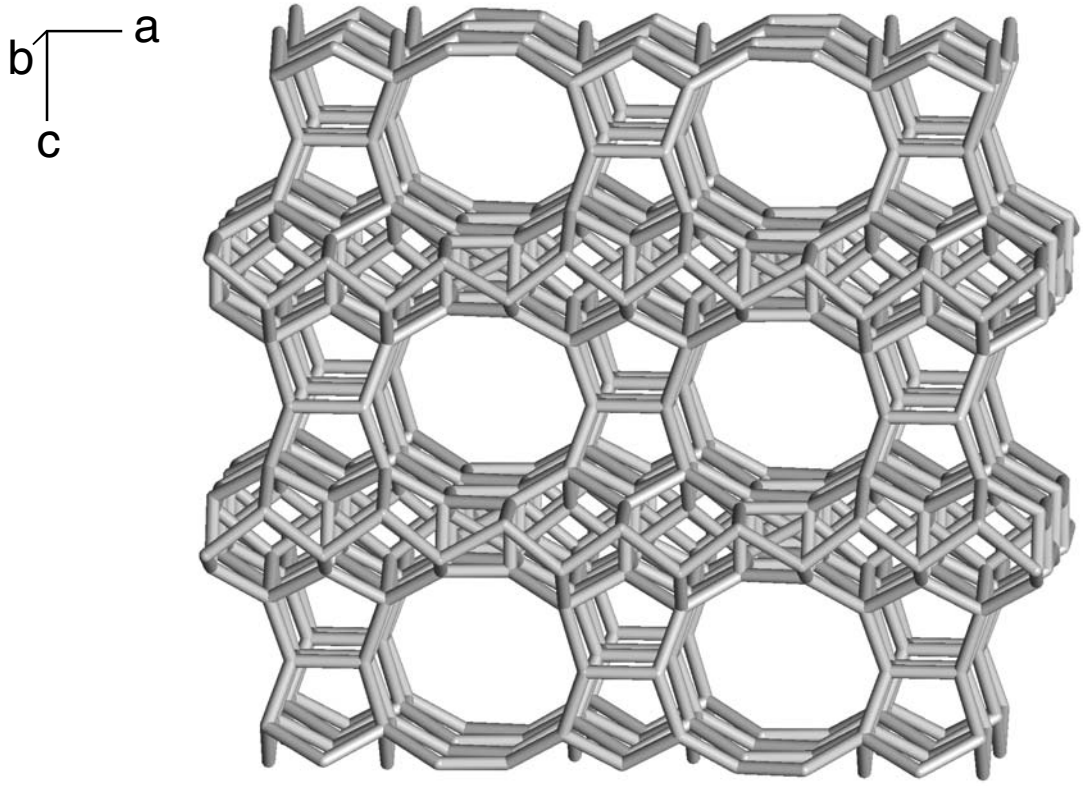
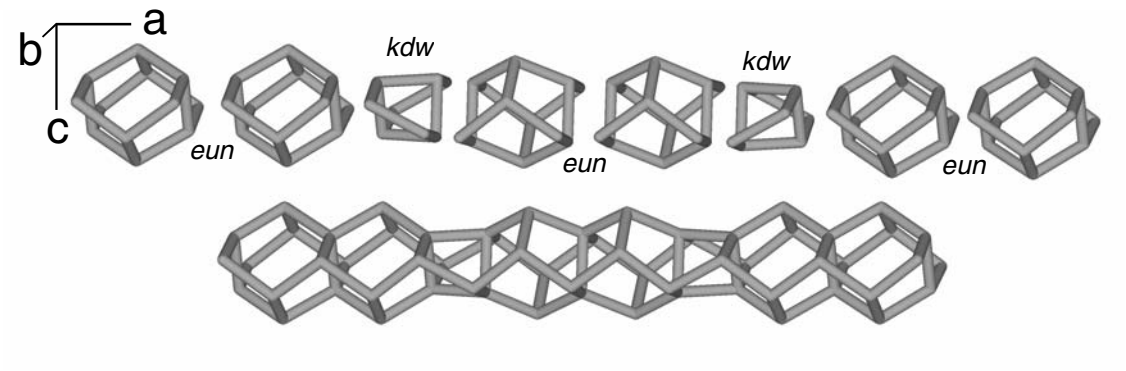
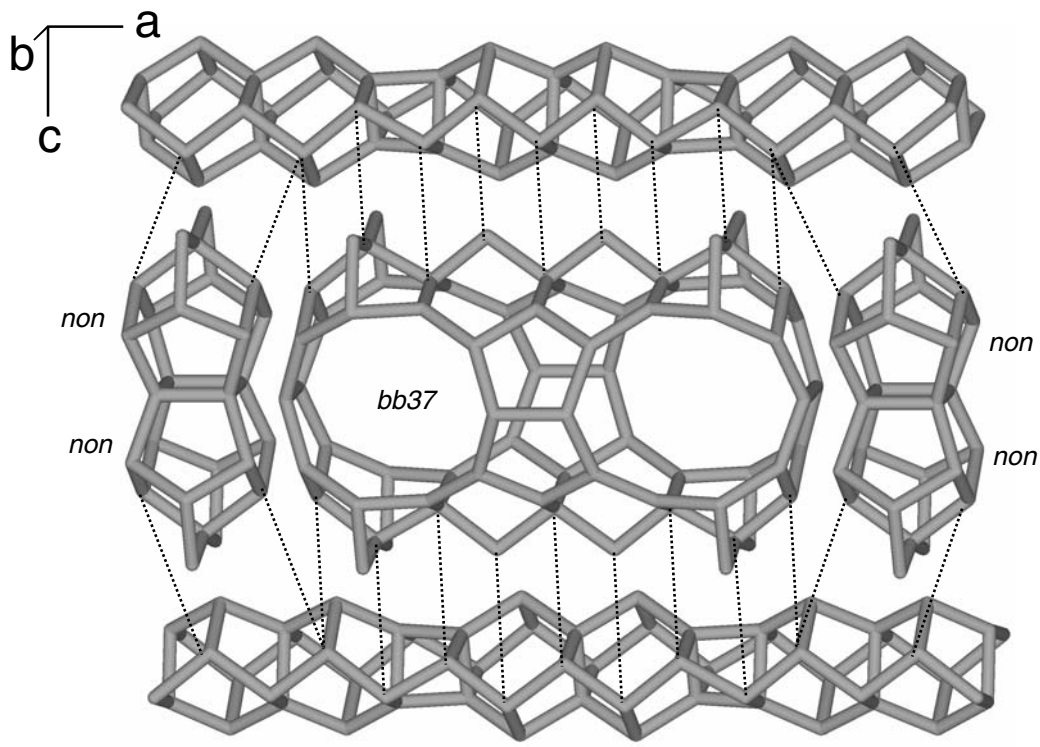


Fig. NES.1.1. The framework structure of NES-type compounds in the highest possible topological symmetry *F m m m.* View parallel **b** rotated by 4° about **a** and 3° about **c**.

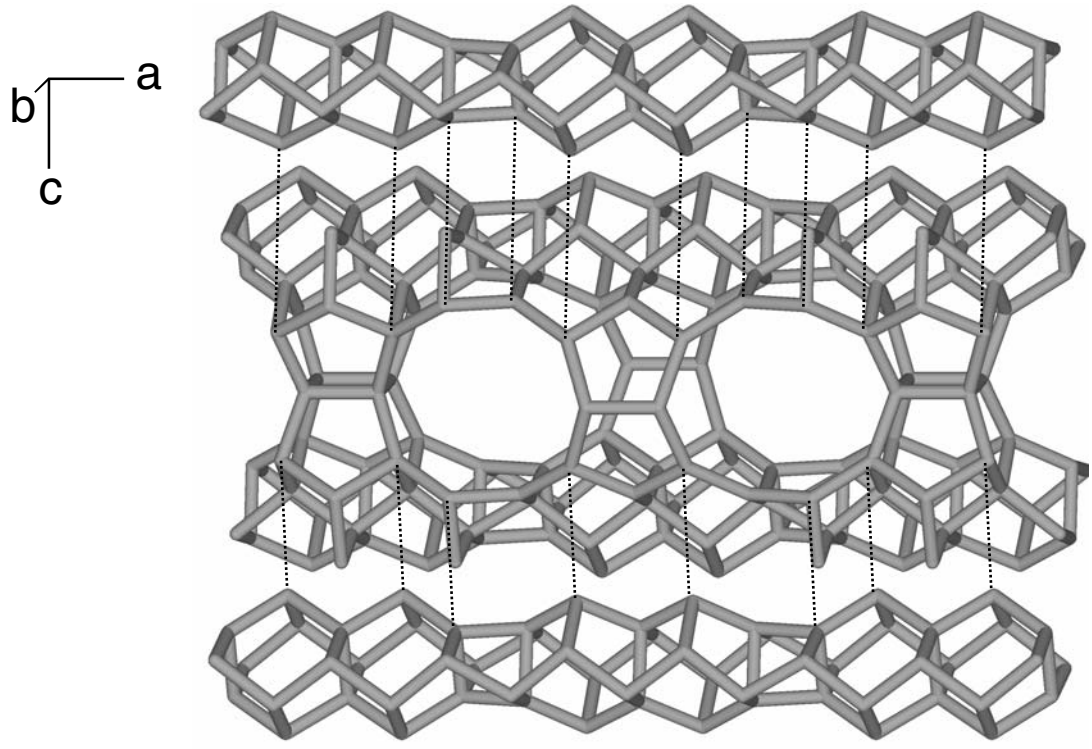


a The linkage of *eun* and *kdw* units forming the chain parallel **a**.

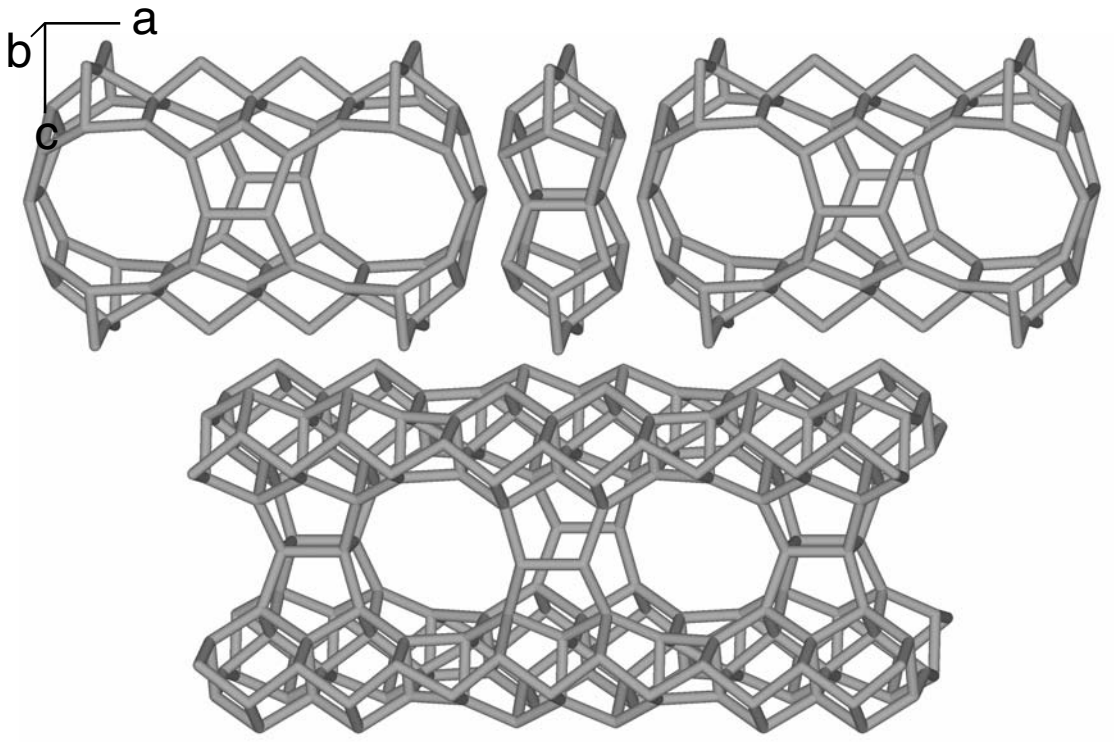


b Linkage of units around the *bb37* unit.

Fig. NES.1.2 Building scheme of NES-type frameworks. View parallel **b** rotated by 3° aboaut **a** and 2° about **c**.



c The assemblage shown in b) extended by two chains.



d The assemblage shown in c) extended by an adjacent sequence of *bb37* and *non* units.

Fig. NES.1.2 (continued). Building scheme of NES-type frameworks. View parallel **b** rotated by 3° aboaut **a** and 2° about **c**.

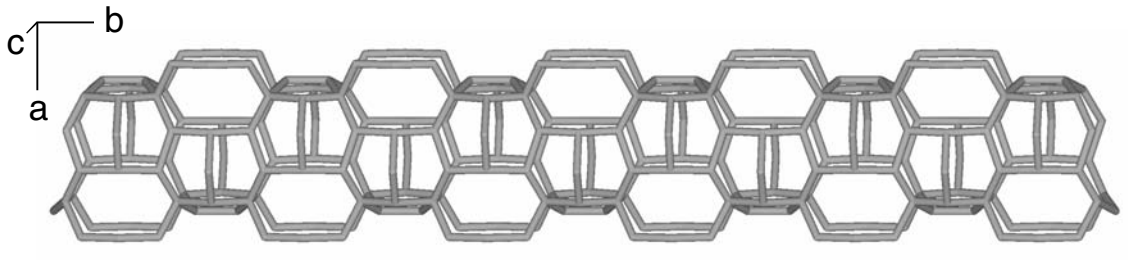


Fig. NES.1.3 The 10-ring channel parallel **b** rotated by 5° about **a** and **b**.

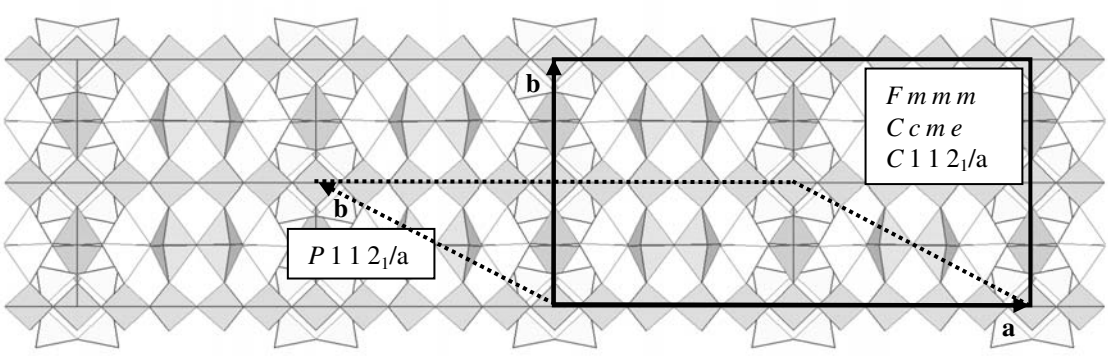


Fig. NES.1.4 Relationship between the two cell settings of the standardized unit cells.

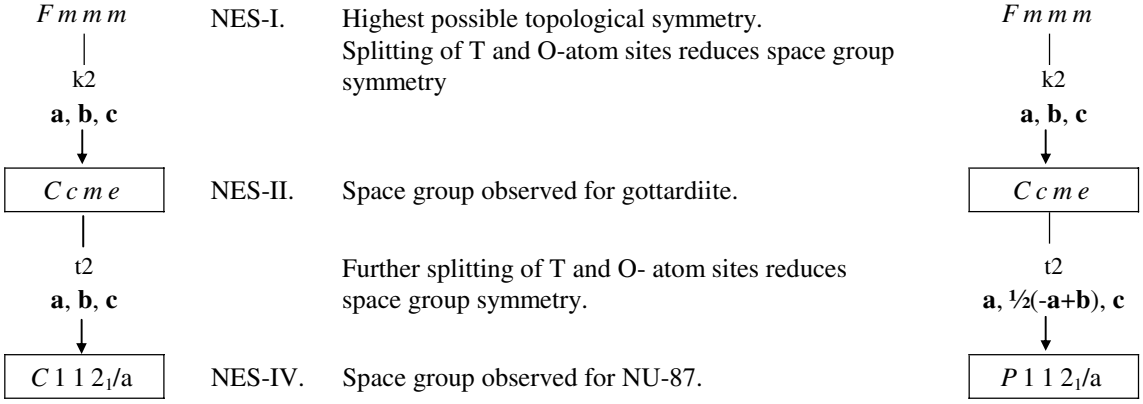


Fig. NES.1.5 The Bärnighausen tree illustrating the symmetry relationship of the NES types.

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

NES-I		NES-II		NES-IV	
F m m m		*C c m e*		*P* 1 1 2_1/*a*	
T1	[32(p), 1]	T11	[16(g), 1]	T11a	[4(e), 1]
				T11b	[4(e), 1]
		T12	[16(g), 1]	T12a	[4(e), 1]
				T12b	[4(e), 1]
T2	[32(p), 1]	T21	[16(g), 1]	T21a	[4(e), 1]
				T21b	[4(e), 1]
		T22	[16(g), 1]	T22a	[4(e), 1]
				T22b	[4(e), 1]
T3	[16(o), . . *m*]	T3	[16(g), 1]	T31	[4(e), 1]
				T32	[4(e), 1]
T4	[16(n), . *m* .]	T41	[8(f), . *m* .]	T41	[4(e), 1]
		T42	[8(f), . *m* .]	T42	[4(e), 1]
T5	[16(n), . *m* .]	T51	[8(f), . *m* .]	T51	[4(e), 1]
		T52	[8(f), . *m* .]	T52	[4(e), 1]
T6	[16(m), *m* . .]	T6	[16(g), 1]	T61	[4(e), 1]
				T62	[4(e), 1]
T7	[8(i), *m m* 2]	T7	[8(f), . *m* .]	T7	[4(e), 1]
O1	[32(p), 1]	O1_1	[16(g), 1]	O1_1a	[4(e), 1]
				O1_1b	[4(e), 1]
		O1_2	[16(g), 1]	O1_2a	[4(e), 1]
				O1_2b	[4(e), 1]
O2	[32(p), 1]	O21	[16(g), 1]	O21a	[4(e), 1]
				O21b	[4(e), 1]
		O22	[16(g), 1]	O22a	[4(e), 1]
				O22b	[4(e), 1]
O3	[32(p), 1]	O31	[16(g), 1]	O31a	[4(e), 1]
				O31b	[4(e), 1]
		O32	[16(g), 1]	O32a	[4(e), 1]
				O32b	[4(e), 1]

Table NES.1.1 (continued). Atomic site relationships of the NES types.

NES-I		NES-II		NES-IV
F m m m		*C c m e*		*P* 1 1 2_1/*a*
O4 [32(p), 1]	→	O41 [16(g), 1]	→	O41a [4(e), 1] O41b [4(e), 1]
		O42 [16(g), 1]	→	O42a [4(e), 1] O42b [4(e), 1]
O5 [32(p), 1]	→	O51 [16(g), 1]	→	O51a [4(e), 1] O51b [4(e), 1]
		O52 [16(g), 1]	→	O52a [4(e), 1] O52b [4(e), 1]
O6 [16(n), . *m* .]	→	O61 [8(f), . *m* .]	→	O61 [4(e), 1]
		O62 [8(f), . *m* .]	→	O62 [4(e), 1]
O7 [16(n), . *m* .]	→	O71 [8(f), . *m* .]	→	O71 [4(e), 1]
		O72 [8(f), . *m* .]	→	O72 [4(e), 1]
O8 [16(m), *m* . .]	→	O8 [16(g), 1]	→	O81 [4(e), 1] O82 [4(e), 1]
O9 [16(l), 2 . .]	→	O91 [8(e), 2 . .]	→	O91 [4(e), 1]
		O92 [8(e), 2 . .]	→	O92 [4(e), 1]
O10 [16(j), . . 2]	→	O10 [16(g), 1]	→	O101 [4(e), 1] O102 [4(e), 1]
O11 [8(h), *m* 2 *m*]	→	O11 [8(d), . 2 .]	→	O11 [4(e), 1]
O12 [8(g), 2 *m m*]	→	O12 [8(f), . *m* .]	→	O12 [4(e), 1]
O13 [8(d), . 2/*m* .]	→	O13 [8(f), . *m* .]	→	O13 [4(e), 1]
O14 [8(c), 2/*m* . .]	→	O14 [8(e), 2 . .]	→	O14 [4(e), 1]

NES.2 Compounds and crystal data

Table NES.2.1 Chemical data.

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

code	chemical composition	M	FD	SM	CE	SR	TT	T	REF
NES-II *C c m e*									
NES1996a01	$Ca_{4.8}K_{0.2}Mg_{3.1}Na_{2.5} \cdot Al_{18.8}Si_{117.2}O_{272} \cdot 93H_2O$	gottardiite	17.4	M	-	H_2O	-	-	96Alb1
NES-IV *C* 1 1 2_1/a , *P* 1 1 2_1/a									
NES1991a01	$Al_2Si_{32}O_{68} \cdot 20H_2O$	NU-87	17.7	S	H	H_2O	C	n.s.	91Sha1

Table NES.2.2 Structural parameters of NES-type compound.

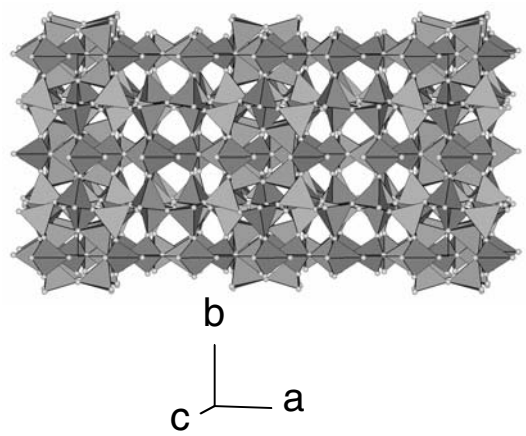
code	*a* [Å]	*b* [Å]	*c* [Å]	γ [°]	*V* [Å^3]	*T* [K]	reference
NES-II *C c m e*							
NES1996a01	25.213(3)	13.698(2)	22.660(2)		7826	n.s.	96Alb1
NES-IV.a *C* 1 1 2_1/a							
NES1991a01	25.092(4)	13.66(1)	22.376(1)	90.37(4)	7671	n.s.	91Sha1
NES-IV.b *P* 1 1 2_1/a							
NES1991a01	25.092(4)	14.324(2)	22.376(1)	151.52(2)	3836	n.s.	91Sha1

Table NES.2.3 Transformation matrices.

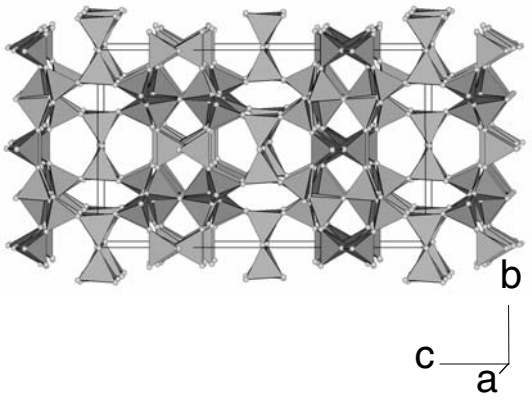
code	shift	matrix	coord. transform.	reference
NES-II *C c m e*				
NES1996a01	0, 0, 0	**b**, **a**, -**c**	*y*, *x*, -*z*	96Alb1
NES-IV.a *C* 1 1 2_1/a				
NES1991a01	0, 0, 0	**c**, 2**a**+**c**, **b**	- ½*x*+*z*, ½*x*, *y*	91Sha1
NES-IV.b *P* 1 1 2_1/a				
NES1991a01	0, 0, 0	**c**, **a**, **b**	*z*, *x*, *y*	91Sha1

NES.3 Framework structures

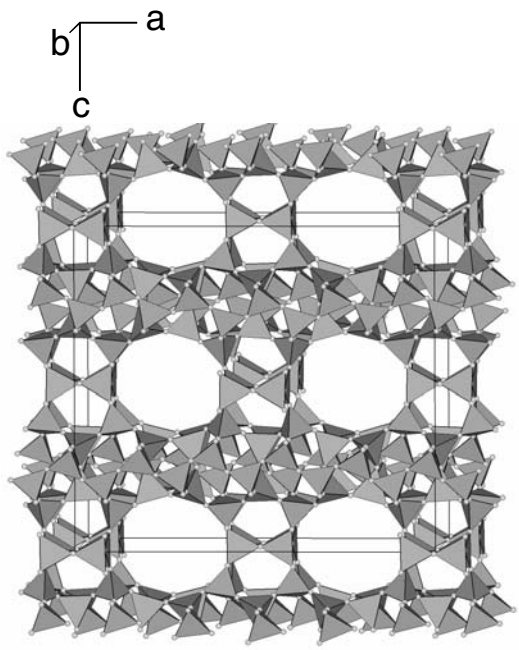
NES.3.1 NES-II compound (*C c m e*, IT #64)



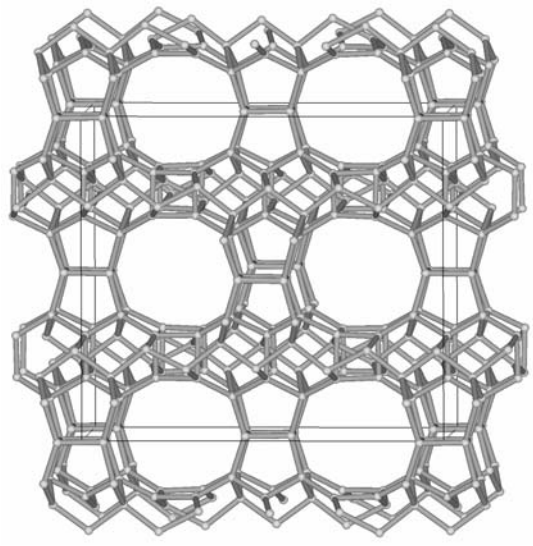
a View parallel **c** rotated by 1° about **a** and **b**.



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



c View parallel **b** rotated by 4° about **a** and **c**.



d Ball and stick model corresponding to c).

Fig. NES.3.1.1 Projections of the NES-II crystal structure of gottardiite, $Ca_{4.8}K_{0.2}Mg_{3.1}Na_{2.5} \cdot Al_{18.8}Si1_{17.2}O_{272} \cdot 93H_2O$ (NES1996a01, 96Alb1).

Table NES.3.1.1 Atomic coordinates and site definitions for NES-II, gottardiite $Ca_{4.8}K_{0.2}Mg_{3.1}Na_{2.5} \cdot Al_{18.8}Si1_{17.2}O_{272} \cdot 93H_2O$ (NES1996a01, 96Alb1).

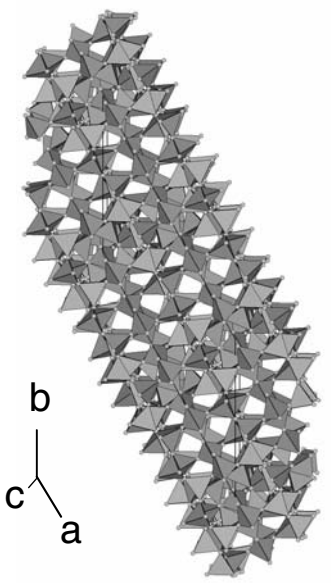
atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)11	0.3111(2)	0.2143(4)	0.8154(2)	1.32	1	16(g)	13.6 / 2.4
(Si,Al)12	0.3052(2)	0.7122(4)	0.3174(2)	1.11	1	16(g)	13.6 / 2.4
(Si,Al)21	0.5978(1)	0.3066(5)	0.8747(2)	1.34	1	16(g)	13.6 / 2.4
(Si,Al)22	0.5951(1)	0.8127(5)	0.3752(2)	1.18	1	16(g)	13.6 / 2.4
(Si,Al)3	0.5634(1)	0.6151(3)	-0.0009(2)	1.53	1	16(g)	13.6 / 2.4
(Si,Al)41	0.3216(2)	0	0.2172(3)	1.47	. *m* .	8(f)	6.8 / 1.2
(Si,Al)42	0.2884(2)	½	0.7204(3)	1.39	. *m* .	8(f)	6.8 / 1.2
(Si,Al)51	0.0804(2)	0	0.8027(3)	1.18	. *m* .	8(f)	6.8 / 1.2
(Si,Al)52	0.1159(3)	½	0.3023(3)	1.34	. *m* .	8(f)	6.8 / 1.2
(Si,Al)6	-0.0023(2)	0.2898(3)	0.1840(2)	1.95	1	16(g)	13.6 / 2.4
(Si,Al)7	-0.0182(2)	0	0.7235(3)	1.68	. *m* .	8(f)	6.8 / 1.2
O1_1	0.0897(7)	0.097(2)	0.841(1)	5.84	1	16(g)	16
O1_2	0.1050(8)	0.584(2)	0.344(1)	6.37	1	16(g)	16
O21	0.1833(6)	0.096(1)	0.6762(6)	2.63	1	16(g)	16
O22	0.1960(6)	0.593(1)	0.1810(6)	2.87	1	16(g)	16
O31	0.1576(5)	0.228(1)	0.8650(7)	2.66	1	16(g)	16
O32	0.1447(5)	0.762(1)	0.3668(6)	2.79	1	16(g)	16
O41	0.0598(5)	0.224(1)	0.6496(7)	3.61	1	16(g)	16
O42	0.0414(5)	0.762(1)	0.1441(8)	5.90	1	16(g)	16
O51	0.0893(6)	0.175(1)	0.9445(6)	3.00	1	16(g)	16
O52	0.0916(6)	0.6627(9)	0.4406(8)	5.34	1	16(g)	16
O61	0.3787(7)	0	0.2501(9)	3.76	. *m* .	8(f)	8
O62	0.3225(6)	½	0.7802(7)	2.53	. *m* .	8(f)	8
O71	0.9225(7)	0	0.746(1)	6.55	. *m* .	8(f)	8
O72	0.9792(6)	½	0.2786(9)	3.92	. *m* .	8(f)	8
O8	0.0080(7)	0.0928(8)	0.3182(5)	3.74	1	16(g)	16
O91	0.6710(6)	¼	¼	1.89	2 . .	8(e)	8
O92	0.6829(6)	¾	¾	2.03	2 . .	8(e)	8
O10	0.2564(5)	0.233(1)	0.6643(5)	3.16	1	16(g)	16
O11	0	0.128(1)	0	3.26	. 2 .	8(d)	8
O12	0.0807(5)	0	-0.005(1)	2.82	. *m* .	8(f)	8
O13	0.2751(6)	0	0.2639(9)	3.11	. *m* .	8(f)	8
O14	-0.005(2)	¼	¼	5.66	2 . .	8(e)	8
OW1	0.386(1)	0	0.001(2)	0.57	. *m* .	8(f)	3.8
OW2	0.183(1)	0	0.570(1)	1.53	. *m* .	8(f)	6.1
OW3	0.263(2)	0	0.004(3)	1.30	. *m* .	8(f)	3.6
OW4	0.081(2)	0	0.596(2)	2.17	. *m* .	8(f)	5.12
OW5	0.281(2)	0.067(4)	0.579(2)	3.03	1	16(g)	9.44
OW6	0.458(2)	0.121(4)	0.981(2)	1.30	1	16(g)	3.84
OW7	0.192(3)	0	0.929(3)	3.67	. *m* .	8(f)	4.56
OW8	0.349(2)	0.151(3)	0.006(3)	2.20	1	16(g)	6.40
OW9	0.390(2)	0	0.897(3)	2.97	. *m* .	8(f)	5.04
OW10	0.268(2)	0.120(4)	0.442(2)	3.13	1	16(g)	8.96
OW11	0.271(3)	0.193(6)	0.527(4)	4.10	1	16(g)	5.76
OW12	0.301(3)	0	0.936(3)	2.97	. *m* .	8(f)	4.08

Table NES.3.1.2 Selected interatomic distances and angles for NES-II, gottardiite $Ca_{4.8}K_{0.2}Mg_{3.1}Na_{2.5} \cdot Al_{18.8}Si1_{17.2}O_{272} \cdot 93H_2O$ (NES1996a01, 96Alb1).

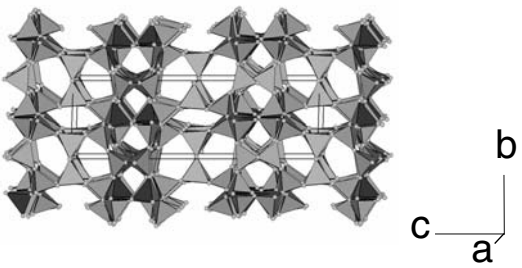
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11 - O10	1.62(1)	144(1)	(Si,Al)12 - O21	1.63(2)	139(1)
(Si,Al)11 - O91	1.63(1)	148(1)	(Si,Al)12 - O10	1.63(1)	144(1)
(Si,Al)11 - O32	1.65(1)	137(1)	(Si,Al)12 - O92	1.64(1)	159(1)
(Si,Al)11 - O22	1.68(2)	142(1)	(Si,Al)12 - O31	1.65(2)	141(1)
mean	1.65	143	mean	1.64	146
(Si,Al)21 - O1_1	1.55(3)	177(2)	(Si,Al)22 - O52	1.52(2)	155(1)
(Si,Al)21 - O41	1.58(2)	141(1)	(Si,Al)22 - O42	1.58(2)	161(1)
(Si,Al)21 - O31	1.60(1)	141(1)	(Si,Al)22 - O1_2	1.60(3)	167(2)
(Si,Al)21 - O51	1.62(1)	151(1)	(Si,Al)22 - O32	1.63(1)	137(1)
mean	1.59	153	mean	1.58	155
(Si,Al)3 - O11	1.61(1)	168(1)	(Si,Al)41 - O13	1.58(2)	150(1)
(Si,Al)3 - O51	1.63(2)	151(1)	(Si,Al)41 - O21	1.61(2)	139(1)
(Si,Al)3 - O1_2	1.64(1)	167(2)	(Si,Al)41 - O21	1.61(2)	139(1)
(Si,Al)3 - O52	1.67(2)	155(1)	(Si,Al)41 - O61	1.62(2)	158(1)
mean	1.64	160	mean	1.61	147
(Si,Al)42 - O22	1.60(2)	142(1)	(Si,Al)51 - O61	1.58(2)	158(1)
(Si,Al)42 - O22	1.60(2)	142(1)	(Si,Al)51 - O11	1.60(3)	177(2)
(Si,Al)42 - O62	1.61(2)	140(1)	(Si,Al)51 - O11	1.60(3)	177(2)
(Si,Al)42 - O13	1.64(2)	150(1)	(Si,Al)51 - O72	1.60(2)	148(1)
mean	1.61	144	mean	1.59	165
(Si,Al)52 - O1_2	1.52(3)	167(2)	(Si,Al)6 - O42	1.59(2)	161(1)
(Si,Al)52 - O1_2	1.52(3)	167(2)	(Si,Al)6 - O14	1.59(1)	175(3)
(Si,Al)52 - O71	1.60(2)	146(1)	(Si,Al)6 - O8	1.63(1)	142(1)
(Si,Al)52 - O62	1.63(2)	140(1)	(Si,Al)6 - O41	1.66(1)	141(1)
Mean	1.57	155	mean	1.62	155
(Si,Al)7 - O71	1.58(2)	146(1)			
(Si,Al)7 - O72	1.59(2)	148(1)			
(Si,Al)7 - O8	1.61(1)	142(1)			
(Si,Al)7 - O8	1.61(1)	142(1)			
mean	1.60	145			

NES.3.2 NES-IV compound ($C\,1\,1\,2_1/a$ [$P\,1\,1\,2_1/a$], IT #14)

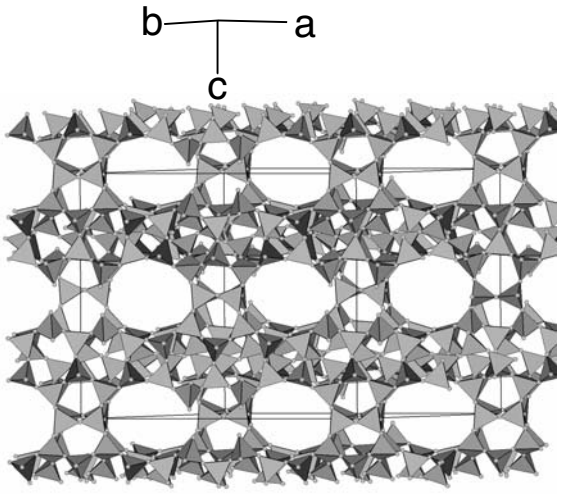
The projections of the framework structure of NU-87 (NES-IV.a) in the C-centered setting are essentially identical to Fig. NES.3.1.1.



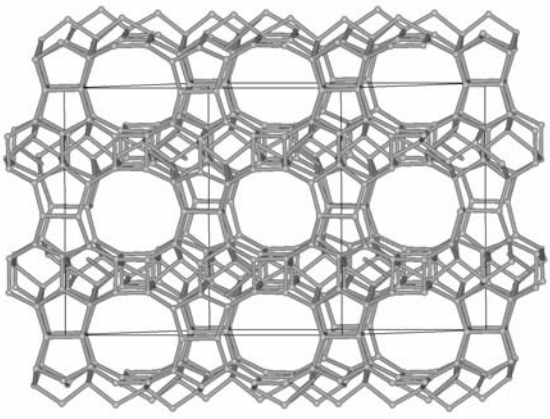
a View parallel **c** rotated by 1° about **b** and **b**×**c**.



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



c View parallel **a**×**c** rotated by 4° about **a** and **c**.



d Ball and stick model corresponding to c).

Fig. NES.3.2.1 Projections of the NES-IV crystal structure of NU-87 $Al_2Si_{32}O_{68} \cdot 20H_2O$ (NES1991a01, 91Sha1) in the primitive setting.

Table NES.3.2.1 Atomic coordinates and site definitions for NES-IV.a, NU-87 $Al_2Si_{32}O_{68} \cdot 20H_2O$ (NES1991a01, 91Sha1) in the **c**-centered setting.

atom full name	*x*	*y*	*z*	site symmetry	Wyckoff position	no. of atoms in unit cell
NES-IV.a	***C* 1 1 2_1/a**					
(Si,Al)11a	0.307(1)	0.197(1)	0.8184(6)	1	8(e)	7.52 / 0.48
(Si,Al)11b	0.308(1)	0.775(1)	0.8163(7)	1	8(e)	7.52 / 0.48
(Si,Al)12a	0.308(1)	0.728(1)	0.3178(7)	1	8(e)	7.52 / 0.48
(Si,Al)12b	0.307(1)	0.302(1)	0.3162(7)	1	8(e)	7.52 / 0.48
(Si,Al)21a	0.598(1)	0.294(1)	0.8720(6)	1	8(e)	7.52 / 0.48
(Si,Al)21b	0.596(1)	0.667(1)	0.8701(6)	1	8(e)	7.52 / 0.48
(Si,Al)22a	0.597(1)	0.827(1)	0.3763(6)	1	8(e)	7.52 / 0.48
(Si,Al)22b	0.597(1)	0.210(1)	0.3800(7)	1	8(e)	7.52 / 0.48
(Si,Al)31	0.564(1)	0.614(1)	0.0010(6)	1	8(e)	7.52 / 0.48
(Si,Al)32	0.565(1)	0.387(1)	-0.0039(6)	1	8(e)	7.52 / 0.48
(Si,Al)41	0.290(1)	0.017(1)	0.2154(6)	1	8(e)	7.52 / 0.48
(Si,Al)42	0.319(1)	0.485(1)	0.7175(6)	1	8(e)	7.52 / 0.48
(Si,Al)51	0.113(1)	-0.019(1)	0.7969(6)	1	8(e)	7.52 / 0.48
(Si,Al)52	0.082(1)	0.517(1)	0.3059(6)	1	8(e)	7.52 / 0.48
(Si,Al)61	0.004(1)	0.320(1)	0.1717(6)	1	8(e)	7.52 / 0.48
(Si,Al)62	0.002(1)	0.736(1)	0.1970(5)	1	8(e)	7.52 / 0.48
(Si,Al)7	0.014(1)	-0.014(1)	0.7218(5)	1	8(e)	7.52 / 0.48
O1_1a	0.107(2)	0.060(2)	0.848(1)	1	8(e)	8
O1_1b	0.099(2)	0.878(2)	0.8239(9)	1	8(e)	8
O1_2a	0.086(2)	0.620(1)	0.337(1)	1	8(e)	8
O1_2b	0.095(2)	0.436(2)	0.354(1)	1	8(e)	8
O21a	0.198(2)	0.081(1)	0.680(1)	1	8(e)	8
O21b	0.197(2)	0.889(1)	0.676(1)	1	8(e)	8
O22a	0.184(2)	0.610(2)	0.176(1)	1	8(e)	8
O22b	0.186(2)	0.419(2)	0.178(1)	1	8(e)	8
O31a	0.148(2)	0.233(2)	0.863(1)	1	8(e)	8
O31b	0.151(2)	0.733(2)	0.866(1)	1	8(e)	8
O32a	0.155(3)	0.754(2)	0.367(1)	1	8(e)	8
O32b	0.154(3)	0.282(2)	0.362(1)	1	8(e)	8
O41a	0.048(2)	0.224(2)	0.641(1)	1	8(e)	8
O41b	0.048(3)	0.711(2)	0.668(1)	1	8(e)	8
O42a	0.052(2)	0.767(2)	0.159(1)	1	8(e)	8
O42b	0.055(2)	0.294(2)	0.133(1)	1	8(e)	8
O51a	0.081(2)	0.162(2)	0.9389(7)	1	8(e)	8
O51b	0.093(3)	0.841(2)	0.9374(8)	1	8(e)	8
O52a	0.094(2)	0.675(2)	0.4477(8)	1	8(e)	8
O52b	0.086(2)	0.325(2)	0.4470(7)	1	8(e)	8
O61	0.326(3)	0.018(2)	0.2734(8)	1	8(e)	8
O62	0.373(3)	0.487(2)	0.7544(8)	1	8(e)	8
O71	0.975(3)	-0.001(2)	0.7773(8)	1	8(e)	8
O72	0.926(3)	0.497(2)	0.2429(8)	1	8(e)	8
O81	-0.007(2)	0.121(1)	0.306(1)	1	8(e)	8
O82	-0.001(2)	0.935(1)	0.3266(8)	1	8(e)	8
O91	0.680(3)	0.260(2)	0.2521(9)	1	8(e)	8
O92	0.676(3)	0.737(2)	0.7501(8)	1	8(e)	8
O101	0.248(3)	0.245(2)	0.667(1)	1	8(e)	8
O102	0.247(3)	0.722(2)	0.663(1)	1	8(e)	8

Table NES.3.2.1 (continued)

atom full name	x	y	z	site symmetry	Wyckoff position	no. of atoms in unit cell
O11	0.000(2)	0.121(2)	0.009(1)	1	8(e)	8
O12	0.082(1)	0.000(1)	0.003(1)	1	8(e)	8
O13	0.230(3)	0.018(2)	0.2360(9)	1	8(e)	8
O14	0.009(3)	0.275(2)	0.2367(7)	1	8(e)	8
OW1	0.452(6)	0.116(4)	0.037(3)	1	8(e)	8
OW2	0.722(7)	0.195(5)	0.016(6)	1	8(e)	8
OW3	0.228(7)	0.040(5)	0.044(3)	1	8(e)	8
OW4	0.328(8)	-0.015(5)	0.037(2)	1	8(e)	8
OW5	0.60(1)	0.01(1)	0.065(4)	1	8(e)	8

Table NES.3.2.2 Atomic coordinates and site definitions for NES-IV.b, NU-87 $Al_2Si_{32}O_{68} \cdot 20H_2O$ (NES1991a01, 91Sha1) in the primitive setting.

atom full name	*x*	*y*	*z*	site symmetry	Wyckoff position	no. of atoms in unit cell
NES-IV.b	***P* 1 1 2_1/a**					
(Si,Al)11a	0.504(1)	0.394(2)	0.8184(6)	1	4(e)	3.76 / 0.24
(Si,Al)11b	0.083(1)	0.549(2)	0.8163(7)	1	4(e)	3.76 / 0.24
(Si,Al)12a	0.036(1)	0.456(2)	0.3178(7)	1	4(e)	3.76 / 0.24
(Si,Al)12b	0.609(1)	0.604(2)	0.3162(7)	1	4(e)	3.76 / 0.24
(Si,Al)21a	0.892(1)	0.588(2)	0.8720(6)	1	4(e)	3.76 / 0.24
(Si,Al)21b	0.263(1)	0.334(2)	0.8701(6)	1	4(e)	3.76 / 0.24
(Si,Al)22a	0.424(1)	0.654(2)	0.3763(6)	1.	4(e)	3.76 / 0.24
(Si,Al)22b	0.808(1)	0.421(2)	0.3800(7)	1.	4(e)	3.76 / 0.24
(Si,Al)31	0.307(1)	0.033(2)	0.2154(6)	1	4(e)	3.76 / 0.24
(Si,Al)32	0.803(1)	-0.031(2)	0.7175(6)	1	4(e)	3.76 / 0.24
(Si,Al)41	0.094(1)	-0.038(2)	0.7969(6)	1	4(e)	3.76 / 0.24
(Si,Al)42	0.600(1)	0.035(2)	0.3059(6)	1	4(e)	3.76 / 0.24
(Si,Al)51	0.178(1)	0.228(2)	0.0010(6)	1	4(e)	3.76 / 0.24
(Si,Al)52	0.952(1)	0.774(2)	0.0039(6)	1	4(e)	3.76 / 0.24
(Si,Al)61	0.324(1)	0.640(2)	0.1717(6)	1	4(e)	3.76 / 0.24
(Si,Al)62	0.738(1)	0.473(2)	0.1970(5)	1	4(e)	3.76 / 0.24
(Si,Al)7	0.000(1)	-0.028(2)	0.7218(5)	1	4(e)	3.76 / 0.24
O1_1a	0.167(2)	0.120(3)	0.848(1)	2	4(e)	4
O1_1b	-0.023(1)	0.756(3)	0.8239(9)	2	4(e)	4
O1_2a	0.706(2)	0.240(2)	0.337(1)	2	4(e)	4
O1_2b	0.531(2)	0.873(3)	0.354(1)	2	4(e)	4
O21a	0.279(2)	0.163(2)	0.680(1)	2	4(e)	4
O21b	0.086(2)	0.777(2)	0.676(1)	2	4(e)	4
O22a	0.793(2)	0.219(3)	0.176(1)	2	4(e)	4
O22b	0.605(2)	0.838(3)	0.178(1)	2	4(e)	4
O31a	0.381(2)	0.467(3)	0.863(1)	2	4(e)	4
O31b	0.884(2)	0.465(3)	0.866(1)	2	4(e)	4
O32a	0.909(2)	0.508(4)	0.367(1)	2	4(e)	4
O32b	0.435(2)	0.563(4)	0.362(1)	2	4(e)	4
O41a	0.272(1)	0.447(3)	0.641(1)	2	4(e)	4
O41b	0.759(2)	0.421(4)	0.668(1)	2	4(e)	4
O42a	0.818(2)	0.533(3)	0.159(1)	2	4(e)	4
O42b	0.349(2)	0.588(3)	0.133(1)	2	4(e)	4

Table NES.3.2.2 (continued)

atom full name	*x*	*y*	*z*	site symmetry	Wyckoff position	no. of atoms in unit cell
O51a	0.243(2)	0.325(3)	0.9389(7)	2	4(e)	4
O51b	0.934(2)	0.682(4)	0.9374(8)	2	4(e)	4
O52a	0.769(2)	0.350(3)	0.4477(8)	2	4(e)	4
O52b	0.411(2)	0.651(3)	0.4470(7)	2	4(e)	4
O61	0.345(2)	0.037(5)	0.2734(8)	2	4(e)	4
O62	0.860(2)	-0.026(5)	0.7544(8)	2	4(e)	4
O71	0.974(2)	-0.002(4)	0.7773(8)	2	4(e)	4
O72	0.423(2)	-0.006(4)[1])	0.2429(8)	2	4(e)	4
O81	0.114(2)	0.242(2)	0.306(1)	2	4(e)	4
O82	0.934(2)	0.870(2)	0.3266(8)	2	4(e)	4
O91	0.940(2)	0.521(5)	0.2521(9)	2	4(e)	4
O92	0.413(2)	0.474(5)	0.7501(8)	2	4(e)	4
O101	0.494(2)	0.491(4)	0.667(1)	2	4(e)	4
O102	-0.031(2)	0.445(4)	0.663(1)	2	4(e)	4
O11	0.121(2)	0.242(3)	0.009(1)	2	4(e)	4
O12	0.083(1)	0.001(2)	0.003(1)	2	4(e)	4
O13	0.248(2)	0.036(5)	0.2360(9)	2	4(e)	4
O14	0.284(2)	0.550(4)	0.2367(7)	2	4(e)	4
OW1	0.568(5)	0.233(8)	0.037(3)	2	4(e)	4
OW2	0.917(5)	0.39(1)	0.016(6)	2	4(e)	4
OW3	0.268(5)	0.08(1)	0.044(3)	2	4(e)	4
OW4	0.313(6)	-0.03(1)	0.037(2)	2	4(e)	4
OW5	0.61(1)	0.01(2)	0.065(4)	2	4(e)	4

[1]) The coordinate was corrected from 0.006 to -0.006.

Table NES.3.2.3 Selected interatomic distances and angles for NES-IV.a, NU-87 $Al_2Si_{32}O_{68} \cdot 20H_2O$ (NES1991a01, 91Sha1) in the **c**-centered setting.

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)11a - O32a	1.59(2)	146(1)	(Si,Al)11b - O32b	1.60(2)	149(1)
(Si,Al)11a - O22b	1.60(2)	143(2)	(Si,Al)11b - O101	1.60(1)	151(2)
(Si,Al)11a - O102	1.61(1)	147(2)	(Si,Al)11b - O22a	1.61(3)	138(2)
(Si,Al)11a - O91	1.63(3)	157(1)	(Si,Al)11b - O91	1.63(3)	157(1)
mean	1.61	148	mean	1.61	149
(Si,Al)12a - O102	1.59(2)	147(2)	(Si,Al)12b - O101	1.58(1)	151(2)
(Si,Al)12a - O31a	1.59(2)	145(2)	(Si,Al)12b - O31b	1.60(2)	140(2)
(Si,Al)12a - O21b	1.60(2)	141(2)	(Si,Al)12b - O21a	1.60(2)	146(2)
(Si,Al)12a - O92	1.64(3)	151(1)	(Si,Al)12b - O92	1.63(3)	151(1)
mean	1.61	146	mean	1.60	147
(Si,Al)21a - O1_1b	1.57(2)	157(1)	(Si,Al)21b - O1_1a	1.57(2)	152(2)
(Si,Al)21a - O41a	1.59(2)	160(2)	(Si,Al)21b - O31a	1.58(2)	145(2)
(Si,Al)21a - O31b	1.59(2)	140(2)	(Si,Al)21b - O41b	1.58(2)	171(2)
(Si,Al)21a - O51b	1.60(2)	159(1)	(Si,Al)21b - O51a	1.59(2)	158(2)
mean	1.59	154	mean	1.58	157

Table NES.3.2.3 (continued)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)22a - O1_2b	1.58(3)	153(2)	(Si,Al)22b - O32a	1.58(1)	146(2)
(Si,Al)22a - O32b	1.58(1)	149(1)	(Si,Al)22b - O1_2a	1.59(2)	166(2)
(Si,Al)22a - O52b	1.61(2)	146(2)	(Si,Al)22b - O52a	1.59(2)	150(1)
(Si,Al)22a - O42a	1.61(2)	164(2)	(Si,Al)22b - O42b	1.59(2)	144(2)
mean	1.60	153	mean	1.59	152
(Si,Al)31 - O51a	1.59(2)	158(2)	(Si,Al)32 - O52b	1.61(2)	146(2)
(Si,Al)31 - O52a	1.60(2)	150(1)	(Si,Al)32 - O12	1.62(2)	147(1)
(Si,Al)31 - O11	1.62(1)	167(2)	(Si,Al)32 - O51b	1.62(2)	159(1)
(Si,Al)31 - O12	1.62(2)	147(1)	(Si,Al)32 - O11	1.64(1)	167(2)
mean	1.61	156	mean	1.62	155
(Si,Al)41 - O61	1.58(2)	144(1)	(Si,Al)42 - O22a	1.59(3)	138(2)
(Si,Al)41 - O21a	1.59(2)	146(2)	(Si,Al)42 - O22b	1.59(3)	143(2)
(Si,Al)41 - O13	1.59(1)	156(1)	(Si,Al)42 - O62	1.60(2)	165(1)
(Si,Al)41 - O21b	1.60(2)	141(2)	(Si,Al)42 - O13	1.60(2)	156(1)
mean	1.59	147	mean	1.60	151
(Si,Al)51 - O1_1b	1.57(2)	157(1)	(Si,Al)52 - O1_2a	1.57(2)	166(2)
(Si,Al)51 - O1_1a	1.58(3)	152(2)	(Si,Al)52 - O1_2b	1.57(3)	153(2)
(Si,Al)51 - O72	1.59(2)	141(1)	(Si,Al)52 - O71	1.59(1)	149(1)
(Si,Al)51 - O61	1.61(2)	144(1)	(Si,Al)52 - O62	1.61(2)	165(1)
mean	1.59	149	mean	1.59	158
(Si,Al)61 - O82	1.58(2)	136(1)	(Si,Al)62 - O42a	1.57(2)	164(2)
(Si,Al)61 - O14	1.58(2)	168(1)	(Si,Al)62 - O14	1.59(2)	168(1)
(Si,Al)61 - O42b	1.59(2)	144(2)	(Si,Al)62 - O41b	1.59(2)	171(2)
(Si,Al)61 - O41a	1.60(2)	160(2)	(Si,Al)62 - O81	1.59(2)	155(2)
mean	1.59	152	mean	1.59	165
(Si,Al)7 - O82	1.57(2)	136(1)			
(Si,Al)7 - O71	1.59(2)	149(1)			
(Si,Al)7 - O72	1.59(1)	141(1)			
(Si,Al)7 - O81	1.60(2)	155(2)			
mean	1.59	145			

NES.4 Chemical composition

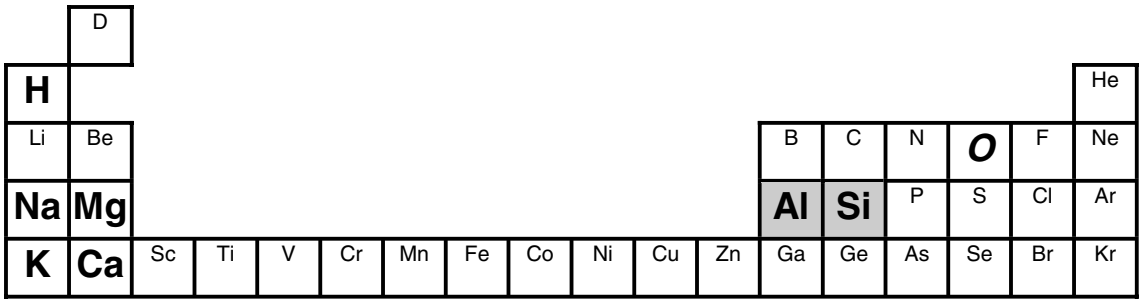


Fig. NES.4.1 Chemical elements (highlighted) occurring in NES-type compounds. Framework cations are in grey fields.

NES.5 Flexibility and apertures

There is insufficient information available about the NES-type to judge its flexibility.

The 10-ring openings in the framework of NES are twisted and have free diameters ranging from slightly less than 5Å to more than 5.5Å. Thus they are more elliptical than in the MFI framework where they measure 5Å to 5.5Å. The channels parallel **b** are straight, while those parallel **a** widen to 12-rings and are interrupted by 4-rings. These channels have to snake around that obstacle.

NES.6 Other information

There are reports about the catalytic properties of NES-type compounds in a variety of applications [2004Che1, 2004Llo1, 2003Par1]. There is also a number of patents and patent applications involving NU-87 compounds, for example [2005Mer1].

NES.7 References

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96Alb1 Alberti, A., Vezzalini, G., Galli, E., Quartieri, S.: Eur. J. Mineral. **8** (1996) 69.
96Gal1 Galli, E., Quartieri, S., Vezzalini, G., Alberti, A.: Eur. J. Mineral. **8** (1996) 687.

2003Par1 Park, S.H., Rhee, H.K.: Reaction Kinetics Catal. Lett. **78** (2003) 81.

2004Che1 Chen, H.Y., Liu, L., Xu, L.Y., Shen, W.J., Xu, Y.D., Bao, X.H.: Chin. J. Catal. **25** (2004) 845.
2004Llo1 Llopis, F.J., Sastre, G., Corma, A.: J. Catal. **227** (2004) 227.

2005Mer1 Merlen, E., Alario, F., Ferrer, N., Martin, O.: U.S. Patent Application 2005-48751 (2005).

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