MTN

MTN.1 Zeolite framework type and topology

The designation of the FTC refers to the type material ZS**M**-**T**hirty-**N**ine (ZSM-39, Zeolite Socony Mobil with sequence number thirty-nine), first synthesized by [81Pel1] and [81Dwy1]. MTN-type compounds belong to the family of clathrasils [83Lie1, 86Lie1], similar to the DDR, DOH, MEP, and NON types. The framework structure of ZSM-39 (Fig. MTN.1.1) is isostructural with the 17 Å cubic gas hydrate type II [81Sch1]. It can be described as being built from close packed *mtn* ($5^{12}6^4$) and *red* (5^{12}) units as shown in Fig. MTN.1.2. Clathrasils formed by *red* (5^{12}) units are also called dodecasils where the MTN-type compound represents dodecasil 3C [82Gie1].

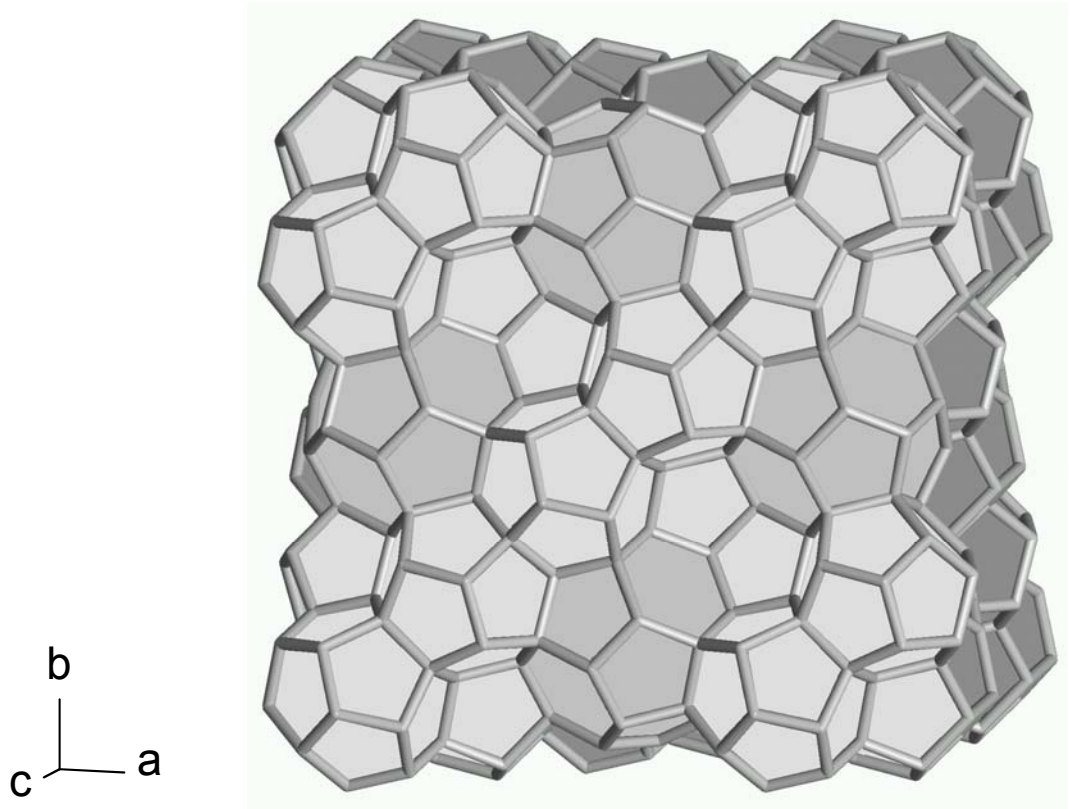
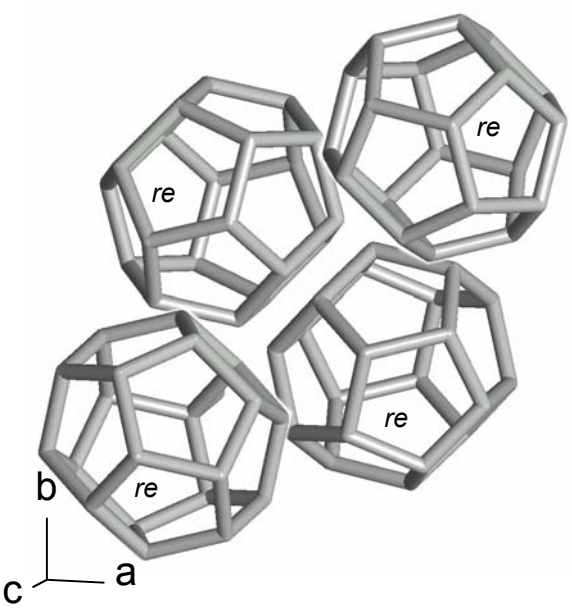
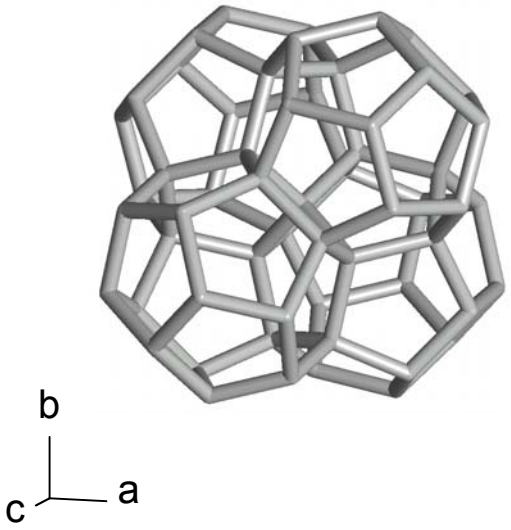


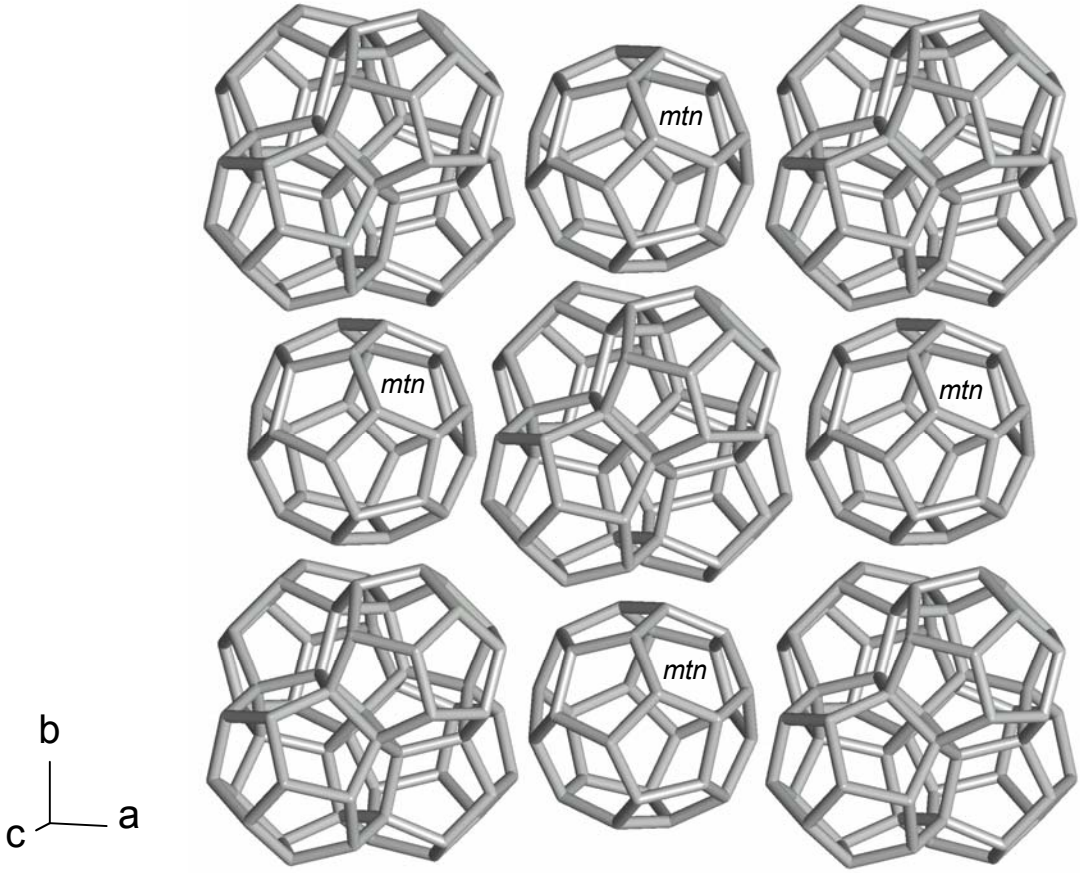
Fig. MTN.1.1. The framework structure of MTN-type compounds in the highest possible topological symmetry $F\,d\,\bar{3}\,m$. The *red* units forming pillars (**kgr** units) parallel [110] are light grey, *mtn* units are dark grey. View parallel **c** rotated by 5° about **a** and 8° about **b**.



a Linkage between 4 *red* units.

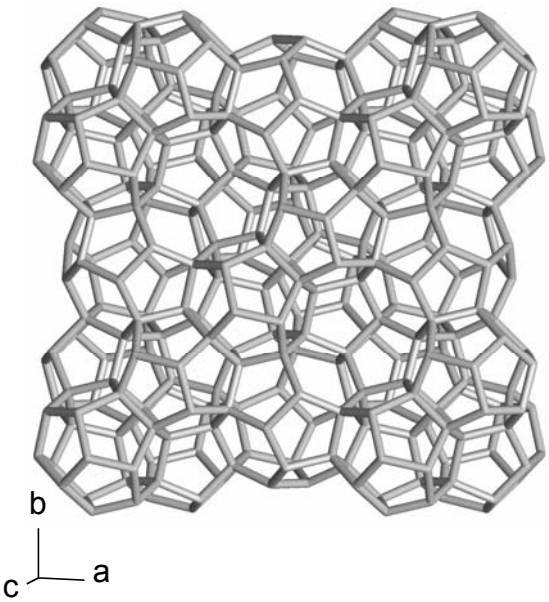


b The complete assemblage shown in a).

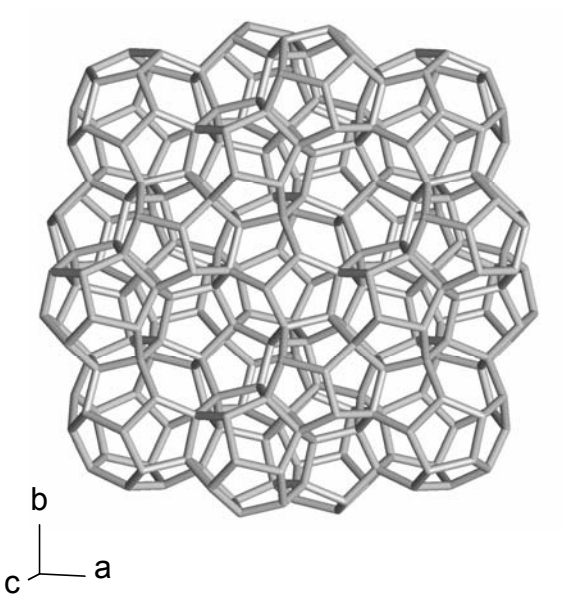


c Linkage of the composite unit shown in b) with *mtn* units.

Fig. MTN.1.2. Building scheme of the MTN-type framework. View parallel **c** rotated by 2° about **a** and 5° about **b**.



d The complete assemblage shown in c) forming the layer in *x*, *y*, 0.



e The layer in *x*, *y*, ½ with face centered arrangement of the units shown in d).

Fig. MTN.1.2 (continued). Building scheme of the MTN-type framework. View parallel **c** rotated by 2° about **a** and 5° about **b**.

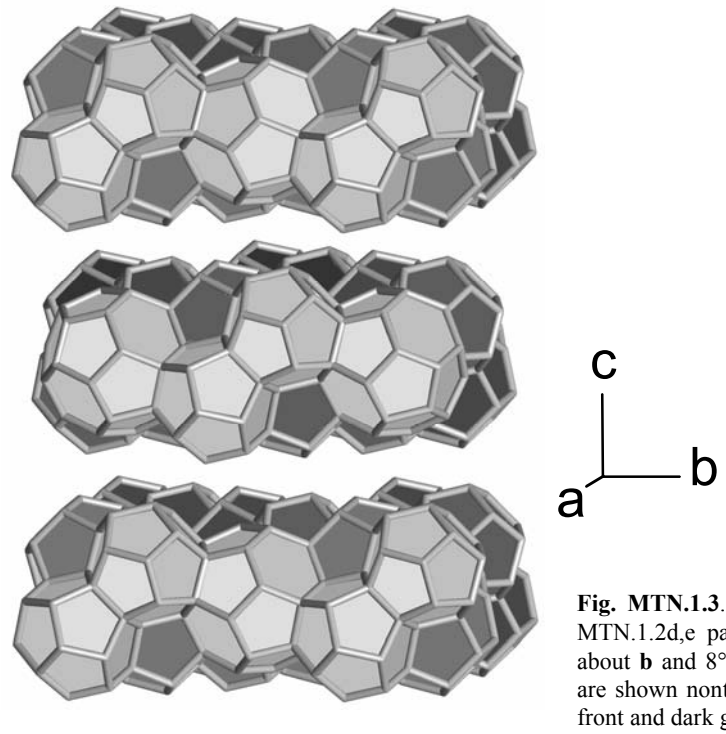


Fig. MTN.1.3. The sequence of layers shown in Fig. MTN.1.2d,e parallel **c**. View parallel **a** rotated by 4° about **b** and 8° about **c**. The cages (*red* and *mtn* units) are shown nontransparently with light grey units in the front and dark grey units in the rear.

Fig. MTN.1.4 shows the symmetry relationships of MTN-type crystal structures. There are three entries in Tables MTN.2.1 and MTN.2.2 originally described in space group $F\,d\,\bar{3}$. However, the framework structures closely resemble space group $F\,d\,\bar{3}\,m$ and therefore they can be better described in the higher symmetry. The dodecasil 3C structure (MTN1984a01) described by [84Gie1] corresponds to the aristotype structure within less than 0.01 Å for framework and nonframework atoms. Consequently, the entry is assigned to $F\,d\,\bar{3}\,m$ in Tables MTN.2.1 and MTN.2.2. Additional subgroups are listed in [95Kön1] corresponding to DLS results given by [92Kön1]. Since they do not represent observed structures, they are not considered here.

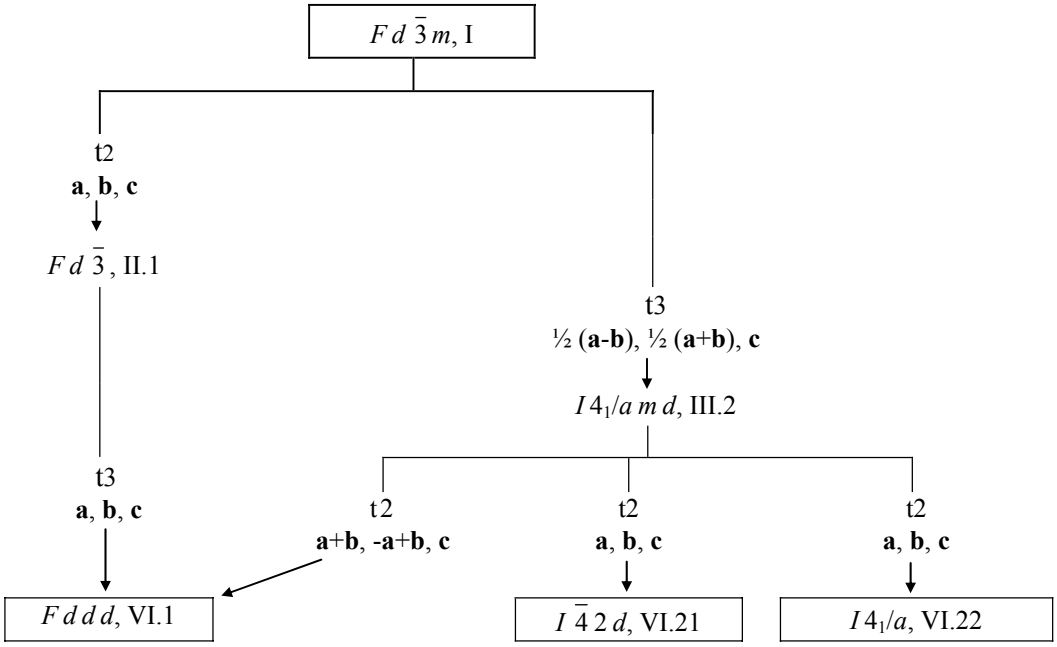


Fig. MTN.1.4 The Bärnighausen tree illustrating the symmetry relationship of the MTN types.

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

MTN-I $F\,d\,\bar{3}\,m$		MTN-II.1 $F\,d\,\bar{3}$		MTN-VI.1 $F\,d\,d\,d$
T1 [96(g), . . *m*]	→	T1 [96(g), 1]	→	T11 [32(h), 1] T12 [32(h), 1] T13 [32(h), 1]
T2 [32(e), . 3 *m*]	→	T2 [32(e), . 3 .]	→	T2 [32(h), 1]
T3 [8(a), $\bar{4}$ 3 *m*]	→	T3 [8(a), 2 3 .]	→	T3 [8(a), 2 2 2]
O1 [96(h), . . 2]	→	O1 [96(g), 1]	→	O11 [32(h), 1] O12 [32(h), 1] O13 [32(h), 1]

Table MTN.1.1 (continued)

MTN-I, $F\,d\,\bar{3}\,m$		MTN-II.1, $F\,d\,\bar{3}$		MTN-VI.1, $F\,d\,d\,d$
O2 [96(g), . . *m*]	→	O2 [96(g), 1]	→	O21 [32(h), 1]
			→	O22 [32(h), 1]
			→	O23 [32(h), 1]
O3 [48(f), 2. *m m*]	→	O3 [48(f), 2 . .]	→	O31 [16(e), 2 . .]
			→	O32 [16(f), . 2 .]
			→	O33 [16(g), . . 2]
O4 [32(e), . 3 *m*]	→	O4 [32(e),. 3 .]	→	O4 [32(h), 1]
MTN-I, $F\,d\,\bar{3}\,m$		MTN-III.2, $I\,4_1/a\,m\,d$		MTN-VI.21, $I\,\bar{4}\,2\,d$
T1 [96(g), . . *m*]	→	T11 [16(h), . *m* .]	→	T11 [16(e), 1]
	→	T12 [32(i), 1]	→	T12a [16(e), 1]
			→	T12b [16(e), 1]
T2 [32(e), . 3 *m*]	→	T2 [16(h), . *m* .]	→	T2 [16(e), 1]
T3 [8(a), $\bar{4}$ 3 *m*]	→	T3 [4(a), $\bar{4}$ *m* 2]	→	T3 [4(a), $\bar{4}$ . .]
O1 [96(h), . . 2]	→	O11 [32(i), 1]	→	O11a [16(e), 1]
			→	O11b [16(e), 1]
	→	O12 [16(f) . 2 .]	→	O12a [8(d), . 2 .]
			→	O12b [8(d), . 2 .]
O2 [96(g), . . *m*]	→	O21 [16(h), . *m* .]	→	O21a [16(e), 1]
	→	O22 [32(i), 1]	→	O22a [16(e), 1]
			→	O22b [16(e), 1]
O3 [48(f), 2. *m m*]	→	O31 [16(g), . . 2]	→	O31 [16(e), 1]
	→	O32 [8(e) 2 *mm* .]	→	O32 [8(c), 2 . .]
O4 [32(e), . 3 *m*]	→	O4 [16(h), . *m* .]	→	O4 [16(e), 1]
MTN-I, $F\,d\,\bar{3}\,m$		MTN-III.2, $I\,4_1/a\,m\,d$		MTN-VI.22, $I\,4_1/a$
T1 [96(g), . . *m*]	→	T11 [16(h), . *m* .]	→	T11 [16(f), 1]
	→	T12 [32(i), 1]	→	T12a [16(f), 1]
			→	T12b [16(f), 1]
T2 [32(e), . 3 *m*]	→	T2 [16(h), . *m* .]	→	T2 [16(f), 1]
T3 [8(a), $\bar{4}$ 3 *m*]	→	T3 [4(a), $\bar{4}$ *m* 2]	→	T3 [4(a), $\bar{4}$ . .]
O1 [96(h), . . 2]	→	O11 [32(i), 1]	→	O11a [16(f), 1]
			→	O11b [16(f), 1]
	→	O12 [16(f) . 2 .]	→	O12 [16(f), 1]

Table MTN.1.1 (continued)

MTN-I, $F\,d\,\bar{3}\,m$		MTN-III.2, $I\,4_1/a\,m\,d$		MTN-VI.22, $I\,4_1/a$
O2 [96(g), . . *m*]	→	O21 [16(h), . *m* .]	→	O21 [16(f), 1]
	→	O22 [32(i), 1]	→	O22a [16(f), 1]
			→	O22b [16(f), 1]
O3 [48(f), 2. *m m*]	→	O31 [16(g), . . 2]	→	O31 [16(f), 1]
	→	O32 [8(e) 2 *mm* .]	→	O32 [8(e), 2 . .]
O4 [32(e), . 3 *m*]	→	O4 [16(h), . *m* .]	→	O4 [16(f), 1]

MTN.2 Compounds and crystal data

Table MTN.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
MTN-I ***F d*** $\bar{\mathbf{3}}$ ***m***									
MTN1981a01	$Si_{136}O_{272}$ [1])	ZSM-39	18.7	S	-	TMA, TEA [4])	-	-	81Sch1
MTN1984a01 [2])	$Si_{136}O_{272}$	D3C [3])	18.6	S	-		-	-	84Gie1
MTN1987a01	$Si_{136}O_{272} \cdot nCH_3NH_2$	ZSM-39	18.6	S	-	TrMA	-	-	87Lon1
MTN1988a01	$Si_{136}O_{272} \cdot nCH_3NH_2$	ZSM-39	18.6	S	-	TrMA	-	-	88Zhe1
MTN1991a01	$Si_{136}O_{272} \,.\, 8(CH_3)_4NF$	ZSM-39	18.7	S	-	TMAF	-	-	91Zha1
MTN1992a01	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön1
MTN1992a02	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön1
MTN1992b01	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön2
MTN1992b02	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön2
MTN1992b07	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön2
MTN1992b08	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	-	C	1173	92Kön2
MTN1992b09	$Si_{136}O_{272}$	D3C [3])	18.6	S	-	t-but	-	-	92Kön2
MTN-II.1 ***F d*** $\bar{\mathbf{3}}$									
MTN1990a01 [4])	$Si_{136}O_{272} \cdot 8C_4H_9N_{0.5}N_2$	D3C [3])	18.8	S	-	pyr, N_2	-	-	90Mel1
MTN1990a02 [5])	$Si_{136}O_{272} \cdot 8C_4H_9N\ N_2$	D3C [3])	18.8	S	-	pyr, N_2	-	-	90Mel1
MTN-VI.1 ***F d d d***									
MTN1992b03	$Si_{136}O_{272}$	-	18.9	T	-	-	-	-	92Kön2
MTN1992b10	$Si_{136}O_{272}$	D3C [3])	18.7	S	-	pyr	-	-	92Kön2
MTN-VI.2.1 ***I*** $\bar{\mathbf{4}}$ **2** ***d***									
MTN1991a01	$Si_{68}O_{136} \cdot 4C_5H_5N$	D3C [3])	8.6	S	-	pyri-dine	-	-	91Cha1

Table MTN.2.1 (continued)

MTN-III.2 ***I*** 4_1***/a***									
MTN1992b06	$Si_{68}O_{136}$	-	18.7	T	-	-	-	-	92Kön2
MTN1992b11	$Si_{68}O_{136}$	D3C[3])	18.7	S	-	t-but	-	-	92Kön2
MTN1995a01	$Si_{68}O_{136}$	D3C[3])	18.7	S	-	t-but	-	-	95Kön1
MTN1997a01	$Si_{68}O_{136} \cdot 4C_4H_8O$	D3C[3])	18.6	S	-	THF	-	-	97Kno1

[1]) The framework contains 0.4 Al atoms per unit cell compensated by Na, TMA, and TEA cations.
[2]) The space group is given as $F\,d\,\bar{3}$ in [84Gie1] but the coordinates correspond to $F\,d\,\bar{3}\,m$ within less than 0.01 Å for framework and nonframework atoms.
[3]) D3C: dodecasil 3C [4]) TrMA, CO_2, N_2, CH_4, Ar [5]) The framework structure essentially resembles space group $F\,d\,\bar{3}\,m$ within the standard deviations of the atomic parameters.

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

code	*a* [Å]	*V* [Å^3]	*T* [K]	reference
MTN-I ***F d*** $\bar{3}$ ***m***				
MTN1981a01	19.36(2)	7256	n.s.	81Sch1
MTN1984a01[1])	19.402(1)	7304	n.s.	84Gie1
MTN1987a01	19.403(3)	7305	n.s.	87Lon1
MTN1988a01	19.403(3)	7305	n.s.	88Zhe1
MTN1991a01	19.391(8)	7291	n.s.	91Zha1
MTN1992a01	19.369(6)	7266	523	92Kön1
MTN1992a02	19.369(6)	7266	523	92Kön1
MTN1992b01	19.369(6)	7266	473	92Kön2
MTN1992b02	19.36(1)	7261	623	92Kön2
MTN1992b07	19.369(6)	7266	473	92Kön2
MTN1992b08	19.369(6)	7266	473	92Kön2
MTN1992b09	19.423(5)	7327	443	92Kön2
MTN-II.1 ***F d*** $\bar{3}$				
MTN1990a01[2])	19.349(1)	7244	408	90Mel1
MTN1990a02[2])	19.346(1)	7241	408	90Mel1

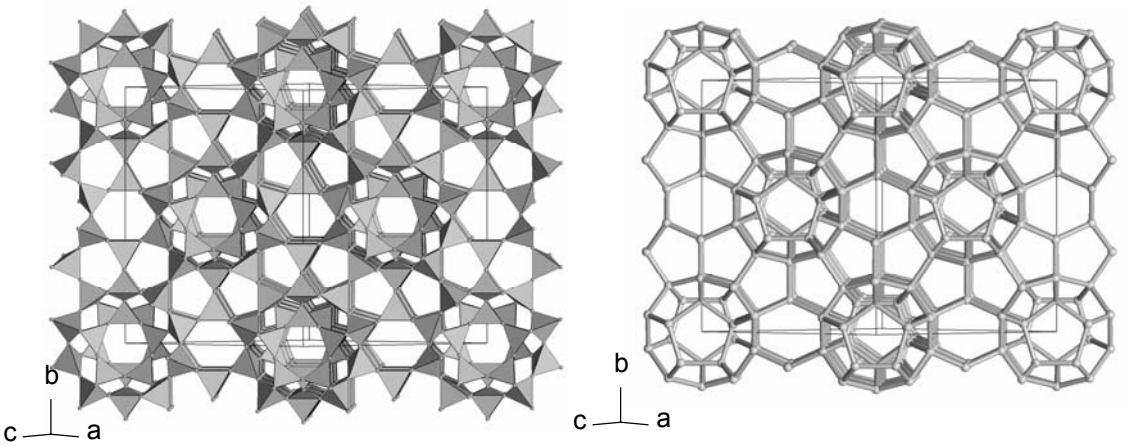
code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
MTN-VI.1 ***F d d d***						
MTN1992b03	19.2399(2)	19.3075(3)	19.3903(3)	7203	RT	92Kön2
MTN1992b10	19.303(1)	19.304(1)	19.4938(8)	7264	RT	92Kön2

code	*a* [Å]	*c* [Å]	shift	matrix	coord. trans.	*V* [Å^3]	*T* [K]	reference
MTN-VI.2.1 ***I*** $\bar{4}$ **2** ***d***								
MTN1991a01	13.6620(5)	19.5669(7)	0, 1/4, 5/8	**a**, **b**, **c**	*x*, *y*-1/4, *z*-5/8	3652	299	91Cha1
MTN-III.2 ***I*** 4_1***/a***								
MTN1992b06	13.6519(2)	19.4757(3)	0, 1/4, 1/8	**a**, **b**, **c**	*x*, *y*-1/4, *z*-1/8	3630	RT	92Kön2
MTN1992b11	13.6519(2)	19.4757(3)	0, 1/4, 1/8	**a**, **b**, **c**	*x*, *y*-1/4, *z*-1/8	3630	RT	92Kön2
MTN1995a01	13.6519(2)	19.4757(3)	0, 1/4, 1/8	**a**, **b**, **c**	*x*, *y*-1/4, *z*-1/8	3630	RT	95Kön1
MTN1997a01	13.684(2)	19.482(5)	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	3648	298	97Kno1

[1]) The space group is given as $F\,d\,\bar{3}$ in [84Gie1] but the coordinates correspond to $F\,d\,\bar{3}\,m$ within less than 0.01 Å for framework and nonframework atoms. [2]) The framework structure essentially resembles space group $F\,d\,\bar{3}\,m$ within the standard deviations of the atomic parameters.

MTN.3 Framework structures

MTN.3.1 MTN-I compound ($F\,d\,\bar{3}\,m$, IT #227)



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

Fig. MTN.3.1.1 Projections of the MTN-I crystal structure of $Si_{136}O_{272}$ (MTN1992b07, 92Kön2). View parallel [110] rotated by 1° about [10 $\bar{1}$] and [010].

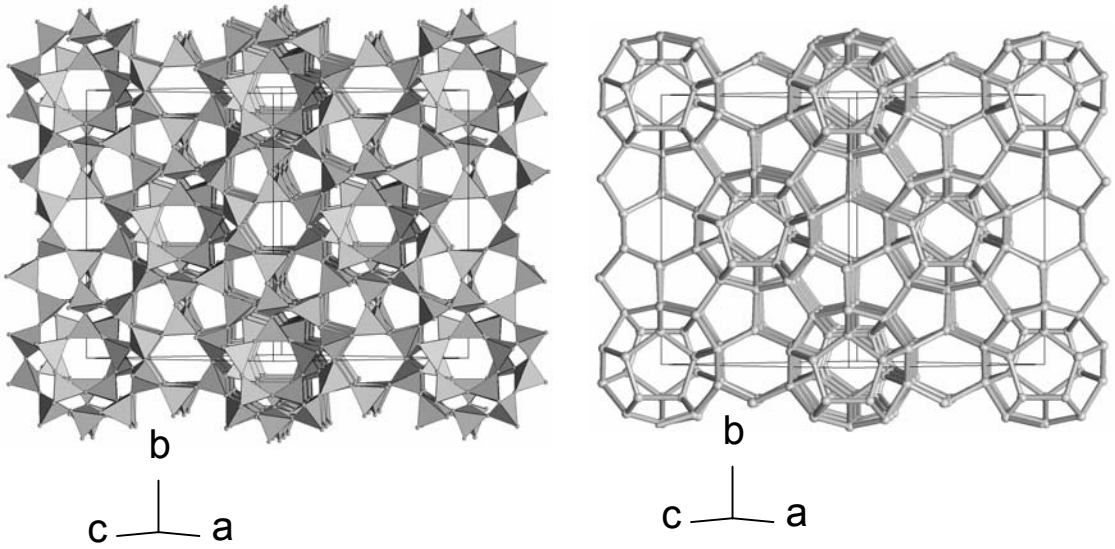
Table MTN.3.1.1 Atomic coordinates and site definitions for MTN-I, $Si_{136}O_{272}$ (MTN1992b07, 92Kön2).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1	0.06750(4)	*x*	0.37010(6)	2.59	. . *m*	96(g)	96
Si2	0.21641(6)	*x*	*x*	2.16	. 3 *m*	32(e)	32
Si3	1/8	1/8	1/8	1.97	$\bar{4}$ 3 *m*	8(a)	8
O1	0	0.3434(2)	-*y*	6.47	. . 2	96(h)	96
O2	0.2004(2)	*x*	0.2936(2)	7.11	. . *m*	96(g)	96
O3	0.3736(3)	1/8	1/8	5.05	2. *m m*	48(f)	48
O4	0.1702(2)	*x*	*x*	10.03	. 3 *m*	32(e)	32

Table MTN.3.1.1 Selected interatomic distances and angles, MTN-I, $Si_{136}O_{272}$ (MTN1992b07, 92Kön2).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 - O2	1.561(4)	178.0(3)	Si2 - O4	1.550(4)	180
Si1 - O1	1.569(2)	169.4(3)	Si2 - O2	1.558(4)	178.0(3)
Si1 - O1	1.569(2)	169.4(3)	Si2 - O2	1.558(4)	178.0(3)
Si1 - O3	1.576(1)	175.1(4)	Si2 - O2	1.558(4)	178.0(3)
mean	1.569	173.0	Mean	1.556	178.5
Si3 - O4	1.516(4)	180			
Si3 - O4	1.516(4)	180			
Si3 - O4	1.516(4)	180			
Si3 - O4	1.516(4)	180			
mean	1.516	180			

MTN.3.2 MTN-VI.1 compound (*F d d d*, IT #70)



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

Fig. MTN.3.2.1 Projections of the MTN-VI.1 crystal structure of $Si_{136}O_{272}$ (MTN1992b10, 92Kön2). View parallel [110] rotated by 1° about [10 $\bar{1}$] and [010].

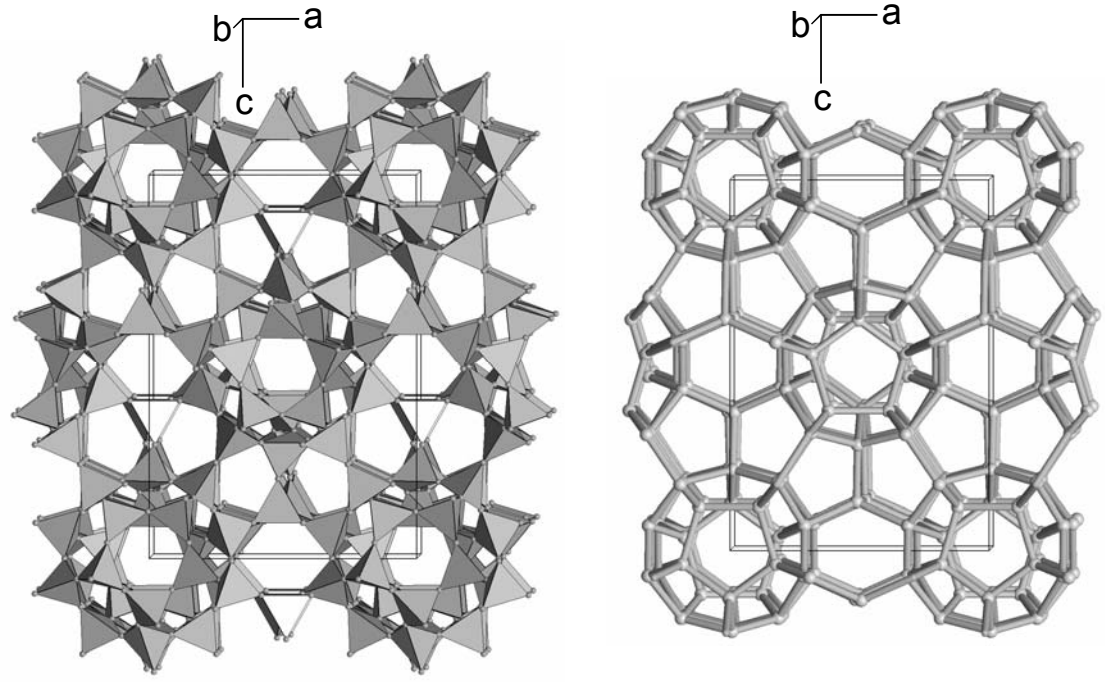
Table MTN.3.2.1 Atomic coordinates and site definitions for MTN-VI.1, $Si_{136}O_{272}$ (MTN1992b10, 92Kön2).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0.061(1)	0.070(2)	0.369(1)	0.8(2)	1	32(h)	32
Si12	0.371(2)	0.06(1)	0.07(1)	0.8(2)	1	32(h)	32
Si13	0.071(1)	0.369(2)	0.065(2)	0.8(2)	1	32(h)	32
Si2	0.218(2)	0.218(2)	0.2136(4)	0.8(2)	1	32(h)	32
Si3	1/8	1/8	1/8	0.8(2)	2 2 2	8(a)	8
O11	0.00(3)	0.346(4)	0.662(4)	3.5(5)	1	32(h)	32
O12	0.662(3)	0.002(4)	0.345(4)	3.5(5)	1	32(h)	32
O13	0.341(3)	0.661(3)	0.006(3)	3.5(5)	1	32(h)	32
O21	0.212(3)	0.193(2)	0.294(2)	3.5(5)	1	32(h)	32
O22	0.294(3)	0.212(3)	0.194(3)	3.5(5)	1	32(h)	32
O23	0.192(3)	0.298(2)	0.216(3)	3.5(5)	1	32(h)	32
O31	0.367(7)	1/8	1/8	3.5(5)	2 . .	16(e)	16
O32	1/8	0.372(6)	1/8	3.5(5)	. 2 .	16(f)	16
O33	1/8	1/8	0.371(3)	3.5(5)	. . 2	16(g)	16
O4	0.171(3)	0.172(3)	0.171(1)	3.5(5)	1	32(h)	32
C1	0.57(1)	7/8	7/8	3.3(8)	2 . .	16(e)	11(1)
C2	0.56(1)	0.61(2)	0.67(3)	3.3(8)	1	32(h)	22(3)
N3	0	0	0	3.3(8)	$\bar{1}$	16(c)	6(1)

Table MTN.3.2.2 Selected interatomic distances and angles for MTN-VI.1, $Si_{136}O_{272}$ (MTN1992b10, 92Kön2).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O11	1.5(4)	161(17)	Si12 - O1 2	1.5(2)	167(5)
Si11 - O21	1.55(5)	165(4)	Si12 - O1 3	1.6(2)	164(4)
Si11 - O12	1.58(8)	167(5)	Si12 - O2 2	1.6(1)	168(8)
Si11 - O33	1.63(3)	177(4)	Si12 - O3 1	1.7(2)	175(10)
mean	1.57	168	mean	1.6	169
Si13 - O23	1.52(6)	154(4)	Si2 - O4	1.52(6)	178(3)
Si13 - O32	1.57(3)	176(9)	Si2 - O22	1.52(7)	168(8)
Si13 - O13	1.65(7)	164(4)	Si2 - O23	1.62(6)	154(4)
Si13 - O11	1.7(5)	161(17)	Si2 - O21	1.64(4)	165(4)
mean	1.61	164	mean	1.58	166
Si3 - O4	1.55(5)	178(3)			
Si3 - O4	1.55(5)	178(3)			
Si3 - O4	1.55(5)	178(3)			
Si3 - O4	1.55(5)	178(3)			
mean	1.55	178			

MTN.3.3 MTN-VI.21 compound ($I\bar{4}2d$, IT #122)



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

Fig. MTN.3.3.1 Projections of the MTN-VI.21 crystal structure of $Si_{68}O_{136} \cdot 4C_5H_5N$ (MTN1991a01, 91Cha1). View parallel **b** rotated by 1° about **a** and **c**.

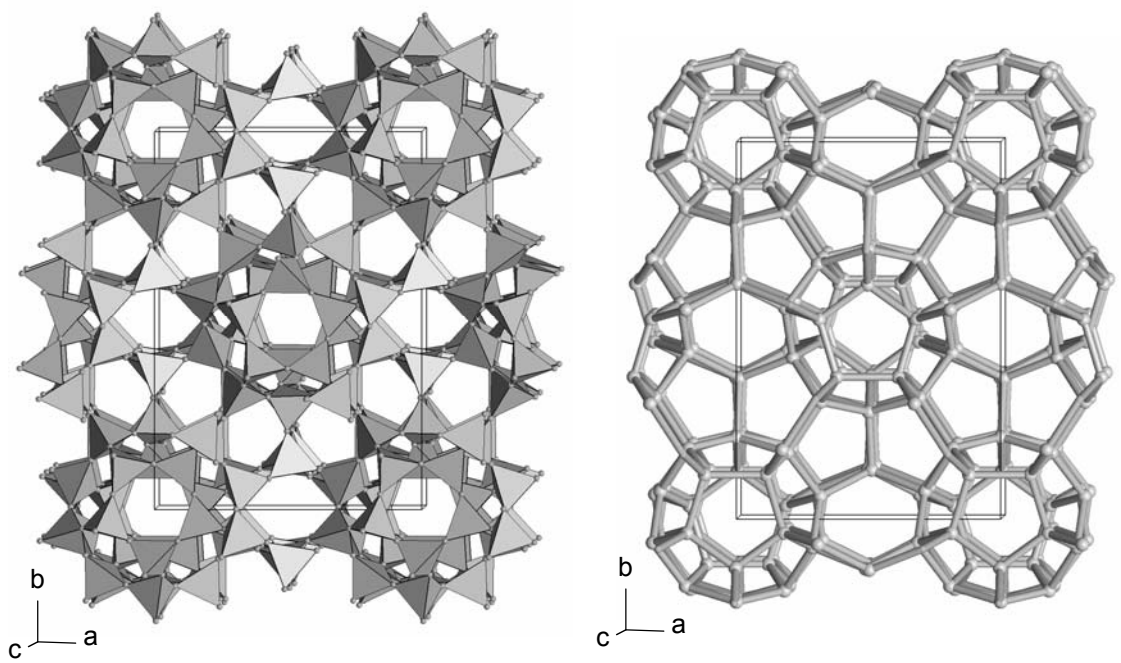
Table MTN.3.3.1 Atomic coordinates and site definitions for MTN-VI.21, $Si_{68}O_{136} \cdot 4C_5H_5N$ (MTN1991a01, 91Cha1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0.01353(6)	0.13473(6)	0.37062(4)	1.15(3)	1	16(e)	16
Si12a	0.31554(6)	0.43522(6)	0.06707(4)	1.11(3)	1	16(e)	16
Si12b	0.71392(6)	0.56210(6)	0.93277(4)	1.04(3)	1	16(e)	16
Si2	-0.00859(6)	0.43069(6)	0.21660(3)	1.08(3)	1	16(e)	16
Si3	0	¼	1/8	1.27(5)	$\bar{4}$ . .	4(a)	4
O11a	0.6688(2)	0.3239(2)	0.6594(2)	2.8(2)	1	16(e)	16
O11b	0.3582(3)	0.6375(2)	0.3408(2)	3.1(2)	1	16(e)	16
O12a	0.6836(5)	0	0	3.6(2)	. 2 .	8(d)	8
O12b	0.3055(4)	0	0	3.2(2)	. 2 .	8(d)	8
O21	-0.0197(4)	0.4027(4)	0.2945(1)	4.4(2)	1	16(e)	16
O22a	0.1022(2)	0.4621(2)	0.2007(2)	2.8(2)	1	16(e)	16
O22b	0.9184(2)	0.4813(2)	0.8015(2)	3.1(2)	1	16(e)	16
O31	0.2551(3)	0.4904(3)	0.1253(2)	3.2(2)	1	16(e)	16
O32	0	¼	0.3635(7)	2.1(5)	2 . .	8(c)	4.5(2)
O32’	0	¼	0.3846(8)	2.7(5)	2 . .	8(c)	3.5(2)
O4	0.0382(2)	0.3387(3)	0.1707(2)	2.8(2)	1	16(e)	16
N1	0.009(2)	0.338(3)	0.588(1)	7.3(3)	1	16(e)	4
C2	0.0382	0.2532	0.5592	7.3(3)	1	16(e)	4
C3	0.0172	0.1614	0.5856	7.3(3)	1	16(e)	4
C4	-0.0377	0.1570	0.6456	7.3(3)	1	16(e)	4
C5	0.9308	0.2431	0.6770	7.3(3)	1	16(e)	4
C6	-0.04411	0.3311	0.6463	7.3(3)	1	16(e)	4

Table MTN.3.3.2 Selected interatomic distances and angles for MTN-VI.21, $Si_{68}O_{136} \cdot 4C_5H_5N$ (MTN1991a01, 91Cha1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O21	1.577(3)	170.1(4)	Si12a - O12a	1.583(1)	180.0(5)
Si11 - O11b	1.590(3)	165.6(3)	Si12a - O22b	1.583(1)	154.5(2)
Si11 - O32	1.592(1)	170.0(10)	Si12a - O11a	1.595(3)	155.8(2)
Si11 - O11a	1.593(3)	155.8(2)	Si12a - O31	1.596(4)	174.3(3)
mean	1.588	165.4	mean	1.589	166.2
Si12b - O31	1.580(4)	174.3(3)	Si2 - O21	1.579(2)	170.1(4)
Si12b - O22a	1.586(3)	155.5(2)	Si2 - O4	1.597(4)	146.2(2)
Si12b - O12b	1.588(1)	160.8(4)	Si2 - O22b	1.602(3)	154.5(2)
Si12b - O11b	1.590(3)	165.6(3)	Si2 - O22a	1.604(3)	155.5(2)
mean	1.586	164.1	Mean	1.596	156.6
Si3 - O4	1.594(4)	146.2(2)			
Si3 - O4	1.594(4)	146.2(2)			
Si3 - O4	1.594(4)	146.2(2)			
Si3 - O4	1.594(4)	146.2(2)			
mean	1.594	146.2			

MTN.3.4 MTN-VI.22 compound ($I\,4_1/a$, IT #88)



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

Fig. MTN.3.4.1 Projections of the MTN-VI.22 crystal structure of $Si_{68}O_{136} \cdot 4C_4H_8O$ (MTN1997a01, 97Kno1). View parallel **b** rotated by 1° about **a** and **c**.

Table MTN.3.4.1 Atomic coordinates and site definitions for MTN-VI.22, $Si_{68}O_{136} \cdot 4C_4H_8O$ (MTN1997a01, 97Kno1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	-0.0086(1)	0.1343(1)	0.3709(1)	0.92	1	16(f)	16
Si12a	0.3155(1)	0.4307(1)	0.0609(1)	0.92	1	16(f)	16
Si12b	0.7112(1)	0.4431(1)	0.0733(1)	0.84	1	16(f)	16
Si2	-0.0010(1)	0.4325(1)	0.2169(1)	0.97	1	16(f)	16
Si3	0	¼	1/8	1.21	$\bar{4}$ . .	4(a)	4
O11a	0.6645(3)	0.3226(3)	0.6684(2)	2.29	1	16(f)	16
O11b	0.3527(3)	0.3637(3)	0.6469(2)	3.29	1	16(f)	16
O12	0.6868(3)	0.0079(3)	-0.0081(2)	3.26	1	16(f)	16
O21	-0.0068(4)	0.4023(4)	0.2944(2)	4.11	1	16(f)	16
O22a	0.1068(3)	0.4660(3)	0.1982(2)	2.76	1	16(f)	16
O22b	0.9246(3)	0.5185(3)	0.2020(2)	3.00	1	16(f)	16
O31	0.2582(3)	0.4878(3)	0.1200(2)	2.92	1	16(f)	16
O32	0	¼	0.3738(3)	3.40	2 . .	8(e)	8
O4	-0.0317(3)	0.3411(3)	0.1707(2)	3.24	1	16(f)	16
C1	0.521(4)	0.677(3)	0.145(5)	25.6	1	16(f)	11.2(2)
O11	0.552(7)	0.258(7)	0.829(4)	14.3	1	16(f)	2

Table MTN.3.4.2 Selected interatomic distances and angles for MTN-VI.22, $Si_{68}O_{136} \cdot 4C_4H_8O$ (MTN1997a01, 97Kno1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O11b	1.585(4)	171.6(3)	Si12a - O12	1.586(4)	168.6(3)
Si11 - O21	1.586(5)	169.0(4)	Si12a - O31	1.597(4)	174.9(3)
Si11 - O32	1.589(1)	175.9(4)	Si12a - O22b	1.598(4)	155.2(3)
Si11 - O11a	1.593(4)	150.8(3)	Si12a - O11a	1.599(4)	150.8(3)
mean	1.588	166.8	Mean	1.595	162.4
Si12b - O31	1.581(4)	174.9(3)	Si2 - O21	1.567(4)	169.0(4)
Si12b - O11b	1.584(4)	171.6(3)	Si2 - O22b	1.583(4)	155.2(3)
Si12b - O12	1.585(4)	168.6(3)	Si2 - O22a	1.587(4)	157.7(3)
Si12b - O22b	1.601(4)	155.2(3)	Si2 - O4	1.597(4)	148.9(3)
mean	1.588	167.6	mean	1.584	157.7
Si3 - O4	1.592(4)	148.9(3)			
Si3 - O4	1.592(4)	148.9(3)			
Si3 - O4	1.592(4)	148.9(3)			
Si3 - O4	1.592(4)	148.9(3)			
mean	1.592	148.9			

MTN.4 Chemical composition

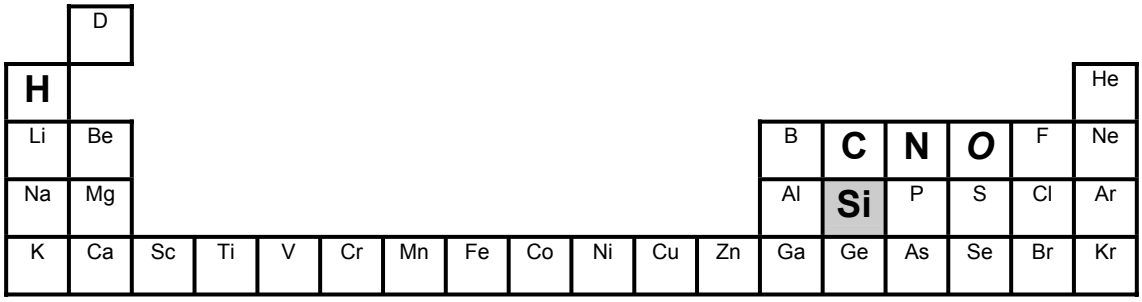


Fig. MTN.4.1 Chemical elements (highlighted) occurring in MTN-type compounds. Framework cations are in grey fields.

MTN.5 Flexibility and apertures

The value of the mean T-O-T angles for two of the most precisely determined crystal structures of the MTN-type (MTN1991a01 and MTN1997a01) is about 162°, with individual angles ranging from 146° to 180° (Tables MTN.3.3.2 and MTN.3.4.2). This range of values T-O-T for the MTN-type is smaller than observed for the LTA-type compounds where it varies from 125° to 179° (see the LTA chapter and [92Bau1]). The full range of values displayed by numerous zeolite frameworks of different types is 115° to 180° as observed in a sample of 2436 T-O-T values [95Bau1]. The mean angle in MFI-type compounds is clearly larger than the maximum of the distribution of T-O-T angles in silicoaluminate zeolites (about 143° [95Bau1]).

The unit cell volumes of MTN-type compounds shown in Table MTN.2.2 vary by about 1.7%. This is a minute deviation, not only when compared with collapsible frameworks such as the natrolites [92Bau2], but also when compared with a rather stable framework, such as the noncollapsible framework of the LTA-type [92Bau2]. There the unit cell constants vary by about 4%. For a meaningful comparison we must contrast this with the ratio of the third root of the unit cell volumes of the MTN-type compounds, which is about 0.6%. It seems that the framework of MTN-type is relatively inflexible.

The largest openings in the MTN-type framework are 6-rings. Actually the framework is made up entirely of 6- and 5-rings.

MTN.6 Other information

MTN-based compounds have been claimed in a few patents as being catalytically useful. There is a report of ferroic properties for pyridine dodecasil-3C [96Day1].

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