MTF

MTF.1 Zeolite framework type and topology

The designation of the FTC refers to the type material **M**CM-**T**hirty-**F**ive (MCM-35, Mobil Composition of Matter with sequence number thirty-five), first synthesized by [91Rub1]. The crystal structure was solved by [99Bar1] in space group *C* 2/*m*. The framework structure (Fig. MTF.1.1) can be described as being built from *bb32* ($4^2 5^4 5^4 6^2 8^2 8^2$) units forming the 8-ring channels parallel **c**, crosslinked by *pen* ($5^4 5^4$) units and a chain of 5-, 6-, and 7-rings as shown in Figs. MTF.1.2 and MTF.1.3.

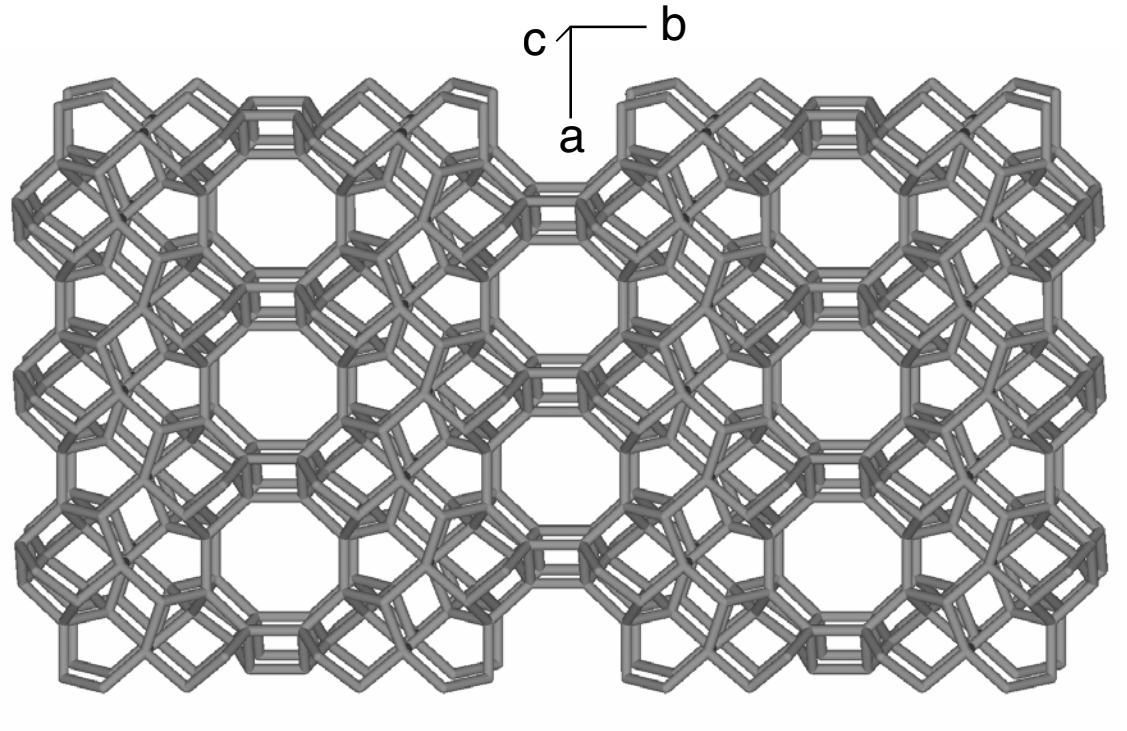
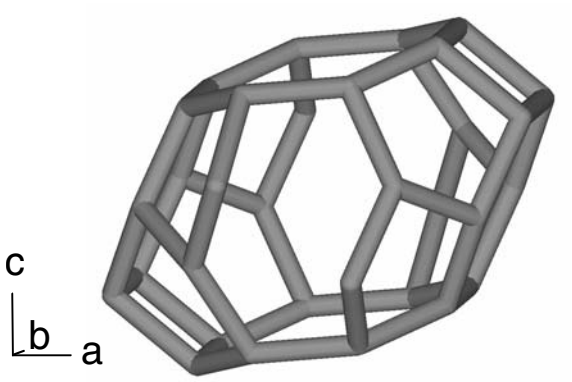
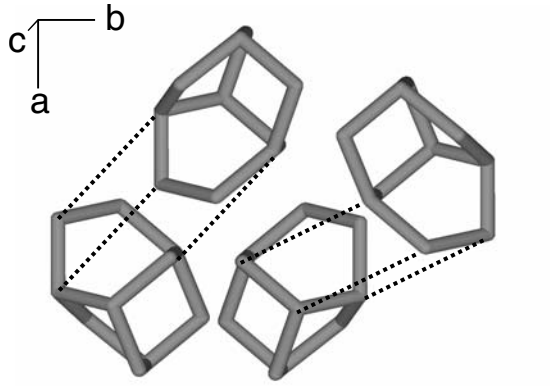


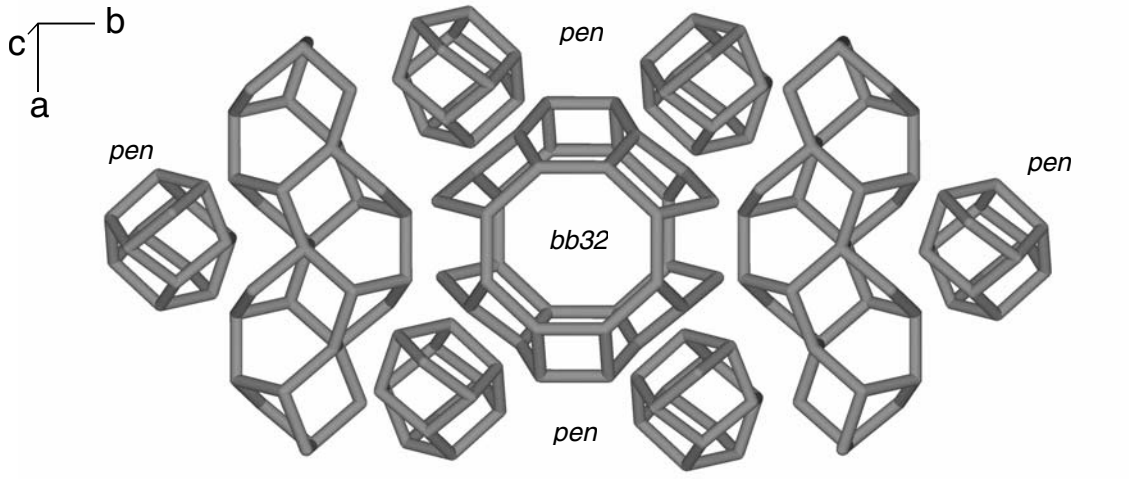
Fig. MTF.1.1. The framework structure of MTF-type compounds in the highest possible topological symmetry *C* 2/*m* (MTF1999b01, 99Plé1). View parallel [001] rotated by 6° about [010] and 4° about **b**×**c**.



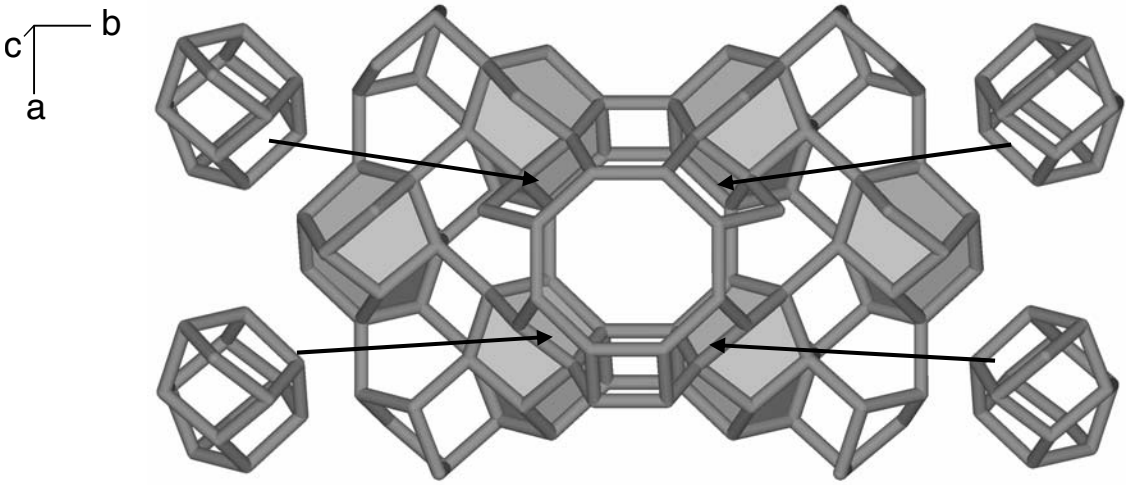
a The *bb32* unit. View parallel $[0\bar{1}0]$ rotated by 10° about [100] and 12° about **b**×**c**.



b Units forming the zigzag chain parallel [100] shown in c) and d).

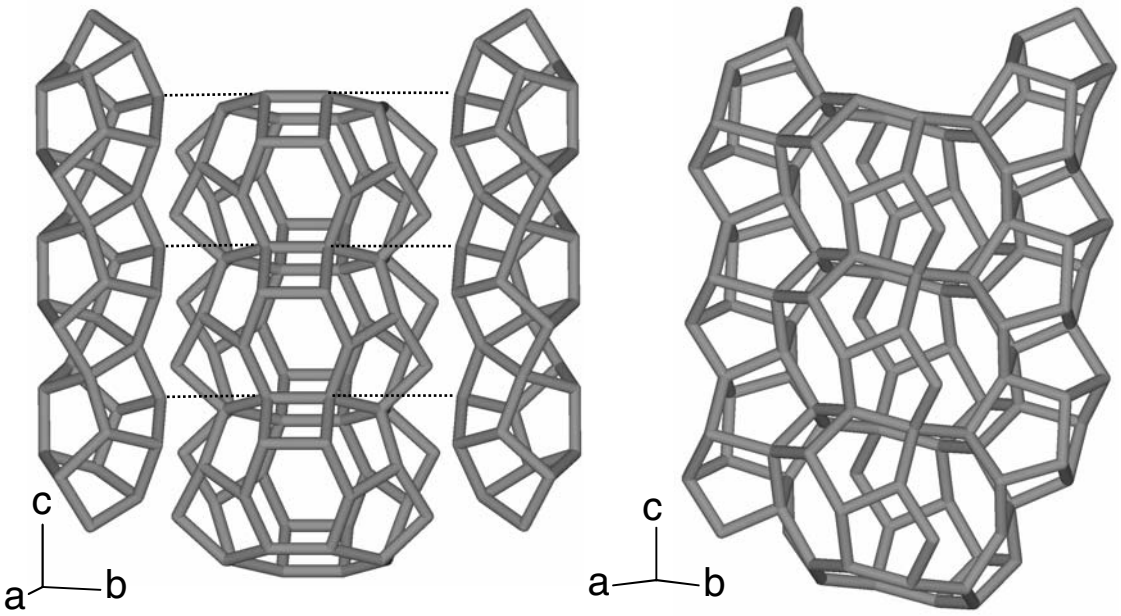


c Linkage of *bb32* and *pen* units with zigzag chain.



d The assemblage shown in c) with additional *pen* units forming the chain parallel [001] shown in Fig. MTF.1.3.

Fig. MTF.1.2 Building scheme of MTF-type structures. View parallel [001] rotated by 6° about [010] and 4° about **b**×**c** in b) to d).



a View parallel [100] rotated by 7° about [010] and 5° about **a**×**c**.

b View approximately parallel [310]. The chains of *pen* units in the front and in the rear are omitted.

Fig. MTF.1.3 Chains of *bb32* and *pen* units parallel [001].

MTF.2 Compounds and crystal data

Table MTF.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]

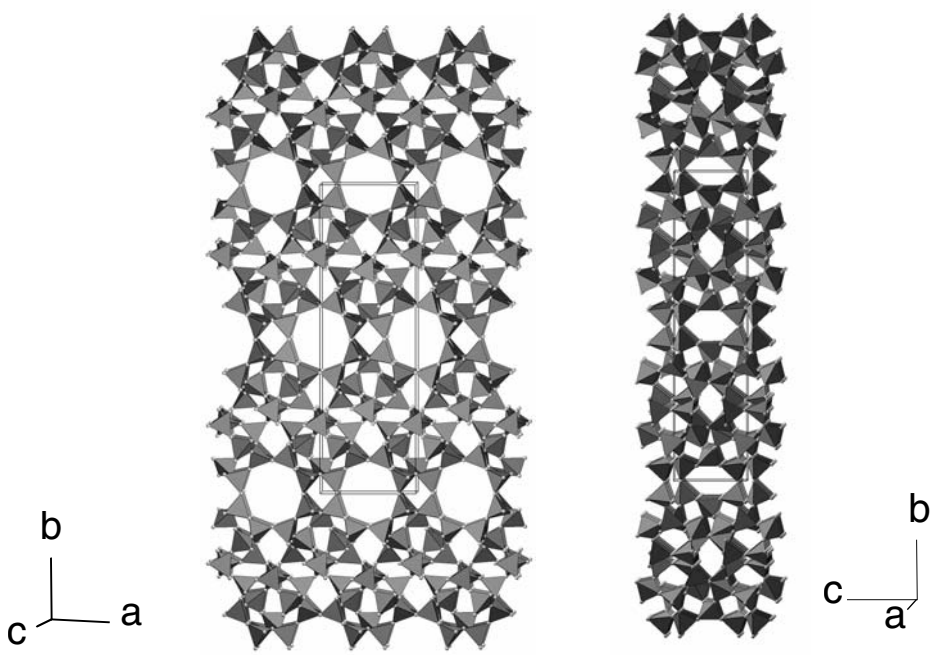
code	chemical composition	compound	FD	SM	CE	SR	TT	T	REF
MTF-I ***C* 2/*m***									
MTF1999a01	$Si_{44}O_{88}$	MCM-35	20.6	S	-	-	C	973	99Bar1
MTF1999b01	$Si_{44}O_{88}$	UTM-1	20.7	S	-	-	C	823	99Plé1

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

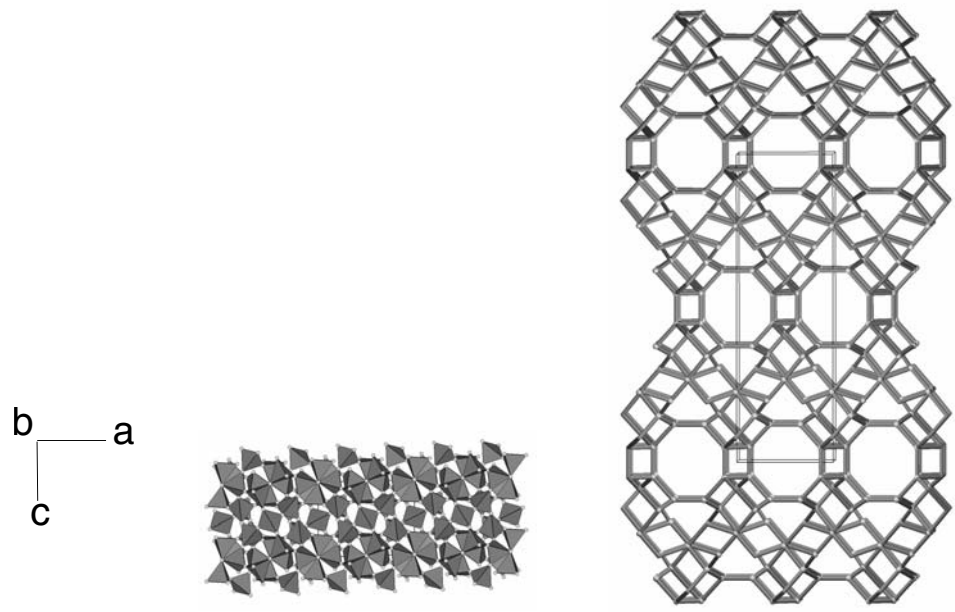
code	*a* [Å]	*b* [Å]	*c* [Å]	β [°]	*V* [Å^3]	*T* [K]	reference
MTF-I ***C* 2/*m***							
MTF1999a01	9.5000(2)	30.7096(7)	7.3133(1)	91.711(1)	2133	298	99Bar1
MTF1999b01	9.4854(2)	30.6991(7)	7.3150(1)	91.734(1)	2129	RT	99Plé1

Transformation matrices for both structures: 0, 0, ½; **a**, **b**, **c**; *x*, *y*, *z*-½

MTF.3 Framework structure of MTF-I compound (*C* 2/*m*, IT #12)



a View parallel [001] rotated by 2° about [010] and **b**×**c**. **b** View parallel [100] rotated by 1° about [010] and **a**×**b**.



c View parallel [010]. **d** Ball and stick model corresponding to a).

Fig. MTF.3.1 Projections of the MTF-I crystal structure of UTM-1, $Si_{44}O_{88}$ (MTF1999b01, 99Plé1).

Table MTF.3.1 Atomic coordinates and site definitions for MTF-I, UTM-1, $Si_{44}O_{88}$ (MTF1999b01, 99Plé1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1	0.1234(4)	0.0489(1)	0.8678(4)	1.4(1)	1	8(j)	8
Si2	0.1932(4)	0.1531(1)	0.3365(5)	1.3(1)	1	8(j)	8
Si3	0.1610(4)	0.3774(1)	0.0227(5)	1.15(9)	1	8(j)	8
Si4	0.1964(4)	0.3024(1)	0.3194(5)	1.2(1)	1	8(j)	8
Si5	0.9937(4)	0.2294(1)	0.2130(4)	1.1(1)	1	8(j)	8
Si6	0	0.0832(2)	½	1.2(1)	2	4(h)	4
O1	0.0725(6)	0.0546(2)	0.6582(7)	1.5(2)	1	8(j)	8
O2	0.2575(6)	0.0801(2)	0.9076(8)	2.1(2)	1	8(j)	8
O3	0.1605(7)	0.2235(2)	0.7183(8)	2.0(2)	1	8(j)	8
O4	0.9365(7)	0.2703(3)	0.6925(8)	1.3(2)	1	8(j)	8
O5	0.9213(8)	0.1863(2)	0.7432(9)	1.9(2)	1	8(j)	8
O6	0.1260(6)	0.1110(2)	0.4222(9)	1.5(2)	1	8(j)	8
O7	0.2957(6)	0.1762(2)	0.4857(9)	1.9(2)	1	8(j)	8
O8	0.2866(6)	0.1382(2)	0.1729(9)	1.6(2)	1	8(j)	8
O9	0.3260(7)	0.1616(2)	0.8338(8)	1.9(2)	1	8(j)	8
O10	0.1730(9)	0	0.901(1)	1.6(3)	*m*	4(i)	4
O11	0	0.0633(3)	0	1.9(3)	2	4(g)	4
O12	0	0.2352(3)	0	1.5(3)	2	4(g)	4
O13	0	0.6080(4)	0	2.2(3)	2	4(g)	4

Table MTF3.2 Selected interatomic distances and angles for MTF-I, UTM-1, $Si_{44}O_{88}$ (MTF1999b01, 99Plé1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 – O10	1.589(5)	141.7(6)	Si2 – O8	1.578(7)	163.8(5)
Si1 – O11	1.602(4)	148.1(7)	Si2 – O6	1.580(8)	154.1(5)
Si1 – O1	1.603(6)	150.1(5)	Si2 – O5	1.588(8)	162.4(6)
Si1 – O2	1.612(7)	156.6(5)	Si2 – O7	1.605(7)	144.5(4)
mean	1.602	149.1	Mean	1.588	156.2
Si3 – O2	1.591(8)	156.6(5)	Si4 – O7	1.569(7)	144.5(4)
Si3 – O13	1.595(5)	147.5(8)	Si4 – O9	1.583(8)	174.7(5)
Si3 – O9	1.596(8)	174.7(5)	Si4 – O4	1.600(8)	146.9(5)
Si3 – O8	1.602(7)	163.8(5)	Si4 – O3	1.604(8)	155.9(6)
mean	1.596	160.7	Mean	1.589	155.5
Si5 – O4	1.570(8)	146.9(5)	Si6 – O6	1.588(7)	154.1(5)
Si5 – O3	1.571(8)	155.9(6)	Si6 – O6	1.588(7)	154.1(5)
Si5 – O12	1.571(3)	166.9(7)	Si6 – O1	1.591(7)	150.1(5)
Si5 – O5	1.576(8)	162.4(6)	Si6 – O1	1.591(7)	150.1(5)
mean	1.572	158.0	mean	1.590	152.1

MTF.4 Chemical composition

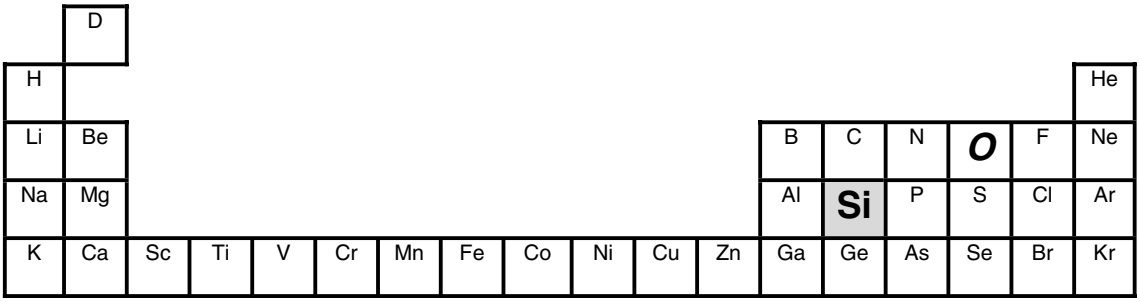


Fig. MTF.4.1 Chemical elements (highlighted) occurring in MTF-type compounds. Framework cation is in grey field.

MTF.5 Flexibility and apertures

There is insufficient information about MTF-type frameworks to deduce anything about their flexibility.

The 8-rings are elliptically compressed with free diameters between about 3.5 Å and 4 Å.

MTF.6 Other Information

Aluminosilicates with the MTF topology have been claimed, among a selection of other zeolites, as useful in processes for reducing NO_x emissions during fluid catalytic cracking [2005Yal1] and as suitable as catalysts for cracking, hydrocracking etc. [91Rub1]. The catalytic properties of acid UTM-1-type materials were investigated recently [2002Yam1].

MTF.7 References

91Rub1 Rubin, M.K.: U.S. Patent 4,981,663 (1991).

99Bar1 Barrett, P.A., Díaz-Cabañas, M.J., Camblor, M.A.: Chem. Mater. **11** (1999) 2919.
99Plé1 Plévert, J., Yamamoto, K., Chiari, G., Tatsumi, T.: J. Phys. Chem. B**103** (1999) 8647.

2002Yam1 Yamamoto, K., Plévert, J., Uneme, M., Tatsumi, T.: Microporous Mesoporous Mater. **55** (2002) 81.

2005Yal1 Yaluris, G., Ziebarth, M.S., Zhao, X.: U.S. Patent Appl. 2005/232839 (2005).

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