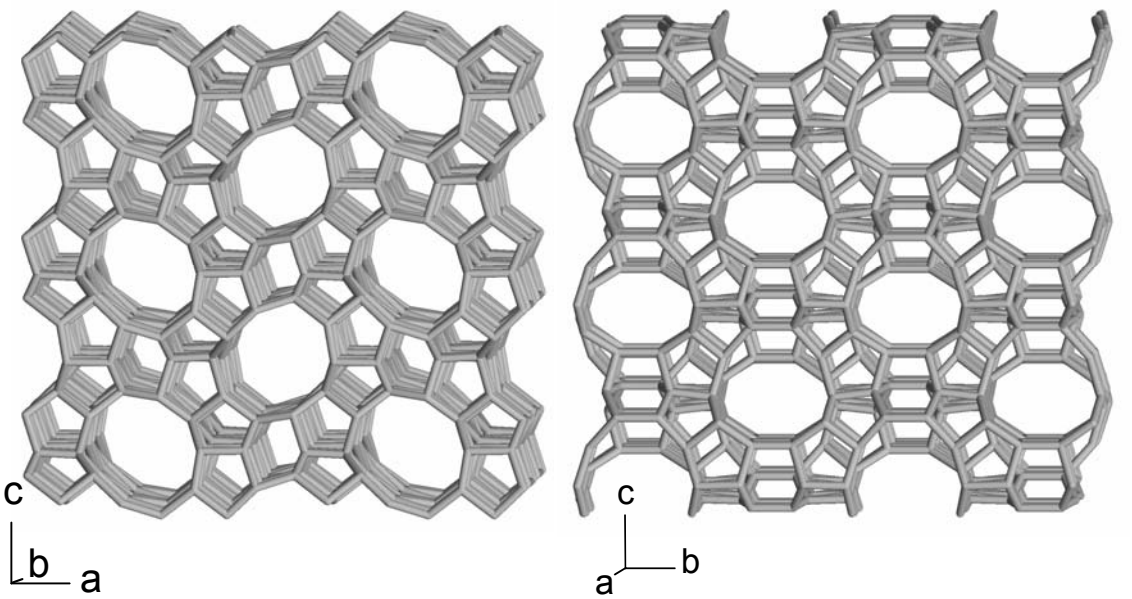
MFI

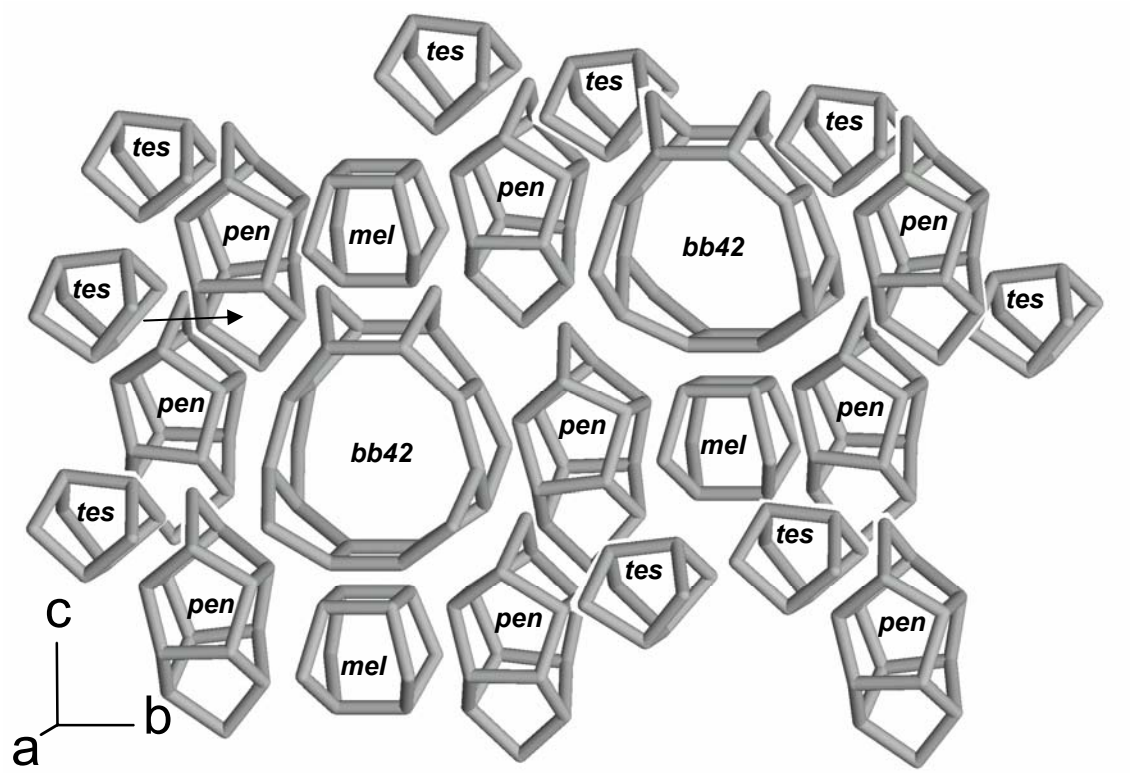
MFI.1 Zeolite framework type and topology

The designation of the framework type code (FTC) refers to the type material ZS**M**-**FI**ve (ZSM-5, Zeolite Socony Mobil with sequence number five), a high silica zeolite [72Arg1] synthesized using TPAOH as a template. It represents the orthorhombic end member of the pentasil family of zeolites [80Kok1] (see MEL for the tetragonal end member). The crystal structure was solved independently by [78Kok1] for ZSM-5 and by [78Fla1] for silicalite, the pure silica compound. However, the space group $P\,n\,2_1\,a$ assigned to silicalite is probably wrong (see [80Smi1] and J.V. Smith, personal communication in [81Ols1]) resulting from a refinement in an unnecessarily low symmetry indicated by strongly distorted SiO_4 polyhedra with Si-O distances varying from 1.20 Å to 2.65 Å. The true space group symmetry is likely to be $P\,n\,m\,a$. Consequently, the $P\,n\,2_1\,a$ structures are listed in Tables MFI.2.1 and MFI.2.2, but they are not further described in chapter MFI.3 and they are not listed in the Bärnighausen tree of Fig. MFI.1.3. The framework structure (Fig. MFI.1.1) can be built from 5-1 SBU's [2001Bae1] forming chains (**pet** units) of *pen* ($5^4 5^4$) units parallel **c**, also known as pentasil chain and unit, respectively [2001McC1].

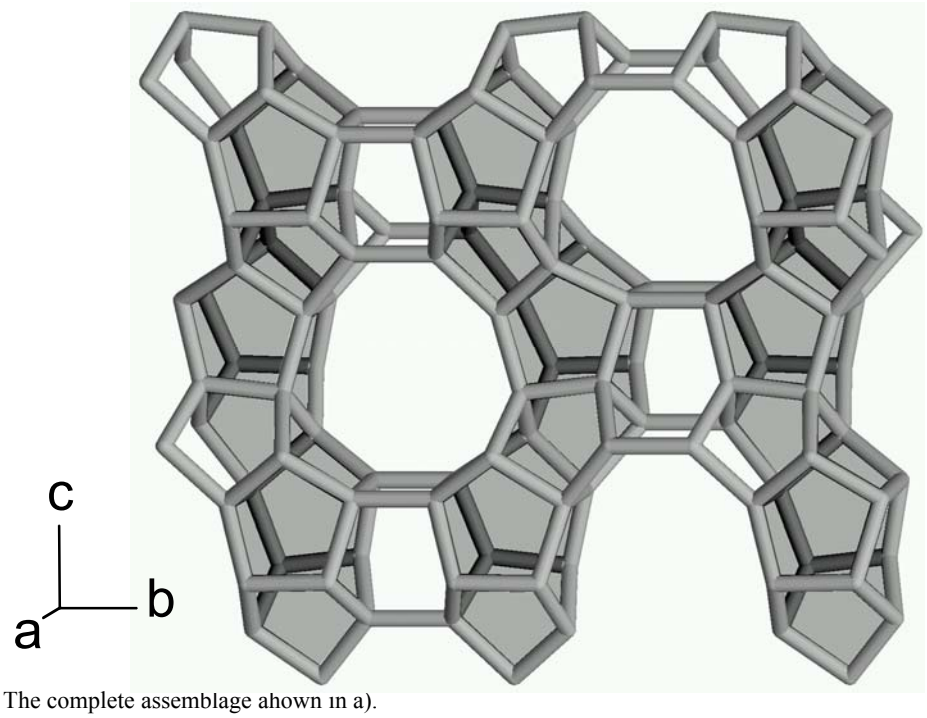


a View parallel -**b** rotated by 2° about **a** and **c**. **b** View parallel **a** rotated by 2° about **b** and **c**.

Fig. MFI.1.1. The framework structure of MFI-type compounds in the highest possible topological symmetry $P\,n\,m\,a$. View directions are chosen to conform to corresponding drawings in the literature, e.g., [90van1].

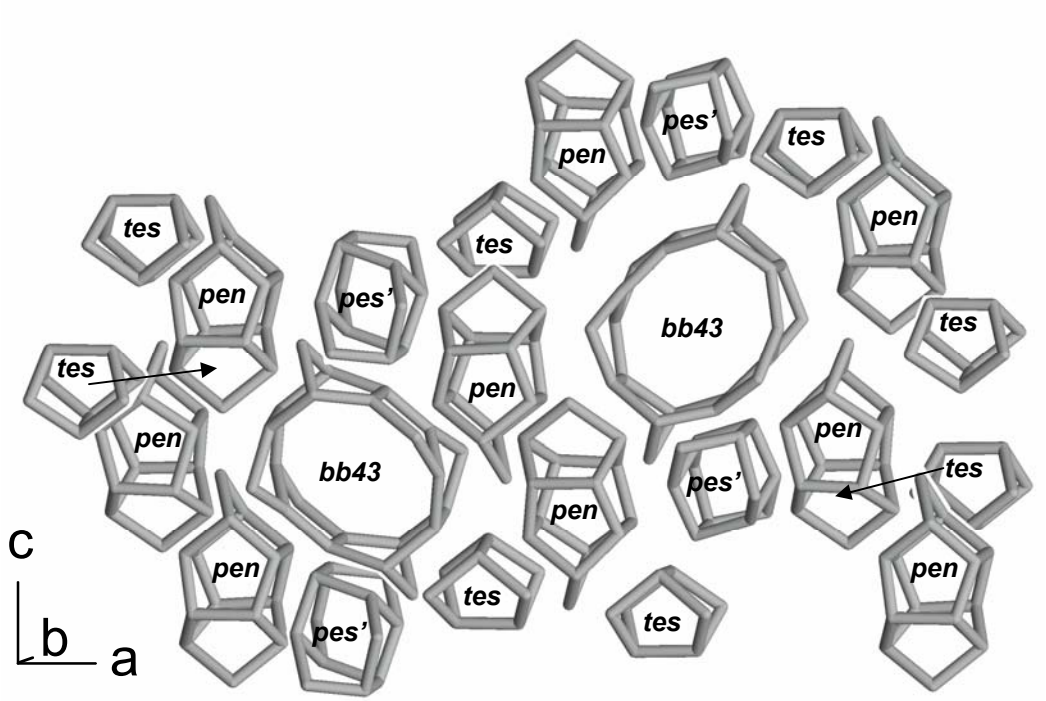


a Building scheme of the pentasil layer in ¼, *y*, *z*. View parallel **a** rotated by 10° about **b** and 15° about **c**. The *bb42* unit is an assemblage of a *kuh* ($4^1 5^2 5^2 8^1 10^1 10^1$) unit with a terminating *koa* ($5^2 6^1 8^1$) unit.

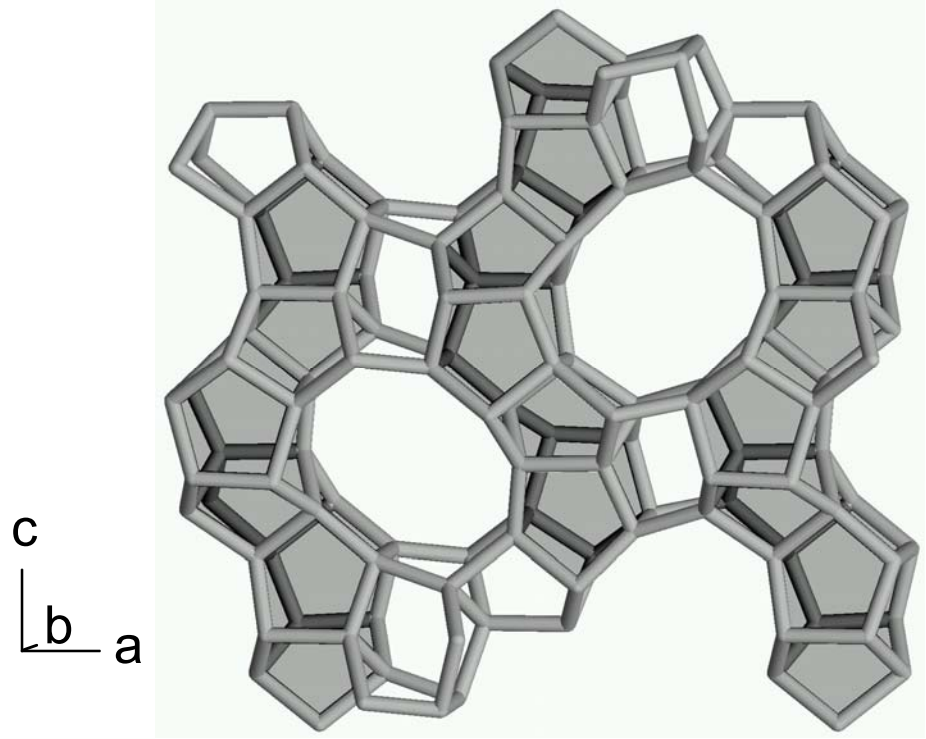


b The complete assemblage shown in a).

Fig. MFI.1.2. Building scheme of the pentasil layers. Pentasil chains (**pet** units) are drawn semi transparently.



c Building scheme of the pentasil layer in *x*, 0, *z*. View parallel **-b** rotated by 10° about **a** and **c**. The *pes*' units consist of two *pes* units. The *bb43* unit is an assemblage of a *kns* ($5^4 6^2 10^2$) unit with terminating handles on the 6-rings.



d The complete assemblage ahown in c).

Fig. MFI.1.2. (continued) Building scheme of the pentasil layers. Pentasil chains (**pet** units) are drawn semi transparently.

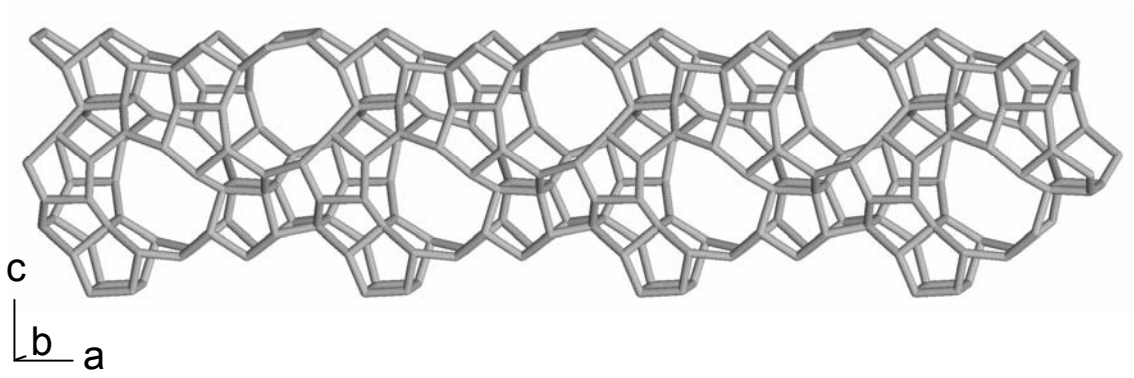


Fig. MFI.1.3 The 10-ring channel parallel **a**. View parallel **-b** rotated by 10° about **a** and 15° about **c**.

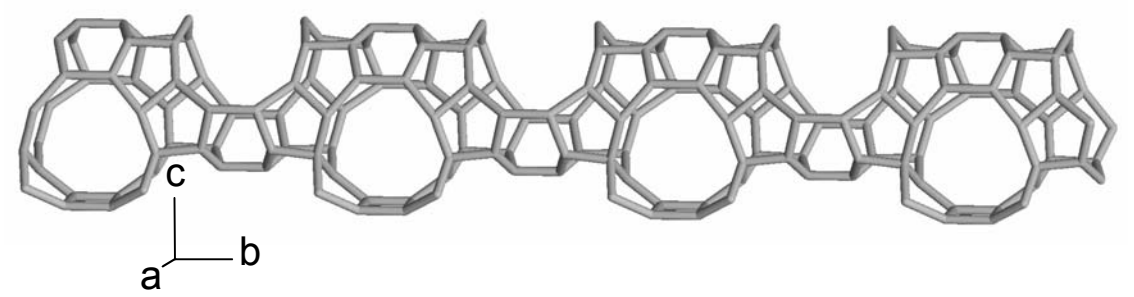


Fig. MFI.1.4 The 10-ring channel parallel **b**. View parallel **a** rotated by 15° about **b** and 10° about **c**.

Other names encountered for this topology in addition to ZSM-5 and silicalite include, among others: pentasil [84Pan1], TS-1 (for the Ti-containing compound [2000Mar1]), boralite (for the B-containing compound [87Men1]), mutinaite (for the corresponding mineral, which has been discovered [97Vez1] after ZSM-5 had been synthesized), and silicalite-1 ([2002Aub1], in order to distinguish it from silicalite-2, which has the MEL-topology). Linkage of the chains by an inversion center (i-stacking) yields the MFI-type framework wheras the MEL-type framework is built by reflection (σ-stacking) of the pentasil chains. The **pet** or *pen* units are crosslinked by *bb42* ($4^1 5^2 5^2 5^2 6^1 10^1 10^1 10^1$), *mel* ($4^1 5^2 6^2$), and *tes* ($5^4$) units in the (100) plane (Fig. MFI.1.2a,b), and by *bb43* ($5^4 5^4 10^2$), *pes* ($5^2 6^2$), and *tes* units in the (010) plane (Fig. MFI.1.2c,d).

Frequently, intergrowth of ZSM-5 with ZSM-11 is observed (see, e.g., [86Jab1]) due to the similarities in their pentasil framework structures. ZSM-8 [71Mob1] synthesized using TEAOH as template was believed to have a unique framework structure different from ZSM-5 and silicalite due to different lattice constants [88Jos1] and peak splittings in the powder diffraction pattern [84Lec1]. However, it could be shown [94Wei2] that the differences between the lattice constants are related to wrongly indexed powder patterns of ZSM-8. Consequently, the framework structures of ZSM-5 and ZSM-8 are essentially identical [94Wei1]. Differences in their physico-chemical properties might be related to intergrowth effects [94Wei3].

Numerals in the atom names of Table MFI.1.1 (and Tables in chapter 3) are separated by a blank to distinguish between first and second order indices.

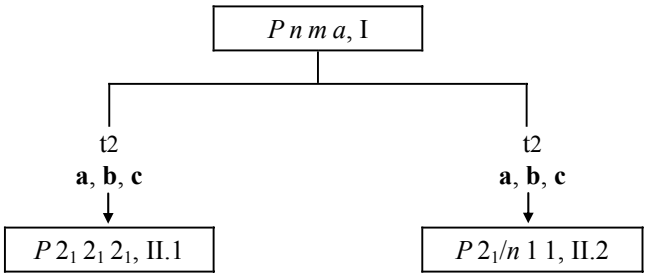


Fig. MFI.1.3 The Bärnighausen tree illustrating the symmetry relationship of the MFI types.

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

MFI-I *P n m a*	MFI-II.1 *P* 2$_1$ 2$_1$ 2$_1$	MFI-I *P n m a*	MFI-II.2 *P* 2$_1$/*n* 1 1
T1 [8(d), 1]	T11 [4(a), 1] T12 [4(a), 1]	T1 [8(d), 1]	T11 [4(e), 1] T12 [4(e), 1]
T2 [8(d), 1]	T21 [4(a), 1] T22 [4(a), 1]	T2 [8(d), 1]	T21 [4(e), 1] T22 [4(e), 1]
T3 [8(d), 1]	T31 [4(a), 1] T32 [4(a), 1]	T3 [8(d), 1]	T31 [4(e), 1] T32 [4(e), 1]
T4 [8(d), 1]	T41 [4(a), 1] T42 [4(a), 1]	T4 [8(d), 1]	T41 [4(e), 1] T42 [4(e), 1]
T5 [8(d), 1]	T51 [4(a), 1] T52 [4(a), 1]	T5 [8(d), 1]	T51 [4(e), 1] T52 [4(e), 1]
T6 [8(d), 1]	T61 [4(a), 1] T62 [4(a), 1]	T6 [8(d), 1]	T61 [4(e), 1] T62 [4(e), 1]
T7 [8(d), 1]	T71 [4(a), 1] T72 [4(a), 1]	T7 [8(d), 1]	T71 [4(e), 1] T72 [4(e), 1]
T8 [8(d), 1]	T81 [4(a), 1] T82 [4(a), 1]	T8 [8(d), 1]	T81 [4(e), 1] T82 [4(e), 1]
T9 [8(d), 1]	T91 [4(a), 1] T92 [4(a), 1]	T9 [8(d), 1]	T91 [4(e), 1] T92 [4(e), 1]
T10 [8(d), 1]	T10 1 [4(a), 1] T10 2 [4(a), 1]	T10 [8(d), 1]	T10 1 [4(e), 1] T10 2 [4(e), 1]
T11 [8(d), 1]	T11 1 [4(a), 1] T11 2 [4(a), 1]	T11 [8(d), 1]	T11 1 [4(e), 1] T11 2 [4(e), 1]

Table MFI.1.1 (continued).

MFI-I *P n m a*	MFI-II.1 *P* 2_1 2_1 2_1	MFI-I *P n m a*	MFI-II.2 *P* $2_1/n$ 1 1
T12 [8(d), 1]	T12 1 [4(a), 1] T12 2 [4(a), 1]	T12 [8(d), 1]	T12 1 [4(e), 1] T12 2 [4(e), 1]
O1 [8(d), 1]	O11 [4(a), 1] O12 [4(a), 1]	O1 [8(d), 1]	O11 [4(e), 1] O12 [4(e), 1]
O2 [8(d), 1]	O21 [4(a), 1] O22 [4(a), 1]	O2 [8(d), 1]	O21 [4(e), 1] O22 [4(e), 1]
O3 [8(d), 1]	O31 [4(a), 1] O32 [4(a), 1]	O3 [8(d), 1]	O31 [4(e), 1] O32 [4(e), 1]
O4 [8(d), 1]	O41 [4(a), 1] O42 [4(a), 1]	O4 [8(d), 1]	O41 [4(e), 1] O42 [4(e), 1]
O5 [8(d), 1]	O51 [4(a), 1] O52 [4(a), 1]	O5 [8(d), 1]	O51 [4(e), 1] O52 [4(e), 1]
O6 [8(d), 1]	O61 [4(a), 1] O62 [4(a), 1]	O6 [8(d), 1]	O61 [4(e), 1] O62 [4(e), 1]
O7 [8(d), 1]	O71 [4(a), 1] O72 [4(a), 1]	O7 [8(d), 1]	O71 [4(e), 1] O72 [4(e), 1]
O8 [8(d), 1]	O81 [4(a), 1] O82 [4(a), 1]	O8 [8(d), 1]	O81 [4(e), 1] O82 [4(e), 1]
O9 [8(d), 1]	O91 [4(a), 1] O92 [4(a), 1]	O9 [8(d), 1]	O91 [4(e), 1] O92 [4(e), 1]
O10 [8(d), 1]	O10 1 [4(a), 1] O10 2 [4(a), 1]	O10 [8(d), 1]	O10 1 [4(e), 1] O10 2 [4(e), 1]
O11 [8(d), 1]	O11 1 [4(a), 1] O11 2 [4(a), 1]	O11 [8(d), 1]	O11 1 [4(e), 1] O11 2 [4(e), 1]
O12 [8(d), 1]	O12 1 [4(a), 1] O12 2 [4(a), 1]	O12 [8(d), 1]	O12 1 [4(e), 1] O12 2 [4(e), 1]
O13 [8(d), 1]	O13 1 [4(a), 1] O13 2 [4(a), 1]	O13 [8(d), 1]	O13 1 [4(e), 1] O13 2 [4(e), 1]

Table MFI.1.1 (continued).

MFI-I *P n m a*	MFI-II.1 *P* 2_1 2_1 2_1	MFI-I *P n m a*	MFI-II.2 *P* $2_1/n$ 1 1
O14[8(d), 1]	O14 1 [4(a), 1] O14 2 [4(a), 1]	O14[8(d), 1]	O14 1 [4(e), 1] O14 2 [4(e), 1]
O15[8(d), 1]	O15 1 [4(a), 1] O15 2 [4(a), 1]	O15[8(d), 1]	O15 1 [4(e), 1] O15 2 [4(e), 1]
O16[8(d), 1]	O16 1 [4(a), 1] O16 2 [4(a), 1]	O16[8(d), 1]	O16 1 [4(e), 1] O16 2 [4(e), 1]
O17[8(d), 1]	O17 1 [4(a), 1] O17 2 [4(a), 1]	O17[8(d), 1]	O17 1 [4(e), 1] O17 2 [4(e), 1]
O18[8(d), 1]	O18 1 [4(a), 1] O18 2 [4(a), 1]	O18[8(d), 1]	O18 1 [4(e), 1] O18 2 [4(e), 1]
O19[8(d), 1]	O19 1 [4(a), 1] O19 2 [4(a), 1]	O19[8(d), 1]	O19 1 [4(e), 1] O19 2 [4(e), 1]
O20[8(d), 1]	O20 1 [4(a), 1] O20 2 [4(a), 1]	O20[8(d), 1]	O20 1 [4(e), 1] O20 2 [4(e), 1]
O21[8(d), 1]	O21 1 [4(a), 1] O21 2 [4(a), 1]	O21[8(d), 1]	O21 1 [4(e), 1] O21 2 [4(e), 1]
O22[8(d), 1]	O22 1 [4(a), 1] O22 2 [4(a), 1]	O22[8(d), 1]	O22 1 [4(e), 1] O22 2 [4(e), 1]
O23[4(c), . 2 .]	O23 [4(a), 1]	O23[4(c), . 2 .]	O23 [4(e), 1]
O24[4(c), . 2 .]	O24 [4(a), 1]	O24[4(c), . 2 .]	O24 [4(e), 1]
O25[4(c), . 2 .]	O25 [4(a), 1]	O25[4(c), . 2 .]	O25 [4(e), 1]
O26[4(c), . 2 .]	O26 [4(a), 1]	O26[4(c), . 2 .]	O26 [4(e), 1]

MFI.2 Compounds and crystal data

Table MFI.2.1 Chemical data.

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

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MFI-I *Pnma*									
MFI1980a01	$Si_{96}O_{192}$	silicalite	18.1	S	-	-	C	873	80Smi1
MFI1981a01	$Na_{0.5}((C_3H_7)_4N)_{0.5} \cdot AlSi_{95}O_{192}$[1])	ZSM-5	17.9	S	-	TPA[1])	-	-	81Ols1
MFI1981b01	$Si_{96}O_{192} \cdot 4(C_3H_7)_4NF$	silicalite	18.0	S	-	TPAF	-	-	81Pri1
MFI1982a01	$Si_{96}O_{192} \cdot 4(C_3H_7)_4NF$	silicalite	18.0	S	-	TPAF	-	-	82Pri1
MFI1982b01	$Na_{0.1}H_{3.9} \cdot Al_4Si_{92}O_{192}$	ZSM-5	17.7	S	-	-	C	813	82Yu1
MFI1984a01	$Si_{96}O_{192} \cdot 4(C_3H_7)_4NOH$	silicalite	17.8	S	-	TPAOH	-	-	84Bae1
MFI1984b01	$H_{6.4} \cdot B_{6.4}Si_{89.6}O_{192}$	B-Si-pentasil	18.3	S	-	-	C	873	84Pan1
MFI1985a01	$Na_{3.5}((C_3H_7)_4N)_{3.5} \cdot Al_7Si_{89}O_{192}$	ZSM-5	17.9	S	-	TPA	-	-	85Ler1
MFI1986a01	$((C_3H_7)_4N)_4 \cdot Al_4Si_{92}O_{192}$	ZSM-5	17.8	S	-	TPA	-	-	86Cha1
MFI1986b01	$Si_{96}O_{192}$	H-ZSM5[2])	17.9	S	-	-	C[2])	n.s.	86Tay1
MFI1986c01	$H_{2.0}Ni_{2.0} \cdot Al_6Si_{90}O_{192}$	ZSM-5	17.8	S	-	-	C	773	86Liu1
MFI1987a01	$Na_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 4(C_3H_7)_4NOH\ nH_2O$	ZSM-5	18.0	S	-	TPAOH, H_2O	-	-	87van1
MFI1987a02	$Na_{0.3}\ .\ Al_{0.3}Si_{95.7}O_{192} \cdot 4(C_3H_7)_4NOH\ nH_2O$	ZSM-5	18.0	S	-	TPAOH, H_2O	-	-	87van1
MFI1987b01	$Na_{1.5} \cdot Al_{1.5}Si_{94.5}O_{192} \cdot 8.05C_6D_6$	ZSM-5	18.1	S	-	deutero-benzene	C	773	87Tay1
MFI1987d01	$H_{3.2} \cdot B_{3.2}Al_{0.02}Si_{92.8}O_{192} \cdot 6C_6H_4(CH_3)_2$	Boralite	18.2	S	-	xylene	C	773	87Men1
MFI1987e01	$H_{4.83} \cdot B_{0.03}Al_{4.8}Si_{91.17}O_{192} \cdot 4C_6H_6$	ZSM-5	17.9	S	-	benzene	C	773	87Men2
MFI1987f01	$H_{4.83} \cdot B_{0.03}Al_{4.8}Si_{91.17}O_{192} \cdot 7.16C_6H_{14}$	ZSM-5	17.8	S	-	hexane	C	773	87Men3
MFI1988a02	$Si_{96}O_{192} \cdot 6H_2O$	ZSM-5	18.0	S	-	H_2O	C	n.s.	88Sch1
MFI1988a03	$Si_{96}O_{192} \cdot 6.8C_8H_{10}$	ZSM-5	17.8	S	-	xylene	C	n.s.	88Sch1
MFI1988b01	$Si_{96}O_{192}$		18.0	T	-	-	-	-	88van1
MFI1988c01	$H_{1.4} \cdot B_{1.38}Al_{0.02}Si_{94.6}O_{192} \cdot 8C_8H_{10}$	B.ZSM-5	17.9	S	-	xylene	C	823	88Men1
MFI1989a01	$H_3 \cdot B_3Si_{93}O_{192} \cdot 10(C_5H_5N)$	B.ZSM-5	18.1	S	-	pyridine	C	n.s.	89Men1

[1]) It is assumed that the tetraalkyl cation is TPA.

[2]) No information on how the sample was synthetized or analysed is given in the paper. Since it is called an H-ZSM-5 it was presumably calcined. However, the chemical composition is that of pure silicalite.

Table MFI.2.1 (MFI-I, *P n m a* continued).

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MFI1989c01	$Si_{96}O_{192}$	-	18.0	T	-	-	-	-	89Uyt1
MFI1990b01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192}$	H-ZSM-5	18.0	S	-	-	C	811	90van2
MFI1991a01	$Tl_{3.4} \cdot Al_{3.4}Si_{92.6}O_{192} \cdot 27H_2O$	ZSM-5	17.8	S	Tl	H_2O	-	-	91Hud1
MFI1991b01	$HCs_3 \cdot Al_4Si_{92}O_{192} \cdot 9.6H_2O$	ZSM-5	17.8	S	-	H_2O	C	873	91Lin1
MFI1991b02	$HCs_3 \cdot Al_4Si_{92}O_{192}$	ZSM-5	17.9	S	-	-	C	873	91Lin1
MFI1991c01	$Si_{96}O_{192} \cdot 4(C_3H_7)_4NF$	silicalite	17.9	S	-	TPAF	C	n.s.	91Men1
MFI1992c01	$H_{1.61}Na_{0.17} \cdot Al_{1.78}Si_{94.22}O_{192} \cdot 24H_2O$	ZSM-5	17.9	S	-	H_2O	C	n.s.	92Li1
MFI1992c02	$H_{1.22}Na_{0.35} \cdot Al_{1.57}Si_{94.43}O_{192} \cdot 16H_2O$	ZSM-5	18.0	S	-	H_2O	C	n.s.	92Li1
MFI1993a01	$H_{1.3} \cdot Al_{1.3}Si_{94.7}O_{192} \cdot 2.2C_6D_6$	ZSM-5	17.9	S	-	deutero-benzene	C	823	93Sac1
MFI1993c01	$Si_{96}O_{192} \cdot 4C_{10}H_8$	silicalite	18.0	S	-	naphthalene	C	823	93Men1
MFI1994a01	$HNa \cdot Al_2Si_{94}O_{192} \cdot 4(C_2H_5)_4NOH\ 3H_2O$	ZSM-8	17.9	S	-	TEAOH	-	-	94Wei1
MFI1994a02	$HNa \cdot Al_2Si_{94}O_{192}$	ZSM-8	17.8	S	-	-	C	813	94Wei1
MFI1994c01	$Al_3Si_{93}O_{192} \cdot 3C_{10}H_8$	HZSM-5	18.1	S	-	naphthalene	C	n.s.	94Kle1
MFI1994c02	$Al_3Si_{93}O_{192} \cdot 3C_{11}H_{10}$	HZSM-5	18.1	S	-	2-methyl-naphthalene	C	n.s.	94Kle1
MFI1995a01	$HNa \cdot Al_2Si_{94}O_{192} \cdot 4(C_2H_5)_4NOH\ 4H_2O$	ZSM-8	17.9	S	-	TEAOH, H_2O	-	-	95Wei1
MFI1995a02	$HNa \cdot Al_2Si_{94}O_{192} \cdot 9H_2O$	ZSM-8	17.9	S	-	H_2O	C	813	95Wei1
MFI1995a03	$H_2Na \cdot Al_3Si_{93}O_{192} \cdot 3(C_2H_5)_4NOH\ 4H_2O$	ZSM-8	17.9	S	-	TEAOH, H_2O	-	-	95Wei1
MFI1995a04	$H_2Na \cdot Al_3Si_{93}O_{192} \cdot 13H2O$	ZSM-8	17.8	S	-	H_2O	C	813	95Wei1
MFI1995a05	$Na_2 \cdot Al_2Si_{94}O_{192}$	ZSM-5	17.9	S	-	-	C	813	95Wei1
MFI1995b01	$Si_{96}O_{192} \cdot 4C_8H_{10}$	silicalite	18.0	S	-	xylene	C	n.s.	95Men1
MFI1995d01	$Si_{96}O_{192} \cdot 2C_{14}H_{12}$	silicalite	18.0	S	-	stilbene	C	n.s.	95Par1
MFI1996a01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 2.56C_6H_4Cl_2$	H-ZSM-5	18.0	S	-	pdcb	C	811	96van1
MFI1996d01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 3.68C_{10}H_8$	H-ZSM-5	18.1	S	-	naphthalene	C	811	96van3
MFI1997a01	$Ca_{3.78}K_{0.11}Mg_{0.21}Na_{2.76} \cdot Al_{11.20}Si_{84.91}O_{192} \cdot 60H_2O$	mutinaite	17.6	M	-	H_2O	-	-	97Vez1
MFI1997b01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 4C_6H_6N_2O_2$	H-ZSM-5	18.0	S	-	nitroaniline	C	823	97van1
MFI1998a01	$Si_{96}O_{192} \cdot 4C_6H_6N_2O_2$	silicalite	18.1	S	-	nitroaniline	C	n.s.	98Men1
MFI1998b01	$Si_{96}O_{192} \cdot 2.85C_8H_{10}$	ZSM-5	18.1	S	-	xylene	C	773	98Lew1
MFI1998c01	$H_{3.8} \cdot Al_{3.8}Si_{92.2}O_{192} \cdot 5.4C_6H_4(CH_3)_2$	ZSM-5	18.0	S	-	xylene	C	973	98Men2
MFI1998c02	$Cs_{3.8} \cdot Al_{3.8}Si_{92.2}O_{192} \cdot 2.6C_6H_4(CH_3)_2$	ZSM-5	17.9	S	-	xylene	C	973	98Men2
MFI1999b01	$Ti_{1.93}Si_{94.07}O_{192}$	TS-1	17.8	S	-	-	C	823	99Lam1
MFI2000a01	$H_{28.80} \cdot Si_{88.32}O_{192}$	defective	18.0	S	-	-	C	823	2000Art

Table MFI.2.1 (MFI-I, *P n m a* continued).

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MFI2000b01	$H_{0.1}Na_{2.5} \cdot Al_{2.5}Si_{93.4}O_{192}$	ZSM-5	17.9	S	-	-	C	823	2000Goy1
MFI2000b02	$H_{0.1}Na_{2.5} \cdot Al_{2.5}Si_{93.4}O_{192} \cdot 3.4C_6D_6$	ZSM-5	17.9	S	-	deutero-benzene	C	823	2000Goy1
MFI2000b03	$H_{0.1}Na_{2.5} \cdot Al_{2.5}Si_{93.4}O_{192} \cdot 7.6C_6D_6$	ZSM-5	17.9	S	-	deutero-benzene	C	823	2000Goy1
MFI2000c01	$Cs_{5.8} \cdot Al_{5.8}Si_{90.2}O_{192}$	Cs-ZSM-5	18.0	S	Cs	-	D	773	2000Ols1
MFI2000d01	$Si_{96}O_{192} \cdot 4C_6H_6N_2O_2$	ZSM-5	18.2	S	-	nitroaniline	C	1073	2000Fyf1
MFI2000e01	$Si_{96}O_{192} \cdot 3.94C_8H_{10}$	silicalite	18.0	S	-	xylene	C	798	2000Nai1
MFI2000e02	$Si_{96}O_{192} \cdot 6.8C_8H_{10}$	silicalite	17.9	S	-	xylene	C	798	2000Nai1
MFI2000f01	$Ti_{2.09}Si_{93.81}O_{192}$	TS-1	17.9	S	-	-	C	n.s.	2000Mar1
MFI2000g01	$Ti_{2.47}Si_{93.53}O_{192}$	TS-1	18.0	S	-	-	C	823	2000Hij1
MFI2000h01	$Na_{2.08} \cdot Fe_{2.5}Si_{93.5}O_{192} \cdot 2.4(C_3H_7)_4NOH$	Fe-silicalite	17.8	S	-	TPAOH	-	-	2000Mil1
MFI2001a01	$Ti_{2.09}Si_{93.81}O_{192}$	TS-1	17.9	S	-	-	C	823	2001Lam1
MFI2001a02	$Ti_{2.09}Si_{93.81}O_{192}$	TS-1	17.9	S	-	-	C	823	2001Lam1
MFI2001a03	$Ti_{2.64}Si_{93.36}O_{192}$	TS-1	17.8	S	-	-	C	823	2001Lam1
MFI2001b01	$Ti_{2.46}Si_{93.54}O_{192}$	TS-1	17.8	S	-	-	C	823	2001Hen1
MFI2001b02	$Ti_{2.46}Si_{93.54}O_{192}$	TS-1	17.8	S	-	-	C	823	2001Hen1
MFI2001b03	$Ti_{2.46}Si_{93.54}O_{192}$	TS-1	17.8	S	-	-	C	823	2001Hen1
MFI2001b04	$Ti_{2.46}Si_{93.54}O_{192}$	TS-1	17.8	S	-	-	C	823	2001Hen1
MFI2002a01	$Si_{96}O_{192} \cdot 4(C_3H_7)_4NF$	silicalite-1	17.9	S	-	TPAF	-	-	2002Aub1
MFI2003a01	$7.28C_2H_{10}N_2 \cdot B_{14}Si_{82}O_{192}$	BOR-C	18.6	S	-	H_2EDA	-	-	2003Per1
MFI2003a02	$7.28C_2H_{10}N_2 \cdot B_{14}Si_{82}O_{192}$	BOR-C	18.6	S	-	H_2EDA	-	-	2003Per1
MFI2004b01	$Si_{96}O_{192}$	silicalite	17.9	T	-	-	-	-	2004Ast1
MFI2005b01	$Si_{96}O_{192} \cdot 3C_6H_4(CD_3)_2$	ZSM-5	18.0	S	-	xylene	C	n.s.	2005Fyf1
MFI2006a01	$Cs_{6.6}H_{0.3} \cdot Al_{6.9}Si_{89.1}O_{192}$	ZSM-5	18.0	S	Cs	-	C	n.s.	2006Men1
MFI2006a01	$Cs_{6.6}H_{0.3} \cdot Al_{6.9}Si_{89.1}O_{192}$	ZSM-5	17.9	S	Cs	-	C	n.s.	2006Men1
MFI2006a01	$Cs_{6.6}H_{0.3} \cdot Al_{6.9}Si_{89.1}O_{192}$	ZSM-5	17.9	S	Cs	-	C	n.s.	2006Men1
MFI2006a01	$Cs_{6.6}H_{0.3} \cdot Al_{6.9}Si_{89.1}O_{192}$	ZSM-5	17.9	S	Cs	-	C	n.s.	2006Men1
MFI2006a01	$Cs_{6.6}H_{0.3} \cdot Al_{6.9}Si_{89.1}O_{192}$	ZSM-5	17.9	S	Cs	-	C	n.s.	2006Men1
MFI2006b01	$H_{0.7}Na_{2.6}(C_{16}H_{28}N)_4 \cdot Al_{3.3}Si_{92.7}O_{192}$ [1])	ZSM-5	17.8	S	-	P3BZY[1])	D	383	2006Men2
MFI-II.1 ***P* 2₁ 2₁ 2₁**									
MFI1989b01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 8C_8H_{10}$	H-ZSM-5	17.9	S	-	xylene	C	811	89van1

[1]) P3BZY is treated as a neutral species in [2006Men2]. In fact, it is a cation which could account for the total charge compensation of the framework disregarding the Na and H atoms which could not be localized by the authors in the crystal structure refinement.

Table MFI.2.1 (MFI-II.1, $P\,2_1\,2_1\,2_1$ continued).

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
MFI1996b01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 8C_6H_4C_{l2}$	H-ZSM-5	18.0	S	-	pdcb	C	811	96van2
MFI1998a02	$Si_{96}O_{192} \cdot 8NO_2C_6H_4NH_2$	ZSM-5	18.1	S	-	nitroaniline	C	n.s.	98Men1
MFI2004a01	$Li_8((C_3H_7)_4N)_4 \cdot Li_4Si_{92}O_{192}$	Li-Si-MFI	18.5	S	-	TPA	-	-	2004Par1
MFI2005a01	$Si_{96}O_{192} \cdot 6.43C_6H_5CH_3$	ZSM-5	17.9	S	-	toluene	C	823	2005Nis1
MFI-II.2 $P\,2_1/n\,1\,1$									
MFI1988a01	$H_{0.6} \cdot Al_{0.6}Si_{95.7}O_{192} \cdot 6H_2O$	ZSM-5	17.9	S	-	H_2O	C	n.s.	88Sch1
MFI1990a01	$H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192}$	H-ZSM-5	18.0	S	-	-	C	811	90van1
MFI1996e01	$Na_4 \cdot Al_4Si_{92}O_{192} \cdot 4C_8H_6S_2$	ZSM-5	18.1	S	-	BT	C	823	96Eyl1
MFI2000a02	$H_{28.80} \cdot Si_{88.32}O_{192}$	defective silicalite	18.0	S	-	-	C	423	2000Art1
MFI2000f02	$Ti_{2.09}Si_{93.81}O_{192}$	TS-1	17.9	S	-	-	C	n.s.	2000Mar1
MFI2001c01	$Si_{96}O_{192} \cdot 8C_6H_{12}C_{l2}$	silicalite-1	17.9	S	-	1,6-dichloro-hexane	C	813	2001Mor1
MFI2001c02	$Si_{96}O_{192} \cdot 8CH_3(CH_2)_4CH_3$	silicalite-1	17.9	S	-	hexane	C	813	2001Mor1
MFI2001c03	$Si_{96}O_{192}$	silicalite-1	18.2	S	-	-	C	813	2001Mor1
MFI2001c04	$Si_{96}O_{192} \cdot 8CH_3(CH_2)_4CH_3$	silicalite-1	17.8	S	-	hexane	C	813	2001Mor1
MFI2001c05	$Si_{96}O_{192} \cdot 8CH_3(CH_2)_4CH_3$	silicalite-1	17.9	S	-	hexane	C	813	2001Mor1
MFI2001c06	$Si_{96}O_{192} \cdot 8CH_3(CH_2)_6CH_3$	silicalite-1	17.9	S	-	octane	C	813	2001Mor1
MFI2001c07	$Si_{96}O_{192} \cdot 8CH_3(CH_2)_{10}CH_3$	silicalite-1	17.8	S	-	dodecane	C	813	2001Mor1
MFI2002b01	$Si_{96}O_{192} \cdot 5.72CH_3(CH_2)_6CH_3$	silicalite-1	17.9	S	-	hexane	C	813	2002Mor1
MFI2002b02	$Si_{96}O_{192} \cdot 7.68CH_3(CH_2)_4CH_3$	silicalite-1	17.9	S	-	hexane	C	813	2002Mor1
MFI2002b03	$Si_{96}O_{192} \cdot 5.04CH_3(CH_2)_4CH_3$	silicalite-1	17.8	S	-	hexane	C	813	2002Mor1
P n* 2_1 *a									
MFI1978a01	$Si_{96}O_{192}$	silicalite	18.1	S	-	-	C	n.s.	78Fla1
MFI1985b01	$H_4 \cdot Al_4Si_{92}O_{192}$	ZSM-5	17.9	S	H	-	C	n.s.	85Liu1
MFI1996c01	$Si_{96}O_{192} \cdot 4\ NO_2C_6H_4NH_2$	ZSM-5	18.1	S	-	nitroaniline	C	673	96Rec1
MFI1999a01	$((C_3H_7)_4N)_4 \cdot Al_4Si_{92}O_{192}$	ZSM-5	17.9	S	-	TPA	C	n.s.	99Yok1

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

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
MFI-I *P n m a*						
MFI1980a01[1])	20.06	19.80	13.36	5306	n.s.	80Smi1
MFI1981a01	20.07(1)	19.92(1)	13.42(1)	5365	n.s.	81Ols1
MFI1981b01	20.04	19.92	13.39	5345	n.s.	81Pri1
MFI1982a01	20.044(2)	19.918(4)	13.395(2)	5348	n.s.	82Pri1
MFI1982b01	20.16(3)	19.97(3)	13.44(2)	5411	n.s.	82Yu1
MFI1984a01	20.096(8)	19.949(8)	13.428(6)	5383	n.s.	84Bae1
MFI1984b01	19.983(1)	19.773(1)	13.303(1)	5256	n.s.	84Pan1
MFI1985a01	20.092(3)	19.952(2)	13.414(2)	5377	n.s.	85Ler1
MFI1986a01	20.100(4)	19.959(4)	13.409(4)	5379	n.s.	86Cha1
MFI1986b01	20.108(2)	19.918(2)	13.392(2)	5364	n.s.	86Tay1
MFI1986c01	20.105(3)	19.961(3)	13.423(2)	5387	773	86Liu1
MFI1987a01	20.022(2)	19.899(2)	13.383(1)	5332	293	87van1
MFI1987a02	20.022(2)	19.899(2)	13.383(1)	5332	293	87van1
MFI1987b01	19.961(2)	19.824(2)	13.398(4)	5302	77	87Tay1
MFI1987d01	19.958(3)	19.863(3)	13.342(2)	5289	n.s.	87Men1
MFI1987e01	20.111(4)	19.893(4)	13.389(3)	5357	n.s.	87Men2
MFI1987f01	20.134(2)	19.926(4)	13.415(3)	5382	n.s.	87Men3
MFI1988a02	20.034	19.873	13.366	5321	773	88Sch1
MFI1988a03	20.140	19.866	13.458	5385	255	88Sch1
MFI1988b01	20.18	19.82	13.3	5320	-	88van1
MFI1988c01	20.105(2)	19.826(2)	13.440(2)	5357	RT	88Men1
MFI1989a01	19.959(3)	19.865(3)	13.389(3)	5309	n.s.	89Men1
MFI1989c01	20.18	19.82	13.3	5320	-	89Uyt1
MFI1990b01	20.078(6)	19.894(7)	13.372(3)	5341	350	90van2
MFI1991a01	20.1122(4)	19.9331(5)	13.4263(4)	5383	RT	91Hud1
MFI1991b01	20.100(2)	19.932(2)	13.431(1)	5381	RT	91Lin1
MFI1991b02	20.080(2)	19.925(2)	13.404(2)	5363	623	91Lin1
MFI1991c01	20.072(2)	19.955(2)	13.402(1)	5368	n.s.	91Men1
MFI1992c01	20.118(4)	19.923(1)	13.410(1)	5375	n.s.	92Li1
MFI1992c02	20.048(2)	19.884(4)	13.352(1)	5323	n.s.	92Li1
MFI1993a01	20.1042(8)	19.9259(8)	13.4007(6)	5368	n.s.	93Sac1
MFI1993c01	19.948(2)	19.980(2)	13.370(1)	5329	RT	93Men1
MFI1994a01	20.0836(6)	19.9394(5)	13.4118(5)	5371	RT	94Wei1
MFI1994a02	20.1245(8)	19.9294(8)	13.4113(6)	5379	RT	94Wei1
MFI1994c01	19.930(4)	19.916(9)	13.35400(0)	5301	n.s.	94Kle1
MFI1994c02	19.930(2)	19.937(2)	13.361(4)	5309	n.s.	94Kle1
MFI1995a01	20.0812(6)	19.9369(5)	13.4100(4)	5369	RT	95Wei1
MFI1995a02	20.1217(8)	19.9267(7)	13.4095(6)	5377	RT	95Wei1
MFI1995a03	20.0873(8)	19.9344(8)	13.4174(9)	5373	RT	95Wei1
MFI1995a04	20.1159(8)	19.9314(7)	13.4147(6)	5378	RT	95Wei1
MFI1995a05	20.1090(6)	19.9156(6)	13.4010(5)	5367	RT	95Wei1
MFI1995b01	20.0210(8)	19.9331(8)	13.3809(6)	5340	RT	95Men1
MFI1995d01	19.86537	19.99053	13.40364	5323	25	95Par1
MFI1996a01	20.009(3)	19.909(4)	13.366(2)	5324	298	96van1
MFI1996d01	19.919(1)	19.955(2)	13.357(1)	5309	293	96van3
MFI1997a01	20.201(2)	19.991(2)	13.469(2)	5439	n.s.	97Vez1
MFI1997b01	19.960(1)	19.941(2)	13.367(1)	5320	n.s.	97van1
MFI1998a01	19.962(1)	19.922(1)	13.3702(8)	5317	n.s.	98Men1

[1]) Cell constants from [87Fla1].

Table MFI.2.2 (MFI-I, *P n m a* continued).

code	a [Å]	b [Å]	c [Å]	V [Å3]	T [K]	reference
MFI1998b01	19.989(4)	19.899(4)	13.362(3)	5315	180	98Lew1
MFI1998c01	20.0445	19.9130	13.3958	5347	n.s.	98Men2
MFI1998c02	20.080(2)	19.920(2)	13.413(1)	5365	n.s.	98Men2
MFI1999b01	20.1468(8)	19.9565(8)	13.4242(5)	5397	n.s.	99Lam1
MFI2000a01	20.0511(1)	19.8757(1)	13.36823(9)	5328	298	2000Art1
MFI2000b01	20.0757(8)	19.9150(9)	13.3862(6)	5352	RT	2000Goy1
MFI2000b02	20.1070(7)	19.9080(7)	13.3870(6)	5359	RT	2000Goy1
MFI2000b03	20.0811(7)	19.8836(7)	13.4057(6)	5353	RT	2000Goy1
MFI2000c01	20.0045(5)	19.9229(4)	13.3929(4)	5338	n.s.	2000Ols1
MFI2000d01	19.9191(2)	19.8912(3)	13.3388(5)	5285	180	2000Fyf1
MFI2000e01	19.997(1)	19.940(1)	13.3738(8)	5333	n.s.	2000Nai1
MFI2000e02	20.0509(7)	19.9268(7)	13.3875(5)	5349	n.s.	2000Nai1
MFI2000f01	20.1014(5)	19.9049(5)	13.3991(4)	5361	170	2000Mar1
MFI2000g01	20.062(1)	19.88(1)	13.387(8)	5339	RT	2000Hij1
MFI2000h01	20.064(2)	19.981(2)	13.421(1)	5380	293	2000Mil1
MFI2001a01	20.1135(2)	19.9300(3)	13.4098(2)	5375	298	2001Lam1
MFI2001a02	20.0715(3)	19.9074(3)	13.3853(2)	5348	298	2001Lam1
MFI2001a03	20.1282(3)	19.9449(3)	13.4195(3)	5387	298	2001Lam1
MFI2001b01	20.137(1)	19.946(1)	13.4203(9)	5390	n.s.	2001Hen1
MFI2001b02	20.138(1)	19.936(1)	13.4169(9)	5387	n.s.	2001Hen1
MFI2001b03	20.140(1)	19.937(1)	13.418(1)	5388	n.s.	2001Hen1
MFI2001b04	20.1403(5)	19.9439(6)	13.4177(4)	5390	n.s.	2001Hen1
MFI2002a01	20.0026(2)	19.9934(2)	13.3923(1)	5356	RT	2002Aub1
MFI2003a01	19.869(2)	19.661(3)	13.207(2)	5159	RT	2003Per1
MFI2003a02	19.875(1)	19.669(1)	13.218(2)	5167	n.s.	2003Per1
MFI2004b01	20.1	19.9	13.4	5360	-	2004Ast1
MFI2005b01	20.009(3)	19.909(4)	13.366(2)	5324	n.s.	2005Fyf1
MFI2006a01	19.9933(3)	19.9367(2)	13.3873(2)	5336	301	2006Men1
MFI2006a02	20.0308(3)	19.9465(3)	13.3988(2)	5353	404	2006Men1
MFI2006a03	20.0656(2)	19.9462(2)	13.4073(2)	5366	510	2006Men1
MFI2006a04	20.0845(2)	19.9412(2)	13.4083(2)	5370	617	2006Men1
MFI2006a05	20.0861(2)	19.9381(2)	13.4069(2)	5369	723	2006Men1
MFI2006b01	20.1138(3)	19.9461(3)	13.4215(2)	5385	301	2006Men2
MFI-II.1 *P* 2$_1$ 2$_1$ 2$_1$						
MFI1989b01	20.121(1)	19.820(1)	13.438(1)	5359	n.s.	89van1
MFI1996b01	20.102(6)	19.797(9)	13.436(3)	5347	293	96van2
MFI1998a02	19.8844(9)	19.852(9)	13.4036(6)	5291	n.s.	98Men1
MFI2004a01	19.793(4)	19.766(4)	13.266(3)	5190	n.s.	2004Par1
MFI2005a01	20.0090(4)	19.8440(3)	13.4240(2)	5354	293	2005Nis1

code	*a* [Å]	*b* [Å]	*c* [Å]	α [°]	*V* [Å^3]	*T* [K]	reference
MFI-II.2 *P* 2$_1$/n 1 1							
MFI1988a01	20.111	19.889	13.385	90.54	5354	RT	88Sch1
MFI1990a01	20.107(2)	19.879(2)	13.369(1)	90.67(1)	5343	n.s.	90van1
MFI1996e01	20.0614(4)	19.8251(4)	13.3623(4)	90.848(2)	5314	25	96Eyl1
MFI2000a02	20.0903(2)	19.8352(2)	13.3588(1)	90.892(1)	5323	100	2000Art1
MFI2000f02	20.0951(6)	19.8885(7)	13.3928(5)	90.264(3)	5353	80	2000Mar1
MFI2001c01	20.1169(4)	19.8993(3)	13.3999(2)	90.892(1)	5363	n.s.	2001Mor1
MFI2001c02	20.1346(1)	19.9111(2)	13.4081(4)	90.5(1)	5375	n.s.	2001Mor1

Table MFI.2.2 (MFI-II.2, *P* 2_1/n 1 1 continued).

code	a [Å]	b [Å]	c [Å]	□ [°]	V [Å3]	T [K]	reference
MFI2001c03	20.0370(3)	19.7960(8)	13.3241(7)	90.44(2)	5285	180	2001Mor1
MFI2001c04	20.1730(3)	19.9310(2)	13.4191(3)	90.20(5)	5395	180	2001Mor1
MFI2001c05	20.1292(2)	9.8247(2)	13.4510(2)	90.29(8)	5368	298	2001Mor1
MFI2001c06	20.1109(8)	19.8742(8)	13.4063(8)	90.23(6)	5358	180	2001Mor1
MFI2001c07	20.1470(5)	19.8940(3)	13.4661(4)	90.41(9)	5397	180	2001Mor1
MFI2002b01	20.1292(2)	19.8247(2)	13.4510(2)	90.29(8)	5368	293	2002Mor1
MFI2002b02	20.1346(1)	19.9111(2)	13.4081(4)	90.5(1)	5375	293	2002Mor1
MFI2002b03	20.1730(3)	19.9310(2)	13.4191(3)	90.20(5)	5395	180	2002Mor1

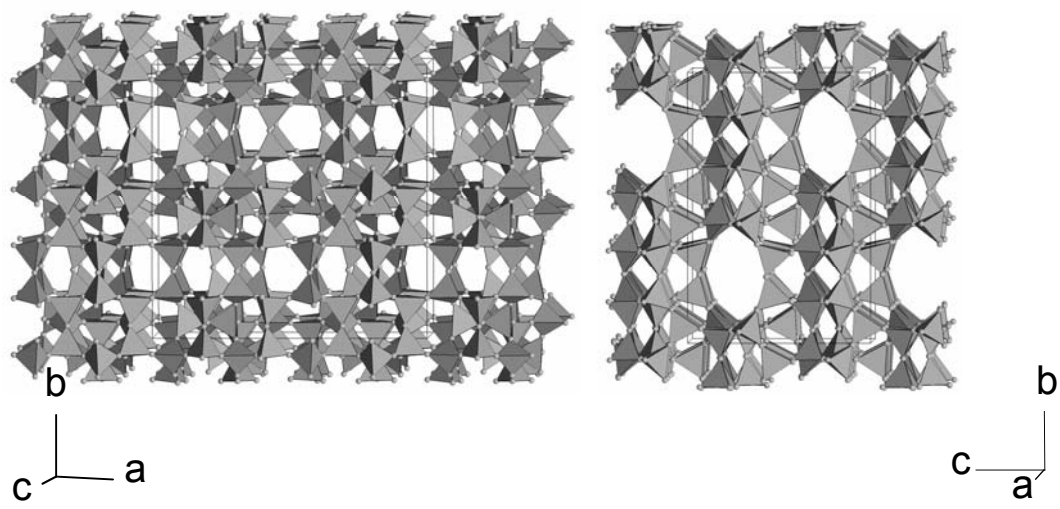
code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
P n* 2_1 *a						
MFI1978a01	20.06	19.80	13.36	5306	n.s.	78Fla1
MFI1985b01	20.09(3)	19.97(3)	13.36(2)	5360	773	85Liu1
MFI1996c01	19.962(1)	19.922(1)	13.370(1)	5317	n.s.	96Rec1
MFI1999a01	20.072(2)	19.937(2)	13.414(2)	5368	293	99Yok1

Table MFI.2.3 Transformation matrices. Entries not listed are not transformed.

code	shift	matrix	coord. transform.	reference
MFI-I *P n m a*				
MFI1980a01	0, 0, 0	**-a**, **b**, **c**	-*x*, *y*, *z*	80Smi1
MFI1981b01	0, 0, 0	**-a**, **b**, **c**	-*x*, *y*, *z*	81Pri1
MFI1982a01	0, 0, 0	**-a**, **b**, **c**	-*x*, *y*, *z*	82Pri1
MFI1982b01	0, ½, 0	**a**, **b**, **c**	*x*, *y*+½, *z*	82Yu1
MFI1984b01	0, ½, 0	**a**, **b**, **c**	*x*, *y*+½, *z*	84Pan1
MFI1986c01	0, ½, 0	**a**, **b**, **c**	*x*, *y*+½, *z*	86Liu1
MFI-II.1 *P* 2_1 2_1 2_1				
MFI1998a02	0, 0, -¼	**a**, **b**, **c**	*x*, *y*, z+¼	98Men1
MFI2004a01	0, 0, ¼	**a**, **b**, **c**	*x*, *y*, z-¼	2004Par1
MFI2005a01	0, 0, ¼	**a**, **b**, **c**	*x*, *y*, z-¼	2005Nis1
MFI-II.2 *P* 2_1/n 1 1				
MFI2000a02	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2000Art1
MFI2000f02	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2000Mar1
MFI2001c01	0, 0, 0	**-b**, **a**, **c**	-*y*, *x*, *z*	2001Mor1
MFI2001c02	0, 0, 0	**-b**, **a**, **c**	-*y*, *x*, *z*	2001Mor1
MFI2001c03	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2001Mor1
MFI2001c04	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2001Mor1
MFI2001c05	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2001Mor1
MFI2001c06	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2001Mor1
MFI2001c07	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2001Mor1
MFI2002b01	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2002Mor1
MFI2002b02	0, 0, 0	**-b**, **a**, **c**	-*y*, *x*, *z*	2002Mor1
MFI2002b03	0, 0, 0	**b**, **a**, **c**	*y*, *x*, *z*	2002Mor1
P n* 2_1 *a				
MFI1985b01	0, 0, 0	**-a**, **b**, **c**	-*x*, *y*, *z*	85Liu1

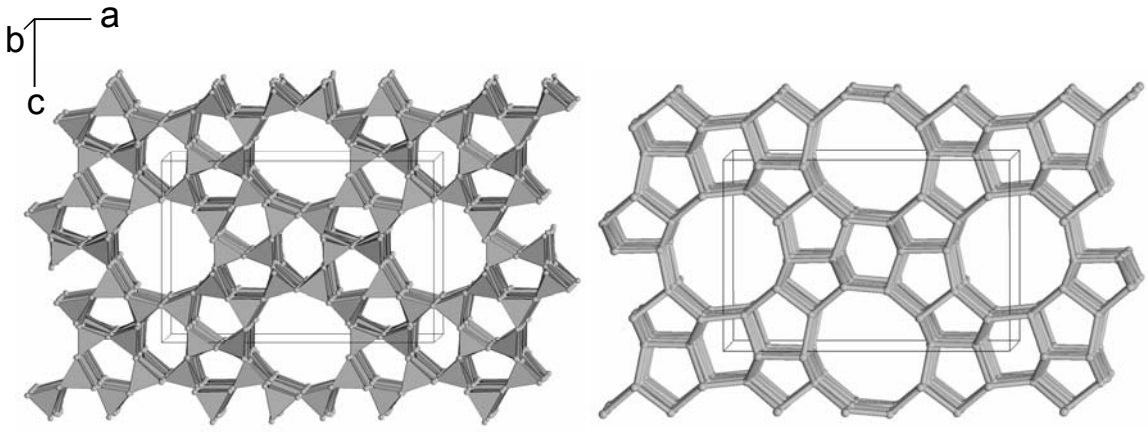
MFI.3 Framework structures

MFI.3.1 MFI-I compound (*P n m a*, IT #62)



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

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



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

d Ball and stick model corresponding to c).

Fig. MEL.3.1.1 Projections of the MFI-I crystal structure of ZSM-5, $Na_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 4(C_3H_7)_4NOH\ nH_2O$ (MFI1987a01, 87van1).

Table MFI.3.1.1 Atomic coordinates and site definitions for MFI-I, $Na_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 4(C_3H_7)_4NOH\ nH_2O$ (MFI1987a01, 87van1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1	0.42238(5)	0.05650(6)	0.66402(9)	1.39	1	8(d)	8
Si2	0.30716(6)	0.02772(6)	0.81070(9)	1.64	1	8(d)	8
Si3	0.27911(6)	0.06127(6)	0.03120(9)	1.52	1	8(d)	8
Si4	0.12215(6)	0.06298(6)	0.02670(9)	1.43	1	8(d)	8
Si5	0.07128(6)	0.02722(6)	0.81449(9)	1.26	1	8(d)	8
Si6	0.18641(5)	0.05896(6)	0.67182(8)	1.41	1	8(d)	8
Si7	0.42265(6)	0.82750(6)	0.67282(9)	1.46	1	8(d)	8
Si8	0.30778(6)	0.86984(6)	0.81452(9)	1.31	1	8(d)	8
Si9	0.27554(6)	0.82721(6)	0.03109(9)	1.39	1	8(d)	8
Si10	0.12058(6)	0.82690(6)	0.02979(9)	1.52	1	8(d)	8
Si11	0.07044(6)	0.86963(6)	0.81800(9)	1.52	1	8(d)	8
Si12	0.18706(6)	0.82673(6)	0.68067(9)	1.58	1	8(d)	8
O1	0.3726(2)	0.0534(3)	0.7558(3)	3.84	1	8(d)	8
O2	0.3084(2)	0.0587(2)	0.9211(2)	3.18	1	8(d)	8
O3	0.2007(2)	0.0592(3)	0.0289(4)	5.11	1	8(d)	8
O4	0.0969(2)	0.0611(2)	0.9144(3)	3.47	1	8(d)	8
O5	0.1149(2)	0.0541(2)	0.7237(2)	2.68	1	8(d)	8
O6	0.2435(2)	0.0553(3)	0.7540(3)	3.61	1	8(d)	8
O7	0.3742(2)	0.8439(2)	0.7628(3)	3.71	1	8(d)	8
O8	0.3085(2)	0.8448(2)	0.9272(3)	3.47	1	8(d)	8
O9	0.1980(2)	0.8446(2)	0.0288(3)	3.18	1	8(d)	8
O10	0.0910(2)	0.8386(2)	0.9223(3)	4.58	1	8(d)	8
O11	0.1169(2)	0.8422(2)	0.7306(3)	3.76	1	8(d)	8
O12	0.2448(2)	0.8406(3)	0.7578(3)	4.40	1	8(d)	8
O13	0.3047(3)	0.9490(2)	0.8134(4)	5.61	1	8(d)	8
O14	0.0768(2)	0.9481(2)	0.8231(3)	3.68	1	8(d)	8
O15	0.4161(2)	0.1276(2)	0.6104(3)	3.50	1	8(d)	8
O16	0.4086(2)	-0.0017(2)	0.5864(3)	3.61	1	8(d)	8
O17	0.4020(2)	0.8686(2)	0.5761(3)	3.21	1	8(d)	8
O18	0.1886(2)	0.1298(2)	0.6164(3)	2.61	1	8(d)	8
O19	0.1940(2)	0.0007(2)	0.5918(3)	3.58	1	8(d)	8
O20	0.1951(2)	0.8709(2)	0.5810(3)	3.37	1	8(d)	8
O21	-0.0037(1)	0.0502(2)	0.7920(2)	2.63	1	8(d)	8
O22	-0.0040(2)	0.8472(2)	0.7922(3)	3.18	1	8(d)	8
O23	0.5808(3)	¼	0.3540(4)	3.50	. 2 .	4(c)	4
O24	0.8116(3)	¼	0.3538(4)	2.68	. 2 .	4(c)	4
O25	0.7117(3)	¼	0.9421(4)	2.58	. 2 .	4(c)	4
O26	0.8915(3)	¼	0.9389(4)	2.37	. 2 .	4(c)	4
N1	0.4762(5)	¼	0.8905(6)	5.45	. 2 .	4(c)	4
Si1	0.42238(5)	0.05650(6)	0.66402(9)	1.39	1	8(d)	8
C1	0.495(1)	0.233(1)	0.779(2)	4.58	1	8(d)	2.40(8)
C2	0.568(2)	¼	0.759(2)	7.66	. 2 .	4(c)	2.40(4)
C3	0.578(2)	¼	0.638(2)	7.74	. 2 .	4(c)	2.40(4)
C4	0.399(1)	0.274(1)	0.900(2)	5.05	1	8(d)	2.40(8)
C5	0.355(1)	0.228(1)	0.850(2)	10.74	1	8(d)	4.00(8)

Table MFI.3.1.1 (continued).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
C6	0.278(2)	¼	0.853(3)	8.21	. 2 .	4(c)	2.40(4)
C7	0.505(2)	0.319(2)	0.911(2)	5.13	1	8(d)	2.40(8)
C8	0.473(2)	0.334(2)	0.019(3)	6.55	1	8(d)	2.40(8)
C9	0.496(1)	0.412(1)	0.045(2)	6.95	1	8(d)	4.00(8)
C10	0.508(1)	0.199(1)	-0.032(2)	9.55	1	8(d)	4.00(8)
C11	0.490(1)	0.124(1)	-0.045(2)	8.61	1	8(d)	4.00(8)
C12	0.529(1)	0.088(1)	0.033(1)	5.68	1	8(d)	4.00(8)
C13	0.413(2)	0.229(2)	0.834(4)	6.55	1	8(d)	1.60(8)
C14	0.285(3)	¼	0.805(4)	8.69	. 2 .	4(c)	1.60(4)
C15	0.534(2)	0.279(2)	0.815(3)	5.29	1	8(d)	1.60(8)
C16	0.546(2)	0.225(2)	0.737(4)	5.76	1	8(d)	1.60(8)
C17	0.601(3)	¼	0.668(5)	10.19	. 2 .	4(c)	1.60(4)
C18	0.468(2)	0.315(2)	0.060(3)	4.82	1	8(d)	1.60(8)
C19	0.516(2)	0.335(2)	0.020(3)	4.82	1	8(d)	1.60(8)

Table MFI.3.1.2 Selected interatomic distances and angles for MFI-I, $Na_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 4(C_3H_7)_4NOH\ nH_2O$ (MFI1987a01, 87van1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 - O16	1.580(4)	164.7(3)	Si2 - O13	1.568(4)	175.9(4)
Si1 - O1	1.583(4)	153.1(3)	Si2 - O6	1.582(4)	158.2(4)
Si1 - O15	1.591(4)	148.2(3)	Si2 - O1	1.587(4)	153.1(4)
Si1 - O21	1.598(2)	145.4(2)	Si2 - O2	1.601(4)	149.7(3)
mean	1.588	152.9	mean	1.584	159.2
Si3 - O3	1.571(4)	175.8(4)	Si4 - O3	1.575(4)	175.8(4)
Si3 - O19	1.571(4)	162.8(3)	Si4 - O16	1.583(4)	164.7(3)
Si3 - O2	1.587(3)	149.7(3)	Si4 - O4	1.586(4)	156.0(3)
Si3 - O20	1.591(4)	147.7(3)	Si4 - O17	1.589(4)	149.4(3)
mean	1.580	159.0	mean	1.583	161.5
Si5 - O14	1.582(4)	169.1(3)	Si6 - O19	1.586(4)	162.8(3)
Si5 - O4	1.583(4)	156.0(3)	Si6 - O6	1.588(4)	158.2(4)
Si5 - O5	1.589(4)	147.9(3)	Si6 - O18	1.593(4)	145.0(3)
Si5 - O21	1.598(3)	145.4(2)	Si6 - O5	1.594(4)	147.9(3)
mean	1.588	154.6	mean	1.590	153.5
Si7 - O7	1.580(4)	156.2(3)	Si8 - O13	1.576(4)	175.9(4)
Si7 - O23	1.585(2)	153.3(4)	Si8 - O12	1.583(4)	164.6(4)
Si7 - O17	1.586(4)	149.4(3)	Si8 - O7	1.586(4)	156.2(3)
Si7 - O22	1.590(4)	150.3(3)	Si8 - O8	1.588(4)	154.5(3)
mean	1.585	152.3	mean	1.583	162.8

Table MFI.3.1.2 (continued)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si9 - O8	1.578(4)	154.5(3)	Si10 - O10	1.573(4)	164.4(3)
Si9 - O9	1.591(4)	154.6(3)	Si10 - O15	1.588(4)	148.2(3)
Si9 - O18	1.597(4)	145.0(3)	Si10 - O9	1.590(4)	154.6(3)
Si9 - O25	1.598(2)	148.0(4)	Si10 - O26	1.605(2)	144.9(4)
mean	1.591	150.5	mean	1.589	153.0
Si11 - O14	1.568(4)	169.1(3)	Si12 - O12	1.574(4)	164.6(4)
Si11 - O10	1.581(4)	164.4(3)	Si12 - O11	1.586(4)	153.4(3)
Si11 - O11	1.591(4)	153.4(3)	Si12 - O24	1.595(2)	146.3(4)
Si11 - O22	1.594(4)	150.3(3)	Si12 - O20	1.606(4)	147.7(3)
mean	1.583	159.3	mean	1.590	153.0

MFI.3.2 MFI-II.1 compound ($P2_12_12_1$, IT #19)

Table MFI.3.2.1 Atomic coordinates and site definitions for MFI-II.1, H-ZSM-5, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 8C_8H_{10}$ (MFI1989b01, 89van1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1 1	0.42512(7)	0.06614(7)	0.7034(1)	0.76	1	4(a)	4
Si1 2	0.42531(7)	0.44952(8)	0.6570(1)	0.79	1	4(a)	4
Si2 1	0.31765(7)	0.03171(7)	0.8528(1)	0.81	1	4(a)	4
Si2 2	0.31445(7)	0.47104(7)	0.8098(1)	0.87	1	4(a)	4
Si3 1	0.27983(7)	0.05290(7)	0.0742(1)	0.85	1	4(a)	4
Si3 2	0.27904(7)	0.42741(7)	0.0216(1)	0.82	1	4(a)	4
Si4 1	0.12322(7)	0.05468(7)	0.0661(1)	0.82	1	4(a)	4
Si4 2	0.12149(7)	0.42683(7)	0.0229(1)	0.77	1	4(a)	4
Si5 1	0.07586(7)	0.02957(7)	0.8472(1)	0.85	1	4(a)	4
Si5 2	0.07431(7)	0.46892(7)	0.8123(1)	0.76	1	4(a)	4
Si6 1	0.19627(7)	0.07052(6)	0.7194(1)	0.73	1	4(a)	4
Si6 2	0.19248(7)	0.44987(7)	0.6620(1)	0.81	1	4(a)	4
Si7 1	0.42775(7)	0.83092(7)	0.7077(1)	0.84	1	4(a)	4
Si7 2	0.42801(7)	0.67407(7)	0.6759(1)	0.82	1	4(a)	4
Si8 1	0.31761(7)	0.87219(7)	0.8505(1)	0.88	1	4(a)	4
Si8 2	0.31712(7)	0.62773(7)	0.8176(1)	0.82	1	4(a)	4
Si9 1	0.27322(7)	0.82622(7)	0.0604(1)	0.75	1	4(a)	4
Si9 2	0.27474(7)	0.67197(7)	0.0248(1)	0.84	1	4(a)	4
Si10 1	0.11852(7)	0.82521(7)	0.0588(1)	0.85	1	4(a)	4
Si10 2	0.12035(7)	0.67150(7)	0.0246(1)	0.88	1	4(a)	4
Si11 1	0.07438(7)	0.87117(7)	0.8480(1)	0.85	1	4(a)	4
Si11 2	0.07384(7)	0.62793(7)	0.8156(1)	0.87	1	4(a)	4
Si12 1	0.19567(7)	0.82712(7)	0.7200(1)	0.81	1	4(a)	4
Si12 2	0.19578(7)	0.67319(7)	0.6834(1)	0.83	1	4(a)	4
O1 1	0.3855(2)	0.0610(2)	0.8071(3)	1.47	1	4(a)	4
O1 2	0.3831(2)	0.4527(3)	0.7581(3)	2.16	1	4(a)	4
O2 1	0.3174(2)	0.0483(2)	-0.0305(3)	1.55	1	4(a)	4
O2 2	0.3076(2)	0.4285(2)	0.9102(3)	1.42	1	4(a)	4

Table MFI.3.2.1 (continued).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
O3 1	0.2019(2)	0.0543(3)	0.0539(3)	2.45	1	4(a)	4
O3 2	0.1999(2)	0.4339(2)	0.0195(4)	2.47	1	4(a)	4
O4 1	0.0877(2)	0.0529(3)	-0.0402(3)	2.26	1	4(a)	4
O4 2	0.0919(2)	0.4299(2)	0.9133(3)	1.79	1	4(a)	4
O5 1	0.1263(2)	0.0676(2)	0.7754(3)	1.82	1	4(a)	4
O5 2	0.1259(2)	0.4515(3)	0.7267(3)	1.89	1	4(a)	4
O6 1	0.2555(2)	0.0654(2)	0.7985(3)	1.68	1	4(a)	4
O6 2	0.2550(2)	0.4554(3)	0.7340(3)	2.24	1	4(a)	4
O7 1	0.3860(2)	0.8424(2)	0.8076(3)	1.87	1	4(a)	4
O7 2	0.3871(2)	0.6458(2)	0.7685(3)	1.95	1	4(a)	4
O8 1	0.3127(2)	0.8558(2)	-0.0334(3)	1.58	1	4(a)	4
O8 2	0.3116(2)	0.6675(2)	0.9202(3)	2.00	1	4(a)	4
O9 1	0.1956(2)	0.8441(2)	0.0475(3)	1.76	1	4(a)	4
O9 2	0.1972(2)	0.6552(2)	0.0089(4)	2.55	1	4(a)	4
O10 1	0.0792(2)	0.8515(2)	-0.0373(3)	2.26	1	4(a)	4
O10 2	0.0839(2)	0.6663(2)	0.9195(3)	2.18	1	4(a)	4
O11 1	0.1290(2)	0.8333(2)	0.7841(4)	2.16	1	4(a)	4
O11 2	0.1296(2)	0.6486(3)	0.7378(4)	2.40	1	4(a)	4
O12 1	0.2568(2)	0.8374(3)	0.7925(4)	2.40	1	4(a)	4
O12 2	0.2585(2)	0.6482(3)	0.7445(4)	2.71	1	4(a)	4
O13 1	0.3155(2)	-0.0481(2)	0.8331(3)	2.29	1	4(a)	4
O13 2	0.3129(3)	0.5489(2)	0.8399(3)	2.68	1	4(a)	4
O14 1	0.0864(2)	-0.0498(3)	0.8372(4)	2.53	1	4(a)	4
O14 2	0.0754(2)	0.5486(2)	0.8346(3)	2.13	1	4(a)	4
O15 1	0.4131(2)	0.1390(2)	0.6554(3)	1.53	1	4(a)	4
O15 2	0.4097(3)	0.3815(2)	0.6012(4)	2.95	1	4(a)	4
O16 1	0.3984(3)	0.0098(2)	0.6282(4)	2.26	1	4(a)	4
O16 2	0.4078(3)	0.5128(2)	0.5878(4)	2.26	1	4(a)	4
O17 1	0.3985(2)	0.8776(2)	0.6208(4)	2.08	1	4(a)	4
O17 2	0.3999(2)	0.6435(2)	0.5732(3)	1.53	1	4(a)	4
O18 1	0.2000(2)	0.1404(2)	0.6612(3)	1.26	1	4(a)	4
O18 2	0.1951(2)	0.3803(2)	0.6021(3)	1.68	1	4(a)	4
O19 1	0.2020(3)	0.0107(2)	0.6407(3)	2.21	1	4(a)	4
O19 2	0.1912(2)	0.5113(2)	0.5845(3)	1.76	1	4(a)	4
O20 1	0.1969(3)	0.8802(2)	0.6314(3)	2.08	1	4(a)	4
O20 2	0.1984(2)	0.6414(2)	0.5738(3)	1.61	1	4(a)	4
O21 1	0.0022(2)	0.0491(3)	0.8137(3)	1.89	1	4(a)	4
O21 2	0.0021(2)	0.4452(2)	0.7753(3)	1.63	1	4(a)	4
O22 1	0.0034(2)	0.8493(2)	0.8084(3)	1.97	1	4(a)	4
O22 2	0.0036(2)	0.6490(2)	0.7706(3)	1.82	1	4(a)	4
O23	0.4223(2)	0.7544(2)	0.6716(4)	2.08	1	4(a)	4
O24	0.1975(2)	0.7529(2)	0.6738(3)	1.76	1	4(a)	4
O25	0.2831(2)	0.7469(2)	0.0673(3)	1.47	1	4(a)	4
O26	0.1099(2)	0.7452(2)	0.0702(3)	1.55	1	4(a)	4
C1	0.1460(6)	0.2481(4)	0.8801(7)	4.50	1	4(a)	4
C2	0.1761(5)	0.2842(4)	0.8028(6)	3.74	1	4(a)	4
C3	0.2466(5)	0.2876(4)	0.7926(6)	3.76	1	4(a)	4
C4	0.2877(5)	0.2557(4)	0.8595(6)	3.84	1	4(a)	4
C5	0.2609(6)	0.2211(5)	0.9374(7)	5.03	1	4(a)	4

Table MFI.3.2.1 (continued).

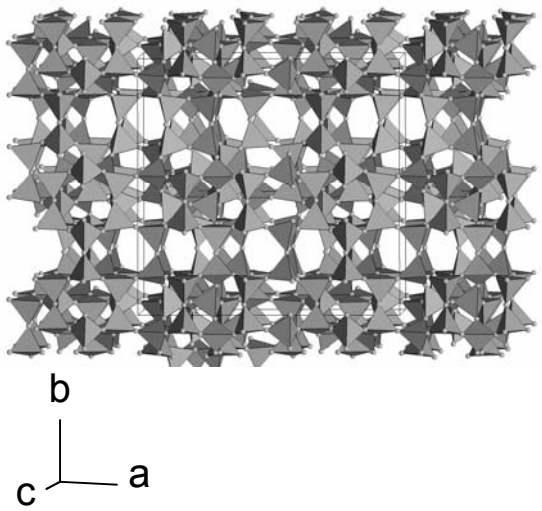
atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
C6	0.1918(8)	0.2175(4)	-0.0513(7)	6.03	1	4(a)	4
C7	0.0729(6)	0.2429(6)	0.8893(9)	5.97	1	4(a)	4
C8	0.3620(6)	0.2604(6)	0.8472(9)	5.82	1	4(a)	4
C11	0.5123(5)	0.3103(8)	-0.0333(9)	6.32	1	4(a)	4
C12	0.4817(6)	0.2827(9)	0.0482(8)	6.71	1	4(a)	4
C13	0.4797(6)	0.2137(9)	0.0631(9)	6.82	1	4(a)	4
C14	0.5076(6)	0.1657(9)	-0.0045(9)	7.40	1	4(a)	4
C15	0.5389(6)	0.1957(8)	0.9123(9)	6.55	1	4(a)	4
C16	0.5424(5)	0.2678(8)	0.9000(8)	6.24	1	4(a)	4
C17	0.5152(9)	0.3863(9)	-0.046(1)	9.71	1	4(a)	4
C18	0.5059(9)	0.0895(9)	0.010(1)	9.74	1	4(a)	4

Table MFI.3.2.2 Selected interatomic distances and angles for MFI-II.1, H-ZSM-5, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 8C_8H_{10}$ (MFI1989b01, 89van1).

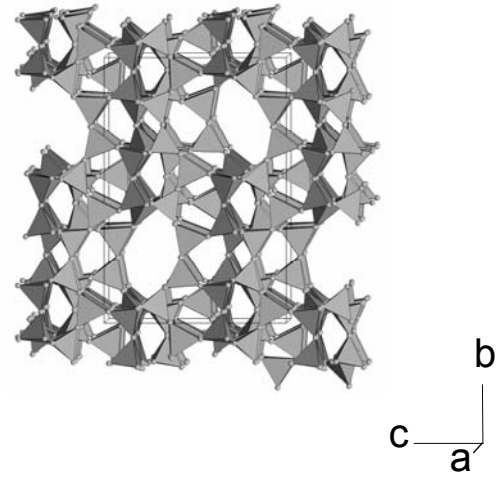
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 1 - O21 2	1.591(4)	150.1(3)	Si1 2 - O15 2	1.574(5)	161.8(4)
Si1 1 - O16 1	1.599(5)	170.7(4)	Si1 2 - O21 1	1.597(4)	146.5(3)
Si1 1 - O15 1	1.600(4)	141.5(3)	Si1 2 - O16 2	1.601(5)	171.0(4)
Si1 1 - O1 1	1.609(4)	140.9(3)	Si1 2 - O1 2	1.603(4)	147.2(3)
mean	1.600	150.8	mean	1.594	156.0
Si2 1 - O6 1	1.595(4)	156.2(3)	Si2 2 - O1 2	1.589(4)	147.2(3)
Si2 1 - O2 1	1.602(4)	150.9(3)	Si2 2 - O13 2	1.596(4)	154.2(3)
Si2 1 - O13 1	1.604(4)	161.8(3)	Si2 2 - O2 2	1.597(4)	145.8(3)
Si2 1 - O1 1	1.606(4)	140.9(3)	Si2 2 - O6 2	1.602(4)	172.3(4)
mean	1.602	152.5	mean	1.596	154.9
Si3 1 - O19 1	1.588(4)	168.9(4)	Si3 2 - O19 2	1.596(4)	156.4(3)
Si3 1 - O3 1	1.592(5)	164.3(3)	Si3 2 - O3 2	1.598(4)	170.0(3)
Si3 1 - O2 1	1.599(4)	150.9(3)	Si3 2 - O20 2	1.599(4)	138.4(3)
Si3 1 - O20 1	1.603(4)	155.8(4)	Si3 2 - O2 2	1.604(4)	145.8(3)
mean	1.596	160.0	mean	1.599	152.7
Si4 1 - O16 1	1.587(5)	170.7(4)	Si4 2 - O3 2	1.585(4)	170.0(3)
Si4 1 - O3 1	1.592(4)	164.3(3)	Si4 2 - O4 2	1.589(4)	152.4(3)
Si4 1 - O17 1	1.592(5)	157.6(3)	Si4 2 - O16 2	1.594(5)	171.0(4)
Si4 1 - O4 1	1.597(4)	156.7(4)	Si4 2 - O17 2	1.608(4)	141.4(3)
mean	1.592	162.3	mean	1.594	158.7
Si5 1 - O5 1	1.590(4)	149.9(3)	Si5 2 - O5 2	1.587(4)	161.3(4)
Si5 1 - O14 1	1.593(6)	160.7(3)	Si5 2 - O4 2	1.602(4)	152.4(3)
Si5 1 - O21 1	1.597(4)	146.5(3)	Si5 2 - O21 2	1.606(4)	150.1(3)
Si5 1 - O4 1	1.600(4)	156.7(4)	Si5 2 - O14 2	1.608(4)	159.9(3)
mean	1.595	153.5	mean	1.601	155.9

Table MFI.3.2.2 (continued)

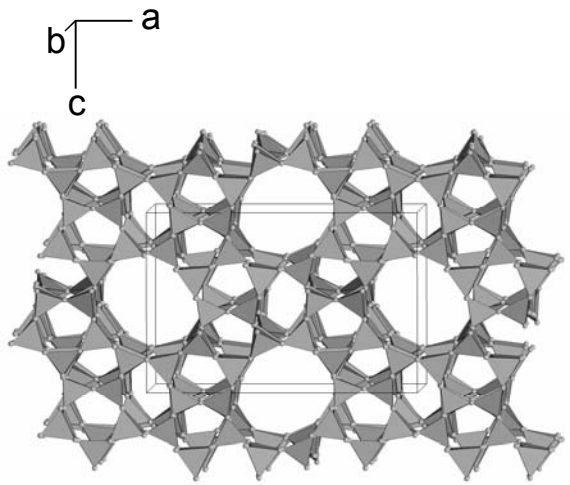
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si6 1 - O18 1	1.592(4)	142.3(3)	Si6 2 - O6 2	1.590(4)	172.3(4)
Si6 1 - O19 1	1.593(4)	168.9(4)	Si6 2 - O5 2	1.597(4)	161.3(4)
Si6 1 - O5 1	1.598(4)	149.9(3)	Si6 2 - O18 2	1.598(4)	154.9(3)
Si6 1 - O6 1	1.600(4)	156.2(3)	Si6 2 - O19 2	1.603(4)	156.4(3)
mean	1.596	154.3	mean	1.597	161.2
Si7 1 - O23	1.596(4)	158.6(4)	Si7 2 - O7 2	1.594(4)	149.1(3)
Si7 1 - O7 1	1.600(4)	143.5(3)	Si7 2 - O23	1.597(4)	158.6(4)
Si7 1 - O17 1	1.602(5)	157.6(3)	Si7 2 - O22 1	1.600(4)	152.8(3)
Si7 1 - O22 2	1.604(4)	147.2(3)	Si7 2 - O17 2	1.610(4)	141.4(3)
mean	1.600	151.7	mean	1.600	150.5
Si8 1 - O8 1	1.597(4)	151.0(3)	Si8 2 - O12 2	1.588(5)	172.7(4)
Si8 1 - O13 1	1.598(4)	161.8(3)	Si8 2 - O8 2	1.592(4)	145.6(3)
Si8 1 - O7 1	1.605(4)	143.5(3)	Si8 2 - O13 2	1.593(4)	154.2(3)
Si8 1 - O12 1	1.606(5)	161.1(4)	Si8 2 - O7 2	1.596(4)	149.1(3)
mean	1.601	154.4	mean	1.592	155.4
Si9 1 - O25	1.587(4)	152.3(3)	Si9 2 - O18 2	1.587(4)	154.9(3)
Si9 1 - O18 1	1.601(4)	142.3(3)	Si9 2 - O8 2	1.592(4)	145.6(3)
Si9 1 - O8 1	1.601(4)	151.0(3)	Si9 2 - O25	1.600(4)	152.3(3)
Si9 1 - O9 1	1.611(4)	151.2(3)	Si9 2 - O9 2	1.610(4)	151.8(3)
mean	1.600	149.2	Mean	1.597	151.2
Si10 1 - O10 1	1.602(4)	152.9(3)	Si10 2 - O15 2	1.590(5)	161.8(4)
Si10 1 - O26	1.603(4)	148.6(3)	Si10 2 - O9 2	1.594(4)	151.8(3)
Si10 1 - O9 1	1.603(4)	151.2(3)	Si10 2 - O10 2	1.595(4)	149.4(3)
Si10 1 - O15 1	1.610(4)	141.5(3)	Si10 2 - O26	1.598(4)	148.6(3)
mean	1.604	148.6	Mean	1.594	152.9
Si11 1 - O11 1	1.584(5)	155.6(3)	Si11 2 - O11 2	1.587(5)	166.1(4)
Si11 1 - O22 1	1.584(4)	152.8(3)	Si11 2 - O22 2	1.593(4)	147.2(3)
Si11 1 - O14 1	1.592(6)	160.7(3)	Si11 2 - O14 2	1.593(4)	159.9(3)
Si11 1 - O10 1	1.593(4)	152.9(3)	Si11 2 - O10 2	1.603(4)	149.4(3)
mean	1.588	155.5	Mean	1.594	155.7
Si12 1 - O12 1	1.582(5)	161.1(4)	Si12 2 - O12 2	1.585(5)	172.7(4)
Si12 1 - O20 1	1.589(4)	155.8(4)	Si12 2 - O24	1.585(4)	152.3(3)
Si12 1 - O24	1.597(4)	152.3(3)	Si12 2 - O11 2	1.595(5)	166.1(4)
Si12 1 - O11 1	1.599(5)	155.6(3)	Si12 2 - O20 2	1.603(4)	138.4(3)
mean	1.592	156.2	mean	1.592	157.4



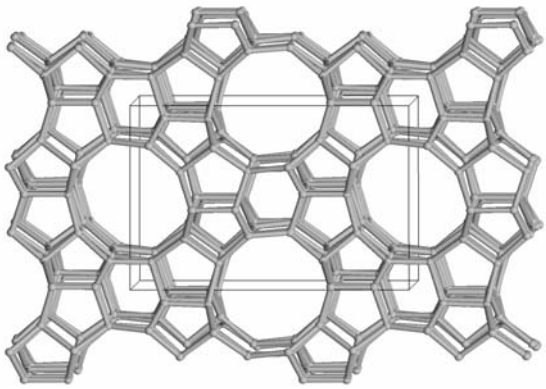
a View parallel **c** rotated by 2° about **a** and **b**.



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



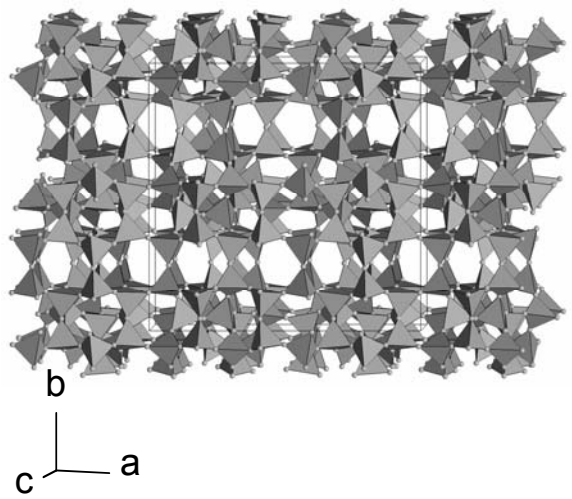
c View parallel **b** rotated by 2° about **a** and **c**.



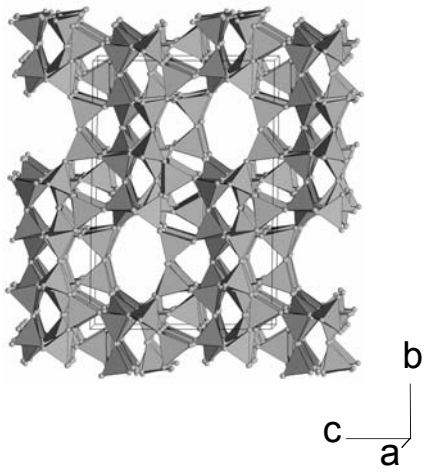
d Ball and stick model corresponding to c).

Fig. MFI.3.2.1 (continued). Projections of the MFI-II.1 crystal structure of H-ZSM-5, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192} \cdot 8C_8H_{10}$ (MFI1989b01, 89van1).

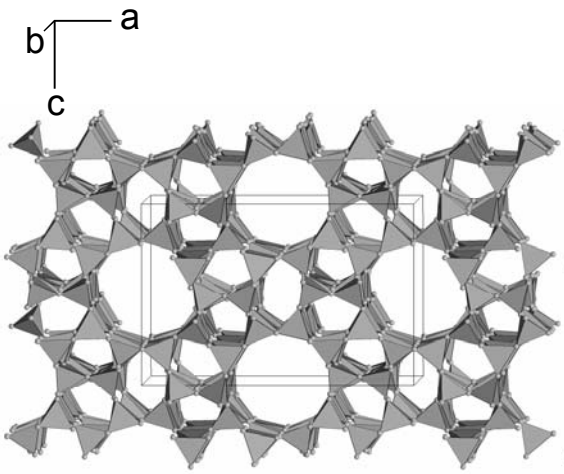
MFI.3.3 MFI-II.2 compound ($P2_1/n\,1\,1$, IT #14)



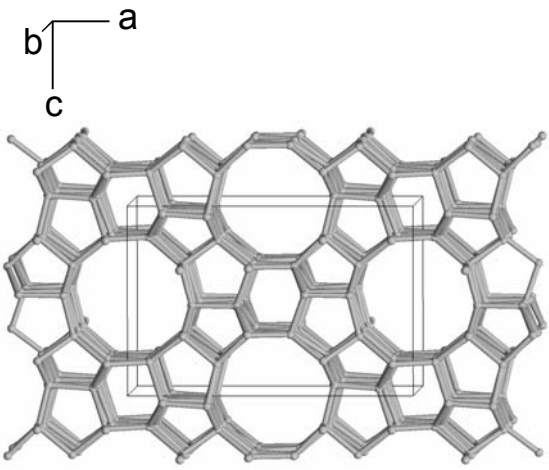
a View parallel **c** rotated by 2° about **a** and **a**×**c**.



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



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



d Ball and stick model corresponding to c).

Fig. MFI.3.3.1 Projections of the MFI-II.2 crystal structure of H-ZSM-5, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192}$ (MFI1990a01, 90van1).

Table MFI.3.3.1 Atomic coordinates and site definitions for MFI-II.2, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192}$ (MFI1990a01, 90van1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0.42056(5)	0.05546(5)	0.68010(8)	0.89	1	4(e)	4
Si12	0.42837(5)	0.44297(5)	0.66544(8)	0.90	1	4(e)	4
Si21	0.31368(5)	0.03090(5)	0.83642(8)	0.97	1	4(e)	4
Si22	0.31237(5)	0.47305(5)	0.81186(8)	1.01	1	4(e)	4
Si31	0.27960(5)	0.06249(5)	0.05346(8)	0.97	1	4(e)	4
Si32	0.27704(5)	0.43889(5)	0.02940(8)	0.93	1	4(e)	4

Table MFI.3.3.1 (continued).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si41	0.12395(5)	0.06233(5)	0.03674(8)	0.96	1	4(e)	4
Si42	0.12155(5)	0.43563(5)	0.03380(8)	0.93	1	4(e)	4
Si51	0.07678(5)	0.02804(5)	0.82403(8)	0.89	1	4(e)	4
Si52	0.07096(5)	0.47315(5)	0.82156(5)	0.87	1	4(e)	4
Si61	0.19556(5)	0.05585(5)	0.68669(8)	0.91	1	4(e)	4
Si62	0.18737(5)	0.43778(5)	0.68257(8)	0.97	1	4(e)	4
Si71	0.42542(5)	0.82852(5)	0.68070(8)	0.94	1	4(e)	4
Si72	0.42389(5)	0.67204(5)	0.68583(8)	0.91	1	4(e)	4
Si81	0.31225(5)	0.87347(5)	0.82612(8)	0.97	1	4(e)	4
Si82	0.31278(5)	0.63130(5)	0.83164(8)	1.02	1	4(e)	4
Si91	0.27325(5)	0.82410(5)	0.03597(8)	0.87	1	4(e)	4
Si92	0.27312(5)	0.66892(5)	0.04608(8)	0.93	1	4(e)	4
Si101	0.11895(5)	0.82366(5)	0.03436(8)	0.99	1	4(e)	4
Si102	0.11867(5)	0.67007(5)	0.03868(8)	0.93	1	4(e)	4
Si111	0.07156(5)	0.87061(5)	0.82484(8)	0.97	1	4(e)	4
Si112	0.07268(5)	0.63082(5)	0.82243(8)	1.03	1	4(e)	4
Si121	0.19079(5)	0.83472(5)	0.68592(8)	0.94	1	4(e)	4
Si122	0.19446(5)	0.68070(5)	0.70211(8)	0.91	1	4(e)	4
O11	0.3779(2)	0.0588(2)	0.7806(2)	2.30	1	4(e)	4
O12	0.3799(2)	0.4503(2)	0.7592(2)	2.67	1	4(e)	4
O21	0.3106(2)	0.0662(2)	0.9436(2)	1.83	1	4(e)	4
O22	0.3143(2)	0.4480(2)	0.9246(2)	2.01	1	4(e)	4
O31	0.2018(2)	0.0472(2)	0.0465(3)	2.64	1	4(e)	4
O32	0.1991(2)	0.4318(2)	0.0094(3)	2.36	1	4(e)	4
O41	0.1032(2)	0.0671(2)	0.9216(2)	1.83	1	4(e)	4
O42	0.0812(2)	0.4478(2)	0.9331(2)	2.42	1	4(e)	4
O51	0.1230(1)	0.0443(2)	0.7307(2)	1.91	1	4(e)	4
O52	0.1206(2)	0.4351(2)	0.7473(2)	1.81	1	4(e)	4
O61	0.2483(2)	0.0477(2)	0.7752(2)	2.59	1	4(e)	4
O62	0.2505(2)	0.4401(2)	0.7549(2)	2.28	1	4(e)	4
O71	0.3769(2)	0.8467(2)	0.7711(3)	2.61	1	4(e)	4
O72	0.3797(2)	0.6590(2)	0.7831(2)	2.19	1	4(e)	4
O81	0.3050(2)	0.8331(2)	0.9275(2)	2.32	1	4(e)	4
O82	0.3148(2)	0.6459(2)	0.9492(2)	1.63	1	4(e)	4
O91	0.1960(2)	0.8442(2)	0.0316(3)	2.21	1	4(e)	4
O92	0.1961(2)	0.6513(2)	0.0270(2)	2.00	1	4(e)	4
O101	0.0885(2)	0.8311(2)	0.9247(2)	2.59	1	4(e)	4
O102	0.0822(2)	0.6559(2)	0.9347(2)	2.72	1	4(e)	4
O111	0.1208(2)	0.8489(2)	0.7370(3)	2.57	1	4(e)	4
O112	0.1232(2)	0.6678(2)	0.7496(3)	2.69	1	4(e)	4
O121	0.2483(2)	0.8624(2)	0.7576(3)	2.78	1	4(e)	4
O122	0.2497(2)	0.6694(2)	0.7856(2)	2.45	1	4(e)	4
O131	0.3189(2)	0.9515(2)	0.8510(3)	2.99	1	4(e)	4
O132	0.3054(2)	0.5530(2)	0.8087(3)	3.10	1	4(e)	4
O141	0.0781(2)	0.9491(2)	0.8471(2)	2.18	1	4(e)	4
O142	0.0851(2)	0.5519(2)	0.8166(3)	2.47	1	4(e)	4
O151	0.4145(2)	0.1253(2)	0.6229(3)	2.36	1	4(e)	4
O152	0.4186(2)	0.3714(2)	0.6115(3)	2.61	1	4(e)	4
O161	0.3923(2)	-0.0041(2)	0.6108(3)	2.54	1	4(e)	4

Table MFI.3.3.1 (continued).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
O162	0.4154(2)	0.5015(2)	0.5865(2)	2.18	1	4(e)	4
O171	0.4022(2)	0.8660(2)	0.5814(2)	2.02	1	4(e)	4
O172	0.3938(2)	0.6320(2)	0.5913(2)	2.15	1	4(e)	4
O181	0.2003(2)	0.1298(1)	0.6417(2)	1.79	1	4(e)	4
O182	0.1900(2)	0.3711(2)	0.6153(2)	1.90	1	4(e)	4
O191	0.2099(2)	0.0026(2)	0.5992(2)	2.41	1	4(e)	4
O192	0.1862(2)	0.5032(2)	0.6137(2)	2.09	1	4(e)	4
O201	0.1948(2)	0.8725(1)	0.5812(2)	2.00	1	4(e)	4
O202	0.2074(2)	0.6326(2)	0.6086(2)	2.66	1	4(e)	4
O211	0.0032(1)	0.0515(2)	0.7959(2)	1.67	1	4(e)	4
O212	-0.0039(1)	0.4576(2)	0.7896(2)	1.87	1	4(e)	4
O221	-0.0023(2)	0.8525(2)	0.7902(2)	2.09	1	4(e)	4
O222	-0.0013(2)	0.6481(2)	0.7880(2)	2.05	1	4(e)	4
O23	0.5761(2)	0.2501(2)	0.3413(3)	2.35	1	4(e)	4
O24	0.8013(2)	0.2435(1)	0.3356(2)	2.01	1	4(e)	4
O25	0.7178(2)	0.2525(2)	0.9324(2)	1.79	1	4(e)	4
O26	0.8899(2)	0.2526(1)	0.9303(2)	1.51	1	4(e)	4

Table MFI.3.3.2 Selected interatomic distances and angles for MFI-II.2, $H_{0.3} \cdot Al_{0.3}Si_{95.7}O_{192}$ (MFI1990a01, 90van1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 1 - O21 2	1.594(2)	149.7(2)	Si1 2 - O1 2	1.593(3)	153.2(2)
Si1 1 - O1 1	1.595(3)	145.0(3)	Si1 2 - O21 1	1.594(2)	144.8(2)
Si1 1 - O15 1	1.597(4)	150.2(3)	Si1 2 - O15 2	1.600(4)	151.0(3)
Si1 1 - O16 1	1.599(4)	168.9(3)	Si1 2 - O16 2	1.601(4)	156.2(3)
mean	1.596	153.5	mean	1.597	151.3
Si2 1 - O6 1	1.586(4)	162.8(2)	Si2 2 - O1 2	1.593(4)	153.2(2)
Si2 1 - O2 1	1.589(4)	145.0(3)	Si2 2 - O2 2	1.593(3)	148.9(3)
Si2 1 - O1 1	1.594(4)	145.0(3)	Si2 2 - O6 2	1.595(4)	156.7(3)
Si2 1 - O13 1	1.596(4)	159.0(3)	Si2 2 - O13 2	1.597(4)	163.6(3)
Mean	1.591	153.0	Mean	1.594	155.6
Si3 1 - O20 2	1.591(4)	155.4(2)	Si3 2 - O19 1	1.586(4)	168.5(2)
Si3 1 - O19 2	1.591(4)	153.5(3)	Si3 2 - O3 2	1.596(4)	157.2(3)
Si3 1 - O3 1	1.596(4)	158.1(3)	Si3 2 - O2 2	1.601(3)	148.9(3)
Si3 1 - O2 1	1.598(3)	145.0(3)	Si3 2 - O20 1	1.601(3)	142.6(2)
Mean	1.594	153.0	Mean	1.596	154.3
Si4 1 - O16 2	1.597(4)	156.2(3)	Si4 2 - O4 2	1.593(3)	155.5(3)
Si4 1 - O17 2	1.598(4)	149.7(3)	Si4 2 - O3 2	1.595(4)	157.2(3)
Si4 1 - O4 1	1.599(3)	146.9(3)	Si4 2 - O16 1	1.595(4)	168.9(3)
Si4 1 - O3 1	1.600(4)	158.1(3)	Si4 2 - O17 1	1.603(4)	146.0(2)
mean	1.598	152.7	mean	1.595	156.9

Table MFI.3.3.2 (continued)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si5 1 - O5 1	1.592(3)	149.0(2)	Si5 2 - O5 2	1.593(4)	147.7(3)
Si5 1 - O21 1	1.597(2)	144.8(2)	Si5 2 - O4 2	1.593(3)	155.5(3)
Si5 1 - O4 1	1.601(3)	146.9(3)	Si5 2 - O14 2	1.593(4)	160.0(3)
Si5 1 - O14 1	1.603(4)	157.4(2)	Si5 2 - O21 2	1.594(2)	149.7(2)
Mean	1.598	149.5	Mean	1.593	153.2
Si6 1 - O5 1	1.591(2)	149.0(2)	Si6 2 - O18 2	1.594(4)	150.6(3)
Si6 1 - O19 1	1.595(3)	168.5(2)	Si6 2 - O6 2	1.596(4)	156.7(3)
Si6 1 - O18 1	1.598(2)	141.3(2)	Si6 2 - O5 2	1.599(4)	147.7(3)
Si6 1 - O6 1	1.599(3)	162.8(2)	Si6 2 - O19 2	1.602(4)	153.5(3)
Mean	1.595	155.4	Mean	1.598	152.1
Si7 1 - O23	1.587(4)	156.1(3)	Si7 2 - O23	1.594(4)	156.1(3)
Si7 1 - O7 1	1.591(4)	158.2(3)	Si7 2 - O22 1	1.596(4)	151.1(2)
Si7 1 - O22 2	1.599(4)	147.8(2)	Si7 2 - O7 2	1.599(3)	149.3(2)
Si7 1 - O17 1	1.600(3)	146.0(2)	Si7 2 - O17 2	1.604(3)	149.7(3)
Mean	1.594	152.0	Mean	1.598	151.6
Si8 1 - O7 1	1.583(4)	158.2(3)	Si8 2 - O13 2	1.590(4)	163.6(3)
Si8 1 - O13 1	1.588(4)	159.0(3)	Si8 2 - O7 2	1.595(4)	149.3(2)
Si8 1 - O8 1	1.590(3)	150.9(3)	Si8 2 - O8 2	1.595(3)	146.0(3)
Si8 1 - O12 1	1.593(4)	167.2(3)	Si8 2 - O12 2	1.604(4)	153.1(2)
mean	1.588	158.8	mean	1.596	153.0
Si9 1 - O18 2	1.588(4)	150.6(3)	Si9 2 - O25	1.596(4)	151.0(2)
Si9 1 - O25	1.595(4)	151.0(2)	Si9 2 - O18 1	1.596(3)	141.3(2)
Si9 1 - O8 1	1.596(3)	150.9(3)	Si9 2 - O8 2	1.605(3)	146.0(3)
Si9 1 - O9 1	1.605(4)	150.6(3)	Si9 2 - O9 2	1.607(4)	150.2(3)
Mean	1.596	150.8	Mean	1.601	147.1
Si10 1 - O15 2	1.585(4)	151.0(3)	Si10 2 - O15 1	1.590(4)	150.2(3)
Si10 1 - O10 1	1.597(3)	154.5(3)	Si10 2 - O10 2	1.594(3)	158.5(3)
Si10 1 - O9 1	1.603(4)	150.6(3)	Si10 2 - O26	1.597(2)	145.3(2)
Si10 1 - O26	1.603(2)	145.3(2)	Si10 2 - O9 2	1.608(4)	150.2(3)
Mean	1.597	150.4	Mean	1.597	151.1
Si11 1 - O14 1	1.590(4)	157.4(2)	Si11 2 - O10 2	1.588(3)	158.5(3)
Si11 1 - O11 1	1.592(4)	156.0(3)	Si11 2 - O14 2	1.590(4)	160.0(3)
Si11 1 - O10 1	1.594(3)	154.5(3)	Si11 2 - O11 2	1.593(4)	153.8(3)
Si11 1 - O22 1	1.596(4)	151.1(2)	Si11 2 - O22 2	1.596(4)	147.8(2)
Mean	1.593	154.8	Mean	1.591	155.0
Si12 1 - O24	1.586(2)	149.8(2)	Si12 2 - O20 2	1.586(3)	155.4(2)
Si12 1 - O11 1	1.588(4)	156.0(3)	Si12 2 - O11 2	1.589(4)	153.8(3)
Si12 1 - O12 1	1.596(4)	167.2(3)	Si12 2 - O12 2	1.592(4)	153.1(2)
Si12 1 - O20 1	1.598(3)	142.6(2)	Si12 2 - O24	1.597(2)	149.8(2)
mean	1.592	153.9	mean	1.591	153.0

MFI.4 Chemical composition

Version of January 23, 2005

	D																
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

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

MFI.5 Flexibility and apertures

Table MFI.5.1 Unit cell volumes and mean, minimum and maximum values of the T-O-T angles for three MFI-type compounds. The value of the mean Δ of T-O-T is the mean deviation of the 48 individual angles T-O-T in MFI1989b01 and MFI1990a01 when compared with their corresponding values in the aristotypic MFI1987a01.

code	space group	V [Å^3]	mean T - O - T [°]	minimum T - O - T [°]	maximum T - O - T [°]	mean Δ of T - O - T [°]	references
MFI1987a01	$P\,n\,m\,a$, I	5332	156.0	144.9	175.9	-	87van1
MFI1989b01	$P\,2_1\,2_1\,2_1$, II.1	5359	154.7	138.4	172.7	7.1	89van1
MFI1990a01	$P\,2_1/n\,1\,1$, II.2	5343	153.0	141.3	168.9	5.2	90van1

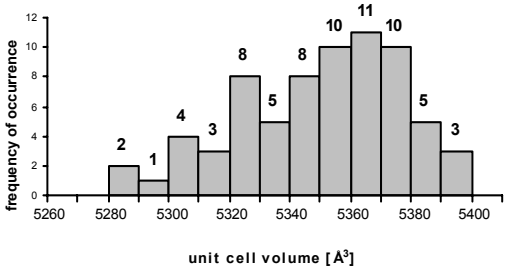


Fig. MFI.5.1 Histogram of 70 unit cell volumes of silicates and aluminosilicates of MFI-type in space groups $P\,n\,m\,a$, $P\,2_1\,2_1\,2_1$, and $P\,2_1/n\,1\,1$. Only those compounds are entered where the Al content is less than 8% of the T-sites and where the e.s.d.'s of the unit cell constants are 0.01 Å or less. Values without an e.s.d. are not listed. Frameworks containing B, Ti or Li have been omitted altogether. The median value of V is 5365 Å^3, while the mean value is 5351 Å^3.

The value of the mean T-O-T angles for three very precisely determined crystal structures of the MFI-type (MFI1987a01, MFI1989b01 and MFI1990a01) is about 154°, with individual angles ranging from 138° to 176° (Table MFI.5.1). This range of values T-O-T for the MFI-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 MFI-type silicoaluminate compounds displayed in a histogram in Fig. MFI.5.1 vary by about 2.1%. 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 MFI-type compounds, which is about 0.7%. It seems that the framework of MFI-type is relatively inflexible. This is also born out by the small deviations between the T-O-T angles of the three compounds in three different space groups (Table MFI.5.1): on average the angles in the space groups of lower symmetry deviate only by 7° and 5° from those in the aristotype.

It is remarkable that in the sample of 70 MFI-type crystal structures the unit cell volumes (and the cell constants) change so little. After all it contains pure silicalite as well as ZSM-5 with various Al-contents, frameworks with empty pores and filled with templates, various exchanged cations, water molecules and about a dozen different organic molecules, some of them in several isomeric forms, and at different levels of loading.

The 10-ring openings in the framework of MFI have free diameters ranging from 5Å to 5.5Å.

MFI.6 Other information

ZSM-5 based compounds are extremely important in petrochemical processing for various reactions involving the formation of more complex molecules from methane. By this we mean the methanol-to-hydrocarbons technology, and more specifically the methanol-to-olefin (that is to alkene) and methanol-to-octane reactions. A thorough review of this field has been given by [99Stö1]. In a way ZSM-5 catalysts are the exact opposite of FAU-based catalysts which are mostly used for cracking long molecules in order to obtain shorter chains useful for gasoline. ZSM-5 catalysts on the other hand are useful for the synthesis, among other products, of gasoline from methane. This is a field of enormous scientific and industrial activity. In the last ten years about 700 patents have been issued mentioning ZSM-5 and silicalite, as opposed to ca. 400 patents involving zeolite Y and faujasite (both according to the Derwent Innovations Index). SciFinder Scholar, the database of the Chemical Abstracts Service lists about 18,000 publications mentioning ZSM-5 or silicalite, which is almost as many as referring to faujasite or zeolite Y (over 19,000). This means that almost a third of all references to zeolites are either to MFI- or FAU-type compounds.

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Gone to press March 1, 2006