MEL

MEL.1 Zeolite framework type and topology

The designation of the framework type code (FTC) refers to the type material ZS**M**-**EL**even (ZSM-11, Zeolite Socony Mobil with sequence number eleven). The synthetic high silica zeolite ZSM-11 represents one endmember of the pentasil family of zeolites [80Kok1] with framework structures 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]. The framework structure can be built by reflection (σ-stacking) of the pentasil chains as shown in Fig. MEL.1.2b. Linkage of the chains by an inversion center (i-stacking) yields ZSM-5 (MFI type) the other end member of the pentasil family.

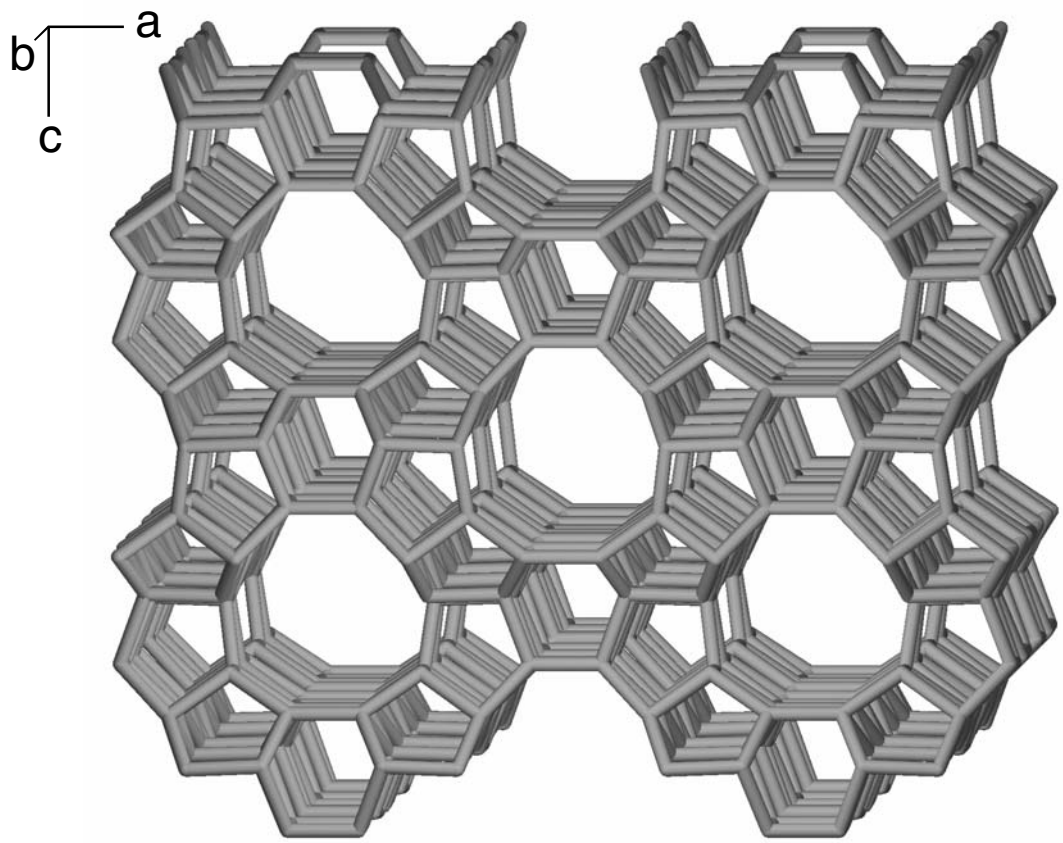
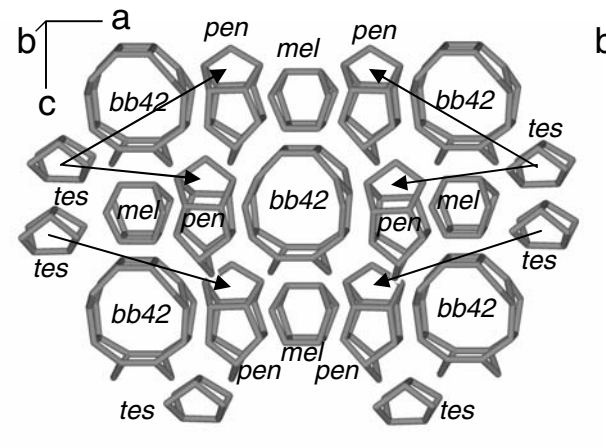
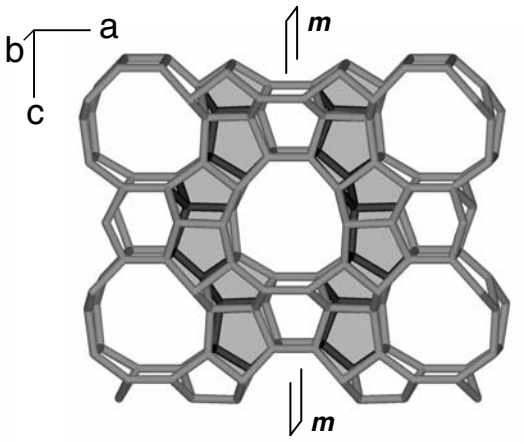


Fig. MEL.1.1 The framework structure of MEL-type zeolites in the highest possible topological symmetry $I\,\bar{4}\,m\,2$. View parallel **b** rotated by 3° about **a** and **c**.

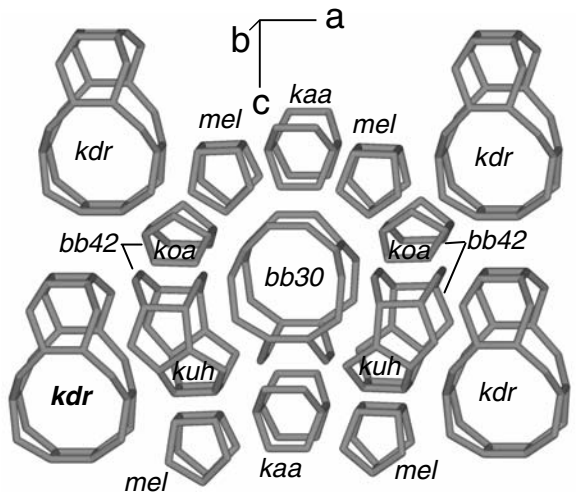
The space between successive pentasil layers (Fig. MEL.1.2b) related by . *m* . mirror planes are filled by the polyhedral units shown in Fig. MEL.1.2c and d. The ordered sequence of mirror planes yields an AA'AA'A... sequence of the pentasil layers where the A' is layer A reflected on the mirror plane. The *bb42* ($4^1 5^2 5^2 5^2 6^1 10^1 10^1$), *kdr* ($4^2 6^4 10^4$), and *bb30* ($8^2 10^4$) units form the two-dimensional channel system (Figs. MEL.1.3, MEL.1.4) in the **ab**-plane interconnected by *mel* ($4^1 5^2 6^2$), *pen*, and *tes* (5^4) units within the pentasil layers and by *kaa* ($6^2 8^2$), *koa* ($5^2 6^1 8^1$), and *mel* units in the intermediate layers. The channels intersect in the *bb30* units (Fig. MEL.1.3) and interpenetrate in the upper and lower parts of the *kdr* unit (Fig. MEL.1.2d). There does exist an 8-ring channel parallel **c** (Fig. MEL.3.1.1a,b) consisting of an alternating sequence of *bb30* and *kaa* units (Fig. MEL.1.2c). However, the aperture is strongly reduced due to the extremely bent geometry of the 8-rings in these two units.



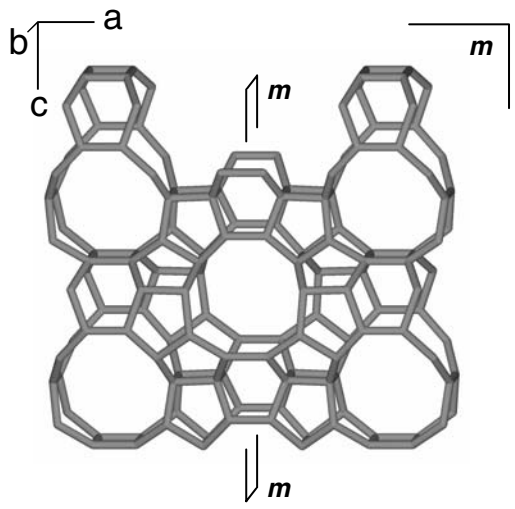
a Linkage of units in *x*, ¾, *z*. Scale is 80% relative to figures b, c, and d. The *bb42* unit is a combination of a *kuh* and a *koa* unit as shown in c).



b The assemblage shown in a) with the pentasil chains (**pet** units) related by the mirror plane shown semi transparently. This pentasil layer is projected by the mirror plane shown in d) to *x*, ¼, *z*.

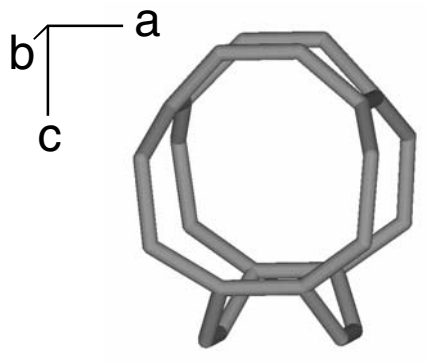


c Linkage of units in *x*, ½, *z*.

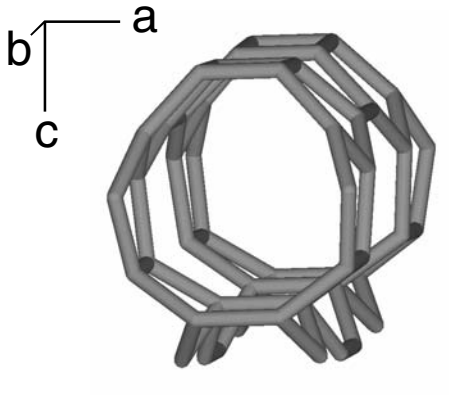


d The complete assemblage shown in c) with . *m* . mirror planes intersecting in ½, ½, *z*.

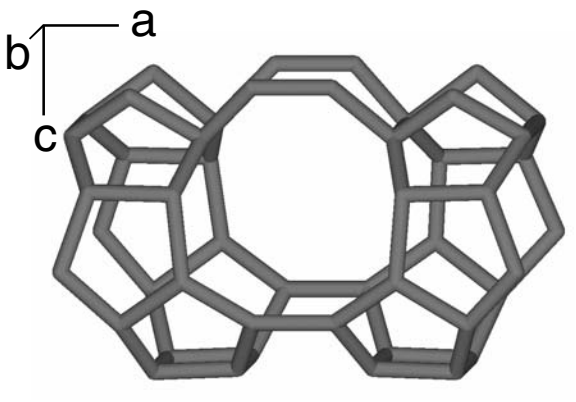
Fig. MEL.1.2 Building scheme of the MEL-type framework. View parallel **b** rotated by 10° about **a** and 8° about **c**.



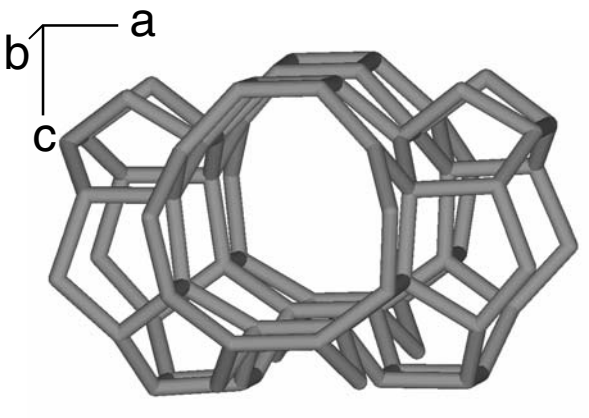
a The *bb30* unit in the intersection of the interpenetrating 10-ring channels and the 8-ring channel parallel **c**.



b The 10-ring channel parallel **b**.



c The 10-ring channel parallel **a**.



d The two 10-ring channels of b) and c) intersecting in *bb30* according to the site symmetry $\bar{4}\,m\,2$ in position 2(d).

Fig. MEL.1.3 The crosspoint of the two-dimensional channel system in the *bb30* unit. View parallel **b** rotated by 5° about **a** and 10° about **c**.

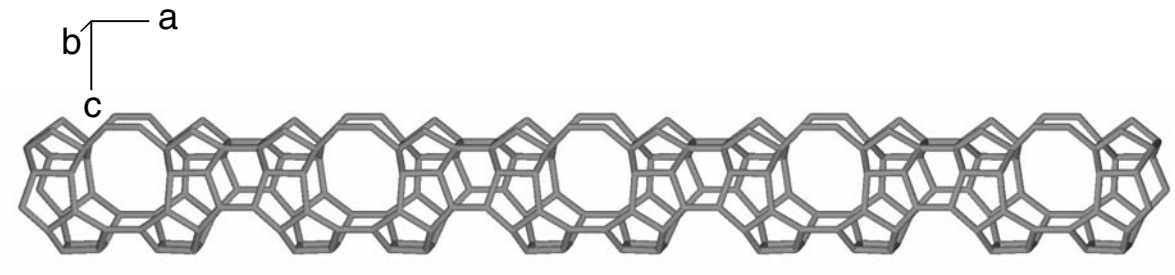
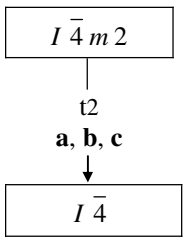


Fig. MEL.1.4 The 10-ring channel (**khi** unit with additional bonds) consisting of a sequence of *bb30*, *kuh*, and the upper part of *kdr* units. View parallel **b** rotated by 10° about **a** and **c**.



MEL-I. Highest possible topological symmetry.

MEL-II. Splitting of T and O-atom sites reduces space group symmetry.

Fig. MEL.1.5 Symmetry relationships of the MEL types.

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

MEL-I $I\bar{4}m2$	MEL-II $I\bar{4}$	MEL-I $I\bar{4}m2$	MEL-II $I\bar{4}$
T1 [16(j), 1]	T11 [8(g), 1] T12 [8(g), 1]	O5 [16(j), 1]	O51 [8(g), 1] O52 [8(g), 1]
T2 [16(j), 1]	T21 [8(g), 1] T22 [8(g), 1]	O6 [16(j), 1]	O61 [8(g), 1] O62 [8(g), 1]
T3 [16(j), 1]	T31 [8(g), 1] T32 [8(g), 1]	O7 [16(j), 1]	O71 [8(g), 1] O72 [8(g), 1]
T4 [16(j), 1]	T41 [8(g), 1] T42 [8(g), 1]	O8 [16(j), 1]	O81 [8(g), 1] O82 [8(g), 1]
T5 [16(j), 1]	T51 [8(g), 1] T52 [8(g), 1]	O9 [16(j), 1]	O91 [8(g), 1] O92 [8(g), 1]
T6 [8(g), . . 2]	T6 [8(g), 1]	O10 [8(i), . *m* .]	O10 [8(g), 1]
T7 [8(g), . . 2]	T7 [8(g), 1]	O11 [8(i), . *m* .]	O11 [8(g), 1]
O1 [16(j), 1]	O1_1 [8(g), 1] O1_2 [8(g), 1]	O12 [8(i), . *m* .]	O12 [8(g), 1]
O2 [16(j), 1]	O21 [8(g), 1] O22 [8(g), 1]	O13 [8(i), . *m* .]	O13 [8(g), 1]
O3 [16(j), 1]	O31 [8(g), 1] O32 [8(g), 1]	O14 [8(h), . . 2]	O14 [8(g), 1]
O4 [16(j), 1]	O41 [8(g), 1] O42 [8(g), 1]	O15 [8(h), . . 2]	O15 [8(g), 1]

MEL.2 Compounds and crystal data

Table MEL.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
MEL-I $I\bar{4}m2$								
MEL1978a01	$Na_{16} \cdot Al_{16}Si_{80}O_{192}$ [1)]	17.6	S	-	-	C	n.s.	78Kok1
MEL1988a01	$Si_{96}O_{192}$	17.8	S	-	-	C	1023	88Tob1
MEL1988b01	$Si_{96}O_{192}$	18.2	T	-	-	-	-	88van1
MEL1989a01	$Si_{96}O_{192}$	17.8	S	-	-	C	1043	89Fyf1
MEL1989b01	$Si_{96}O_{192}$	18.2	T	-	-	-	-	89Uyt1
MEL1990a01	$Na_{3.2} \cdot Ga_{3.0}Si_{93.0}O_{192}$	17.8	S	-	-	C	813	90Liu1
MEL1996b01	$Si_{96}O_{192}$	17.8	S	-	-	C	823	96Ter1
MEL1999a01	$Si_{96}O_{192} \cdot C_{11}NH_{24}OH$	17.9	S	-	DDPOH	-	-	99van1
MEL-II $I\bar{4}$								
MEL1996a01	$Si_{96}O_{192}$	17.9	S	-	-	C	1023	96Hoc1
MEL1996a02	$Si_{96}O_{192}$	17.9	S	-	-	-	-	96Hoc1

[1]) Chemical composition assumed

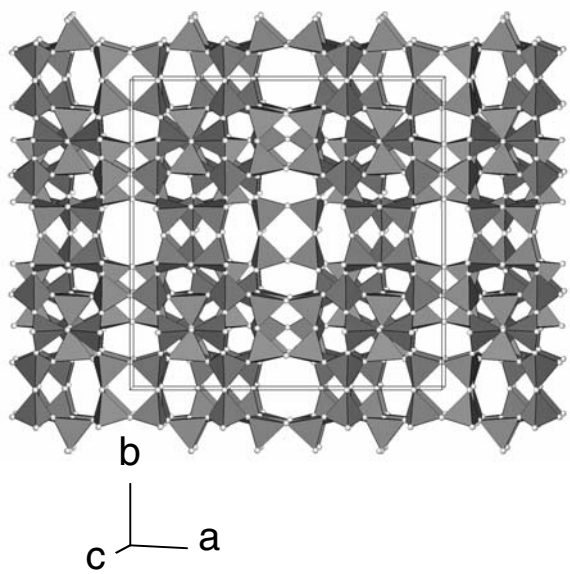
Table MEL.2.2 Structural parameters of the MEL-type compound.

code	*a* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
MEL-I $I\bar{4}m2$					
MEL1978a01	20.12	13.44	5441	n.s.	78Kok1
MEL1988a01	20.0647(2)	13.4082(2)	5398	295	88Tob1
MEL1988b01	20.02	13.15	5271	-	88van1
MEL1989a01	20.067(1)	13.411(1)	5400	373	89Fyf1
MEL1989b01	20.02	13.15	5271	-	89Uyt1
MEL1990a01	20.073(4)	13.403(3)	5400	n.s.	90Liu1
MEL1996b01	20.05988(4)	13.40310(3)	5393	299	96Ter1
MEL1999a01	20.049(1)[1)]	13.379(1)[1)]	5378	n.s.	99van1
MEL-II $I\bar{4}$					
MEL1996a01	20.019(2)	13.380(1)	5362	20	96Hoc1
MEL1996a02	20.019(2)	13.380(1)	5362	-	96Hoc1

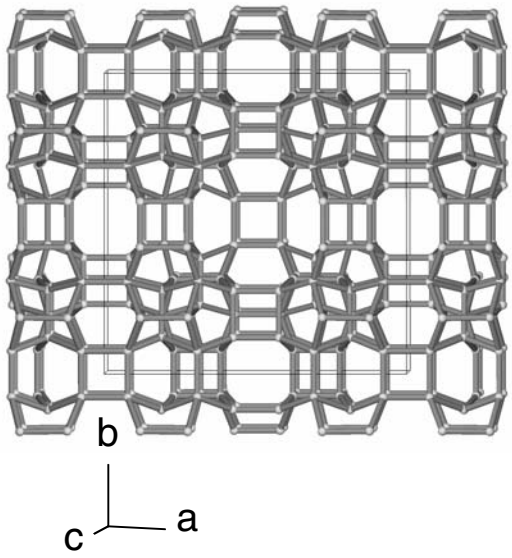
[1]) Lattice constants from private communication by H. van Koningsveld.

MEL.3 Framework structures

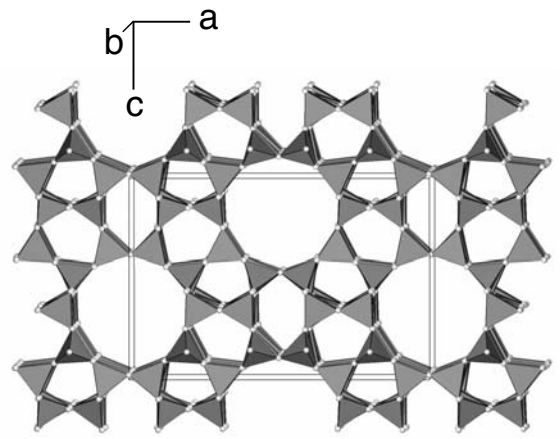
MEL.3.1 MEL-I compound ($I\bar{4}m2$, IT #119)



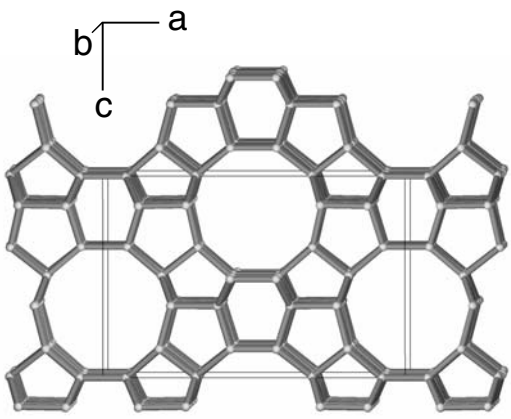
a Polyhedral representation. View parallel **c** rotated by 1° about **a** and **b**.



b Ball and stick model corresponding to a).



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



d Ball and stick model corresponding to c).

Fig. MEL.3.1.1 Projections of the MEL-I crystal structure of ZSM-11, $Si_{96}O_{192} \cdot C_{11}NH_{24}$ OH (MEL1999a01, 99van1).

Table MEL.3.1.1 Atomic coordinates and site definitions for ZSM-11, $Si_{96}O_{192} \cdot C_{11}NH_{24}$ OH (MEL1999a01, 99van1). Atomic coordinates of the template molecules are not given. According to Fig. 2 in [99van1] they reside in the *bb30* and *kdr* units.

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1	0.12066(3)	0.18805(3)	0.14403(5)	1.27(2)	1	16(j)	14.70(5)
Si2	0.07657(3)	0.22544(3)	0.35715(5)	1.40(2)	1	16(j)	14.96(5)
Si3	0.27751(3)	0.18986(3)	0.14020(6)	1.56(2)	1	16(j)	15.12(5)
Si4	0.30711(3)	0.07607(3)	-0.00710(5)	1.55(2)	1	16(j)	15.22(6)
Si5	0.07623(3)	0.37981(3)	0.3564(5)	1.41(2)	1	16(j)	13.30(5)
Si6	0.07697(3)	*x*	0	1.30(2)	. . 2	8(g)	7.80(4)
Si7	0.19003(3)	*x*	½	1.59(2)	. . 2	8(g)	7.72(4)
O1	0.0993(1)	0.11881(9)	0.0956(2)	3.18(6)	1	16(j)	16
O2	0.0934(1)	0.1882(1)	0.2553(1)	3.70(6)	1	16(j)	16
O3	0.1991(1)	0.1953(1)	0.1428(3)	5.29(8)	1	16(j)	16
O4	0.3000(1)	0.1214(1)	0.0900(2)	4.06(6)	1	16(j)	16
O5	0.11974(9)	0.1927(1)	0.4431(2)	3.13(5)	1	16(j)	16
O6	0.3058(1)	0.2505(1)	0.0783(2)	4.16(6)	1	16(j)	16
O7	0.0933(1)	0.30264(8)	0.3479(2)	3.47(6)	1	16(j)	16
O8	0.0903(1)	0.2486(1)	0.0830(2)	4.279(6)	1	16(j)	16
O9	0.3772(1)	0.0883(1)	0.9399(2)	4.32(6)	1	16(j)	16
O10	0.0895(1)	0	0.0246(2)	2.57(6)	. *m* .	8(i)	8
O11	0.3038(1)	0	0.0289(2)	2.53(6)	. *m* .	8(i)	8
O12	0.2129(1)	0	0.6150(2)	2.74(6)	. *m* .	8(i)	8
O13	0.3909(2)	0	0.6107(2)	2.95(7)	. *m* .	8(i)	8
O14	0.3088(1)	*x*+½	¼	3.36(6)	. . 2	8(h)	8
O15	0.0870(1)	*x*+½	¼	5.21(8)	. . 2	8(h)	8

Table MEL.3.2 Selected interatomic distances and angles for ZSM-11, $Si_{96}O_{192} \cdot C_{11}NH_{24}$ OH (99van1, (MEL1999a01)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 - O3	1.579(2)	170.7(2)	Si2 - O5	1.582(2)	147.2(2)
Si1 - O8	1.585(2)	166.1(2)	Si2 - O7	1.589(2)	153.9(2)
Si1 - O2	1.586(2)	151.5(1)	Si2 - O2	1.590(2)	151.5(1)
Si1 - O1	1.591(2)	149.5(2)	Si2 - O12	1.600(1)	147.4(2)
Mean	1.585	159.5	mean	1.590	150.0
Si3 - O3	1.576(2)	170.7(2)	Si4 - O8	1.578(2)	166.1(2)
Si3 - O6	1.577(2)	160.7(2)	Si4 - O4	1.592(3)	149.5(2)
Si3 - O4	1.593(2)	149.5(2)	Si4 - O9	1.593(2)	153.2(2)
Si3 - O14	1.598(1)	149.2(1)	Si4 - O11	1.601(1)	144.6(2)
Mean	1.586	157.5	mean	1.591	153.4
Si5 - O15	1.586(1)	156.9(2)	Si6 - O1	1.594(2)	149.5(2)
Si5 - O7	1.589(2)	153.9(2)	Si6 - O1	1.594(2)	149.5(2)
Si5 - O9	1.590(2)	153.2(2)	Si6 - O10	1.598(2)	150.0(2)
Si5 - O13	1.606(1)	144.3(2)	Si6 - O10	1.598(2)	150.0(2)
Mean	1.593	152.1	Mean	1.596	149.8

Table MEL.3.2 (continued)

	T - O [Å]	T - O - T [°]
Si7 - O6	1.589(2)	160.7(2)
Si7 - O6	1.589(2)	160.7(2)
Si7 - O5	1.603(2)	147.2(2)
Si7 - O5	1.603(2)	147.2(2)
Mean	1.596	154.0

MEL.3.2 MEL-II compound ($I\bar{4}$, IT #82)

The figures for MEL-II are identical with those of MEL-I within the accuracy of the drawings.

Table MEL.3.2.1 Atomic coordinates and site definitions for the low temperature form of calcined ZSM-11, $Si_{96}O_{192}$ (MEL1996a01, 96Hoc1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0.1231(4)	0.1857(4)	0.1445(6)	1.3(4)	1	8(g)	8
Si12	0.8775(4)	0.1897(5)	0.1436(6)	1.3(4)	1	8(g)	8
Si21	0.0791(5)	0.2273(4)	0.3558(6)	1.3(4)	1	8(g)	8
Si22	0.9231(5)	0.2278(4)	0.3572(7)	1.3(4)	1	8(g)	8
Si31	0.2796(4)	0.1913(5)	0.1550(6)	1.3(4)	1	8(g)	8
Si32	0.7196(4)	0.1862(5)	0.1277(5)	1.3(4)	1	8(g)	8
Si41	0.3079(5)	0.0811(4)	-0.0037(6)	1.3(4)	1	8(g)	8
Si42	0.6952(5)	0.0707(5)	-0.0153(6)	1.3(4)	1	8(g)	8
Si51	0.0758(5)	0.3818(4)	0.3606(7)	1.3(4)	1	8(g)	8
Si52	0.9227(4)	0.3826(4)	0.3518(7)	1.3(4)	1	8(g)	8
Si6	0.0818(5)	0.0734(5)	0.0054(7)	1.3(4)	1	8(g)	8
Si7	0.1898(5)	0.1956(5)	0.5155(6)	1.3(4)	1	8(g)	8
O1_1	0.1122(8)	0.1131(6)	0.098(1)	1.9(7)	1	8(g)	8
O1_2	0.9061(9)	0.1248(8)	0.090(1)	1.9(7)	1	8(g)	8
O21	0.0953(8)	0.1864(7)	0.2565(7)	1.9(7)	1	8(g)	8
O22	0.9082(8)	0.1910(8)	0.2537(7)	1.9(7)	1	8(g)	8
O31	0.2007(4)	0.2051(8)	0.148(1)	1.9(7)	1	8(g)	8
O32	0.7981(4)	0.1815(8)	0.150(1)	1.9(7)	1	8(g)	8
O41	0.2982(9)	0.1249(7)	0.0949(9)	1.9(7)	1	8(g)	8
O42	0.6933(8)	0.1179(6)	0.0806(9)	1.9(7)	1	8(g)	8
O51	0.1261(7)	0.2009(8)	0.4438(9)	1.9(7)	1	8(g)	8
O52	0.8789(6)	0.1928(8)	0.441(1)	1.9(7)	1	8(g)	8
O61	0.3165(7)	0.2550(7)	0.1088(9)	1.9(7)	1	8(g)	8
O62	0.7087(8)	0.2437(7)	0.047(1)	1.9(7)	1	8(g)	8
O71	0.0958(7)	0.3052(4)	0.342(1)	1.9(7)	1	8(g)	8
O72	0.9023(7)	0.3050(4)	0.350(1)	1.9(7)	1	8(g)	8
O81	0.0835(7)	0.2397(7)	0.081(1)	1.9(7)	1	8(g)	8
O82	0.8941(8)	0.2578(7)	0.088(1)	1.9(7)	1	8(g)	8
O91	0.3813(6)	0.0883(9)	0.951(1)	1.9(7)	1	8(g)	8
O92	0.6293(6)	0.0768(7)	0.918(1)	1.9(7)	1	8(g)	8
O10	0.0917(5)	-0.0056(5)	0.019(1)	1.9(7)	1	8(g)	8

Table MEL.3.2.1 (continued)

atom	x	y	z	B [Å2]	site symmetry	Wyckoff position	no. of atoms in unit cell
O11	0.2953(7)	0.0044(4)	0.0242(8)	1.9(7)	1	8(g)	8
O12	0.2174(7)	-0.0012(5)	0.620(1)	1.9(7)	1	8(g)	8
O13	0.3915(7)	0.0016(5)	0.6113(8)[1])	1.9(7)	1	8(g)	8
O14	0.3189(6)	0.7995(8)	0.2302(6)	1.9(7)	1	8(g)	8
O15	0.0776(6)	0.5901(8)	0.2396(8)	1.9(7)	1	8(g)	8

[1]) z coordinate of O13 corrected from 0.3887 [96Hoc1] to 0.6113 in the standardized setting.

Table MEL.3.2 Selected interatomic distances and angles for the low temperature form of ZSM-11, $Si_{96}O_{192}$ (MEL1996a01, 96Hoc1)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O81	1.59(2)	159(1)	Si1 2 - O82	1.59(2)	160(1)
Si11 - O1_1	1.60(2)	144(1)	Si1 2 - O1_2	1.59(2)	154(1)
Si11 - O21	1.60(1)	149(1)	Si1 2 - O22	1.60(1)	152(1)
Si11 - O31	1.60(1)	156(1)	Si1 2 - O32	1.60(1)	163(1)
Mean	1.60	152	mean	1.59	157
Si21 - O21	1.59(1)	149(1)	Si22 - O52	1.59(2)	142(1)
Si21 - O51	1.60(2)	159(1)	Si22 - O22	1.60(2)	152(1)
Si21 - O12	1.60(1)	153(1)	Si22 - O72	1.60(1)	150(1)
Si21 - O71	1.61(1)	149(1)	Si22 - O12	1.61(1)	153(1)
Mean	1.60	153	mean	1.60	149
Si31 - O41	1.60(2)	154(1)	Si32 - O62	1.59(2)	169(1)
Si31 - O61	1.60(2)	139(1)	Si32 - O42	1.60(2)	145(1)
Si31 - O14	1.60(1)	144(1)	Si32 - O14	1.60(1)	144(1)
Si31 - O31	1.61(1)	156(1)	Si32 - O32	1.60(1)	163(1)
Mean	1.60	148	Mean	1.60	155
Si41 - O82	1.59(2)	160(1)	Si42 - O81	1.59(2)	159(1)
Si41 - O41	1.60(2)	154(1)	Si42 - O42	1.59(2)	145(1)
Si41 - O91	1.60(2)	145(1)	Si42 - O92	1.60(2)	153(1)
Si41 - O11	1.60(1)	143(1)	Si42 - O11	1.61(1)	143(1)
Mean	1.60	151	Mean	1.60	150
Si51 - O15	1.59(1)	149(1)	Si52 - O92	1.59(2)	153(1)
Si51 - O91	1.60(2)	145(1)	Si52 - O15	1.60(2)	149(1)
Si51 - O71	1.60(1)	149(1)	Si52 - O13	1.60(1)	146(1)
Si51 - O13	1.61(1)	146(1)	Si52 - O72	1.61(1)	150(1)
Mean	1.60	147	Mean	1.60	150
Si6 - O1_1	1.59(2)	144(1)	Si7 - O62	1.59(2)	169(1)
Si6 - O1_2	1.59(2)	154(1)	Si7 - O61	1.60(2)	139(1)
Si6 - O10	1.60(1)	153(1)	Si7 - O51	1.60(2)	159(1)
Si6 - O10	1.60(1)	153(1)	Si7 - O52	1.60(2)	142(1)
Mean	1.60	151	Mean	1.60	152

MEL.4 Chemical composition

	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

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

MEL.5 Flexibility and apertures

The unit cell constants of the known frameworks of the MEL-type vary only by about 0.5% and their chemistry is pretty uniform. Therefore, one cannot say much about their flexibility.

The 10-ring in the MEL framework is almost circular with a free diameter of about 5.5 Å.

MEL.6 Other information

As explained in MEL.1 the frameworks of the MEL- and the MFI-types are closely related. Nevertheless, compounds based on the MEL framework are not used as catalysts the way MFI-type compounds have been, which, among other applications, are commercially employed for the methanol-to-hydrocarbon conversion [99Stö1]. This might be related to the difficulty of synthesizing MEL-type compounds [96Ter1]. Studies of the catalytic properties of Fe-substituted ZSM-11 [2004Req1] and of V-substituted ZSM-11 [94Sen1] have been published, however.

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