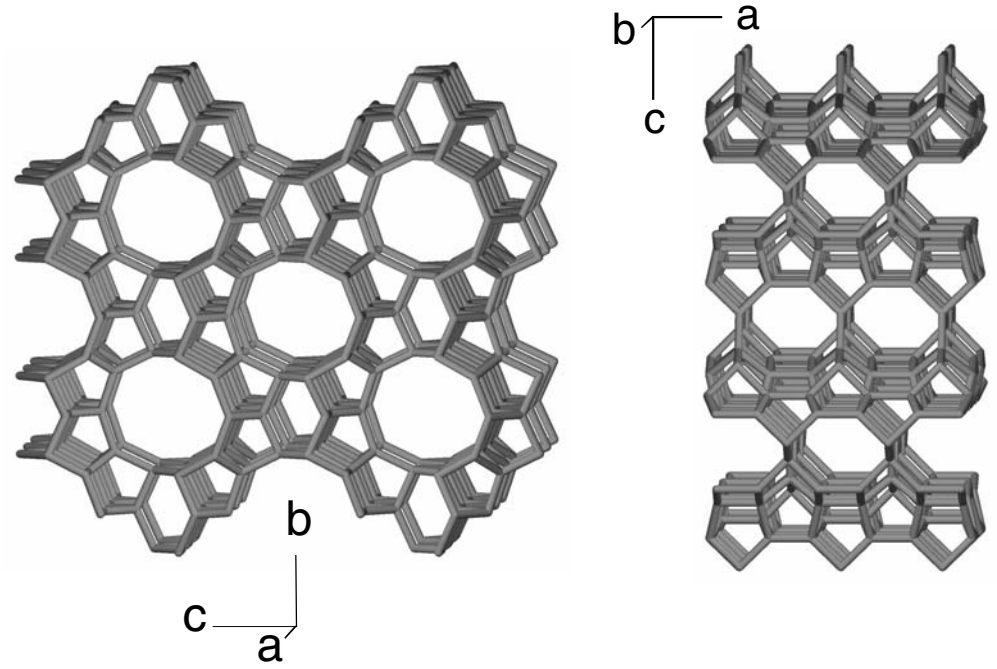
MFS

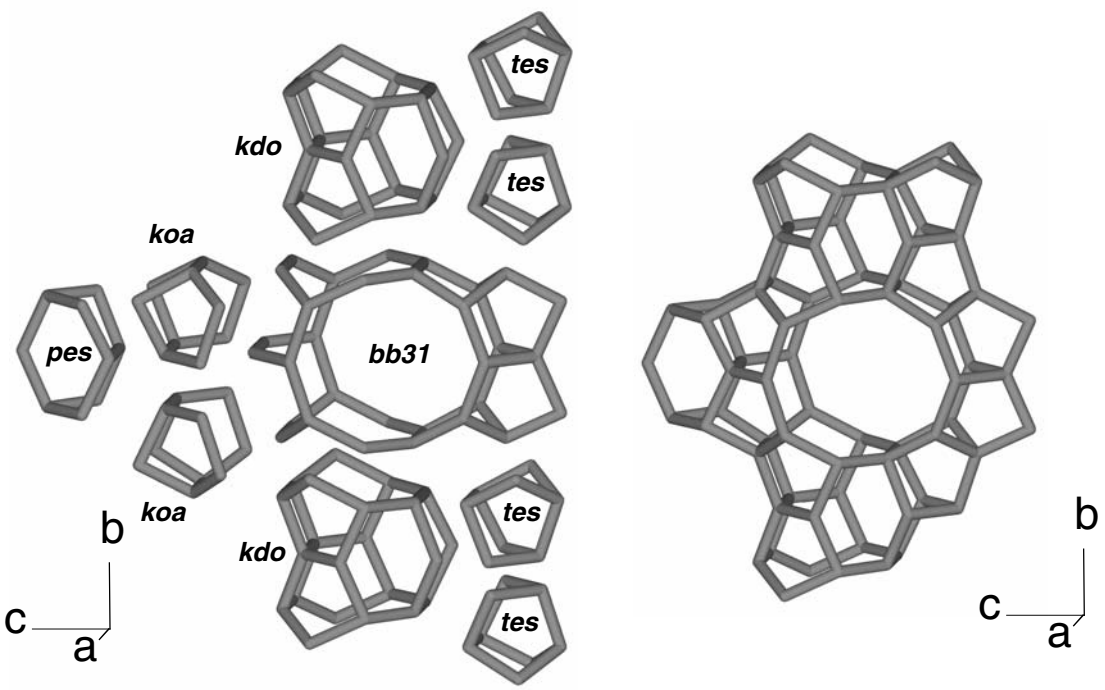
MFS.1 Zeolite framework type and topology

The designation of the FTC refers to the type material ZS**M**-**F**ifty-**S**even (ZSM-57, Zeolite Socony Mobil with sequence number fifty-seven), first synthesized by [86Val1]. The framework structure (Fig. MFS.1.1) can be described as being built from *bb31* ($5^2 5^4 8^2 8^2 10^2$) units forming the 10-ring channels (**kdh** units, Figs. MFS.1.1a and MFS.1.3) parallel **a**, crosslinked by *kdo* ($4^2 5^4 6^2 6^1 8^2$), *koa* ($5^2 6^1 8^1$), *pes* ($5^2 6^2$), and *tes* (5^4) units as shown in Fig. MFS.1.2. The 10-ring channel is interpenetrated by an 8-ring channel (Figs. MFS.1.1b and MFS.1.4) formed by an alternating sequence of *bb31* and *kdo* units (Fig. MFS.1.2a).



a View parallel **a** rotated by 4° about **b** and **c**. **b** View parallel **b** rotated by 2° about **a** and **c**.

Fig. MFS.1.1 The framework structure of MFS-type zeolites in the highest possible topological symmetry *I m m* 2.



a Linkage of *bb31*, *koa*, *kdo*, *pes*, and *tes* units. **b** The complete assemblage shown in a).

Fig. MFS.1.2 Building scheme of the MFS-type framework. View parallel **a** rotated by 10° about **b** and **c**. Subsequent layers in front and in the rear are shifted by ½, ½, ½ according to the I-centering of the unit cell.

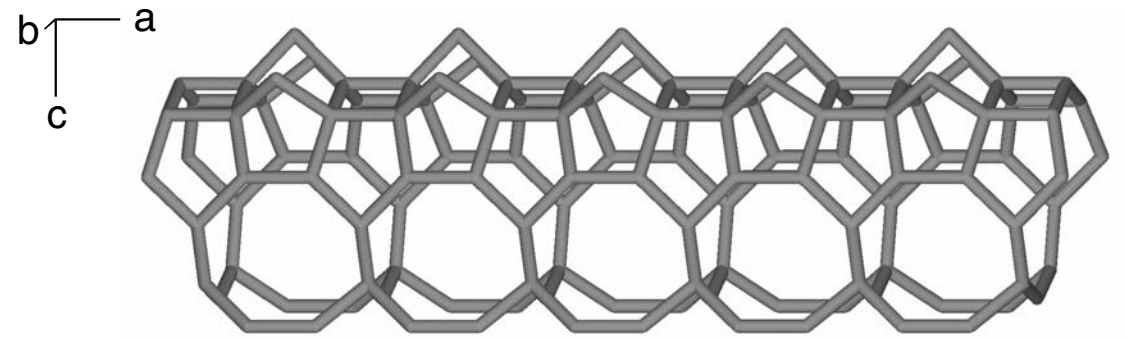


Fig. MFS.1.3 The 10-ring channel parallel **a**. View parallel **b** rotated by 6° about **a** and 12° about **c**.

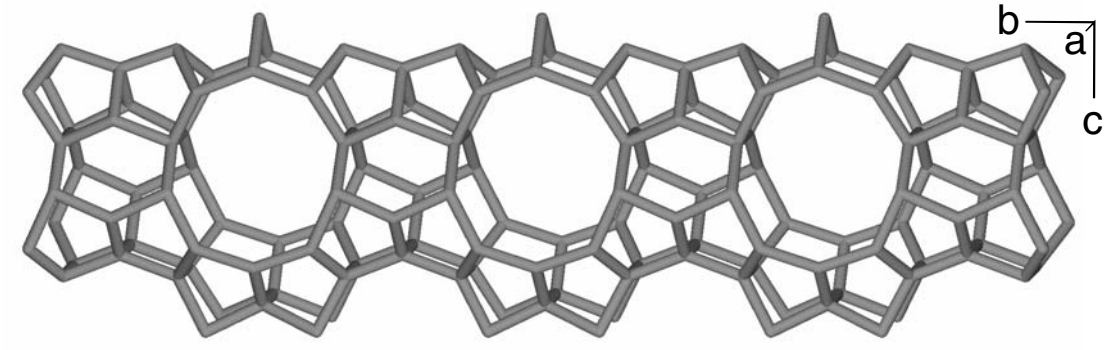


Fig. MFS.1.4 The 8-ring channel parallel **b**. View parallel **a** rotated by 10° about **b** and **c**.

MFS.2 Compounds and crystal data

Table MFS.2.1 Chemical data.

FD = framework density CE = cation exchange SR = sorbate T = temperature of thermal treatment [K]
SM = source of material TE = template TT = thermal treatment REF = reference

code	chemical composition	FD	SM	CE	TE/SR	TT	T	REF
***I m m* 2**								
MFS1989a01	$H_{1.5} \cdot Al_{1.5}Si_{34.5}O_{72}$ [1])	18.2	S	-	-	C	n.s.	89Sch1
MFS1990a01	$H_{1.5} \cdot Al_{1.5}Si_{34.5}O_{72}$	18.2	S	-	-	C	n.s.	90Sch1

[1]) Chemical composition from [90Sch1].

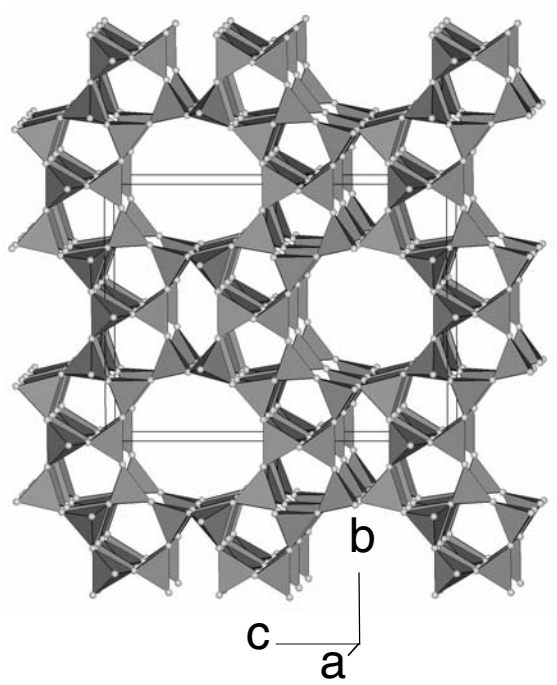
Table MFS.2.2 Structural parameters of the MFS-type compounds.

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
***I m m* 2**						
MFS1989a01	7.45	14.17	18.77	1981	n.s.	89Sch1
MFS1990a01	7.4510(7)	14.1711(8)	18.767(2)	1982	n.s.	90Sch1

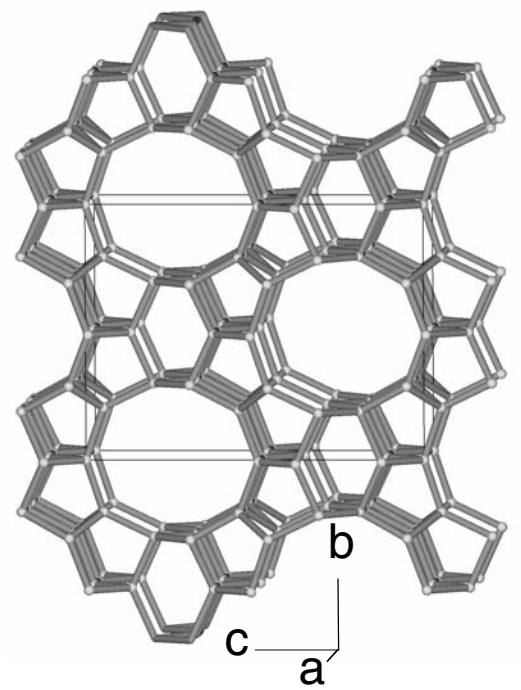
MFS.3 Framework structure of MFS-I compound (*I m m* 2 ,IT #44)

Table MFS.3.1 Atomic coordinates and site definitions for $H_{1.5} \cdot Al_{1.5}Si_{34.5}O_{72}$ (MFS1990a01, 90Sch1).

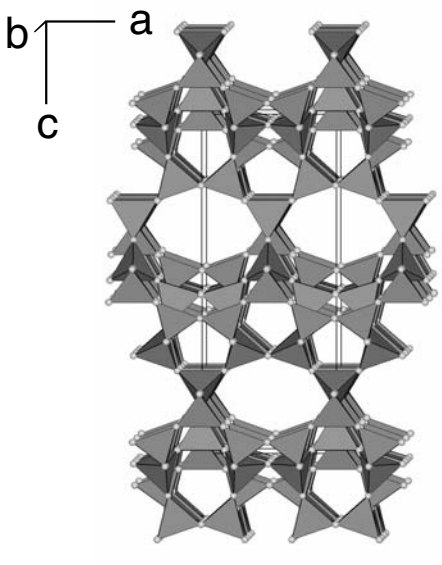
atom	*x*	*y*	*z*	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	0.2057	0.1963	0.1848	1	8(e)	7.68 / 0.32
(Si,Al)2	0.2939	0.7017	0.0427	1	8(e)	7.68 / 0.32
(Si,Al)3	0	0.2043	0.9486	*m* . .	4(d)	3.84 / 0.16
(Si,Al)4	0	0.6998	0.7986	*m* . .	4(d)	3.84 / 0.16
(Si,Al)5	0.2941	0	0.1176	. *m* .	4(c)	3.84 / 0.16
(Si,Al)6	0.7945	0	0.4848	. *m* .	4(c)	3.84 / 0.16
(Si,Al)7	0	½	0.8668	*m m* 2	2(b)	1.92 / 0.08
(Si,Al)8	0	0	0	*m m* 2	2(a)	1.92 / 0.08
O1	0.1755	0.2405	0.9876	1	8(e)	8
O2	0.8255	0.7253	0.7524	1	8(e)	8
O3	0.2531	0.0916	0.1632	1	8(e)	8
O4	0.2441	0.2688	0.1221	1	8(e)	8
O5	0.2570	0.5917	0.0319	1	8(e)	8
O6	0	0.2234	0.5276	*m* . .	4(d)	4
O7	0	0.0915	0.9503	*m* . .	4(d)	4
O8	0	0.2369	0.8678	*m* . .	4(d)	4
O9	0	0.5912	0.8173	*m* . .	4(d)	4
O10	0	0.2031	0.2079	*m* . .	4(d)	4
O11	0.1754	0	0.0473	. *m* .	4(c)	4
O12	0.6748	0	0.4149	. *m* .	4(c)	4
O13	0	½	0.5946	*m m* 2	2(b)	2
O14	0	0	0.4611	*m m* 2	2(a)	2



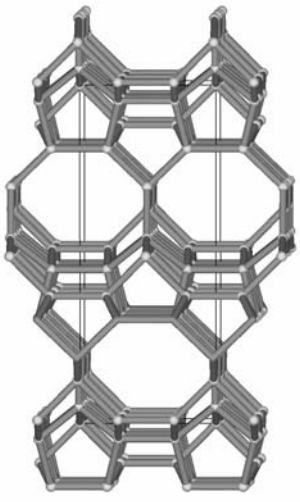
a Polyhedral representation. View parallel **a** rotated by 4° about **b** and **c**.



b Ball and stick model corresponding to a).



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



b Ball and stick model corresponding to c).

Fig. MFS.3.1 Projections of ZSM-57, $H_{1.5} \cdot Al_{1.5}Si_{34.5}O_{72}$ (MFS1990a01, 90Sch1).

Table MFS.3.2 Selected interatomic distances and angles for ZSM-57, $H_{1.5} \cdot Al_{1.5}Si_{34.5}O_{72}$ (MFS1990a01, 90Sch1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)1– O3	1.58	162	(Si,Al)2– O1	1.59	158
(Si,Al)1– O4	1.59	155	(Si,Al)2– O4	1.59	155
(Si.Al)1– O10	1.60	148	(Si.Al)2– O6	1.59	150
(Si,Al)1– O2	1.61	145	(Si,Al)2– O5	1.60	147
mean	1.60	153	mean	1.59	153
(Si,Al)3– O1	1.58	158	(Si,Al)4– O8	1.58	162
(Si,Al)3– O1	1.58	158	(Si,Al)4– O9	1.58	157
(Si.Al)3– O8	1.59	162	(Si.Al)4– O2	1.60	145
(Si,Al)3– O7	1.60	145	(Si,Al)4– O2	1.60	145
mean	1.59	156	mean	1.59	152
(Si,Al)5– O3	1.59	162	(Si,Al)6– O12	1.59	159
(Si,Al)5– O3	1.59	162	(Si,Al)6– O14	1.59	148
(Si.Al)5– O11	1.59	158	(Si.Al)6– O5	1.60	147
(Si,Al)5– O13	1.59	149	(Si,Al)6– O5	1.60	147
mean	1.59	158	mean	1.60	150
(Si,Al)7– O12	1.59	159	(Si,Al)8– O11	1.58	158
(Si,Al)7– O12	1.59	159	(Si,Al)8– O11	1.58	158
(Si.Al)7– O9	1.59	157	(Si.Al)8– O7	1.60	145
(Si,Al)7– O9	1.59	157	(Si,Al)8– O7	1.60	145
mean	1.59	158	mean	1.59	152

MFS.4 Chemical composition

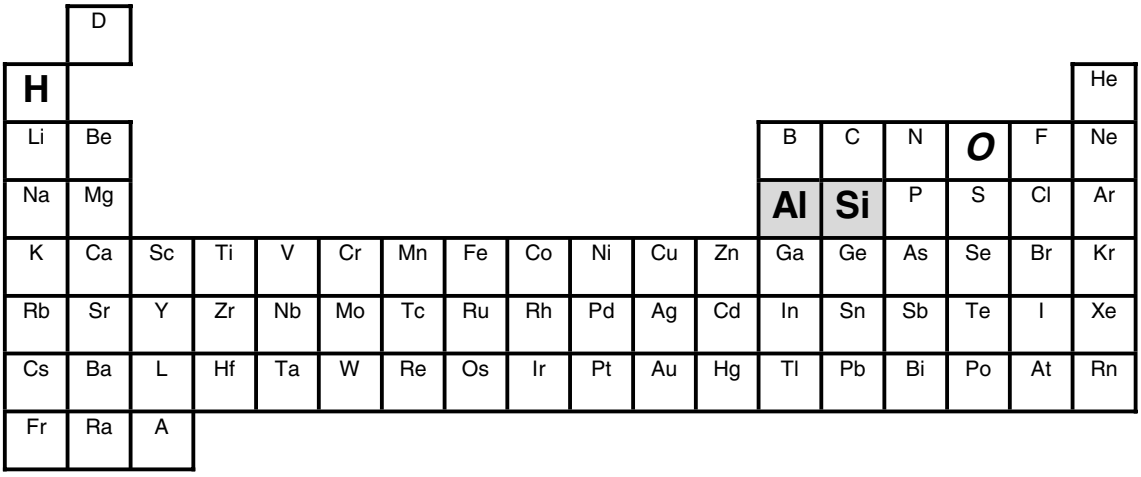


Fig. MFS.4.1 Chemical elements (highlighted) occurring in MFS-I. Framework cations are in grey fields.

MFS.5 Flexibility and apertures

There is insufficient information about the MFS-type framework to deduce anything about its flexibility.

The 10-ring openings parallel [100] are approximately 5.0 by 5.5 Å, that is they are as wide as in the related framework of MFI-topology. The 8-ring openings parallel [010] are elliptical and rather similar to the corresponding 8-rings in the related framework of FER-topology.

MFS.6 Other information

There are numerous patents and a few papers referring to the catalytic properties of aluminosilicates based on the ZSM-57 topology. The original patent [86Val1] claimed that using such compound toluene could be alkylated with methanol to produce xylenes. According to a recent patent application [2005Loe1] normal butanes can be oligomerized by a ZSM-57 catalyst. Furthermore zeolite ZSM-57 was evaluated for its ability for 1-butene skeletal isomerization and for n-octane cracking [2000Lee1].

MFS.7 References

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89Sch1 Schlenker, J.L., Higgins, J.B., Valyocsik, E.W. in: Zeolites for the nineties. Recent Research Reports of the 8th International Zeolite Conference (Eds.: Jansen, J.C., Moscou, L., Post, M.F.M.) (1989) 287.

90Sch1 Schlenker, J.L., Higgins, J.B., Valyocsik, E.W.: Zeolites **10** (1990) 293.

2000Lee1 Lee, S.-H., Lee, D.-K., Shin, C.H., Paik, W.C., Lee, W.M., Hong, S.B.: J. Catal. **196** (2005) 158.

2005Loe1 Loescher, M.E., Woods, D.G., Keenan, M.J., Silverberg, S.E. Allen, P.W.: U.S. Pat. Appl. 2004-898506 (2005).

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