MSO

MSO.1 Zeolite framework type and topology

The designation of the FTC refers to the type material **M**CM-**S**ixty-**O**ne (MCM-61, Mobil Composition of Matter with sequence number sixty-one), first synthesized by [97Val1]. The crystal structure was solved by [99Sha1] in space group $R\,\bar{3}m$. The framework structure (Fig. MSO.1.1, MSO.1.2) consists of pillars (**zni** units) of stacked *ber* ($6^6 6^2$), *hpr* ($4^6 6^2$), and *znl* ($4^6 6^{12} 6^6 6^2$) units in 0, 0, z and its symmetrically equivalent positions in 1/3, 2/3, z and 2/3, 1/3, z shifted by 2/3 and 1/3 along z, respectively, according to the R-centering of the rhombohedral space group as shown in Fig. MSO.1.2. The remaining voids are formed by lau ($4^2 6^4$) units.

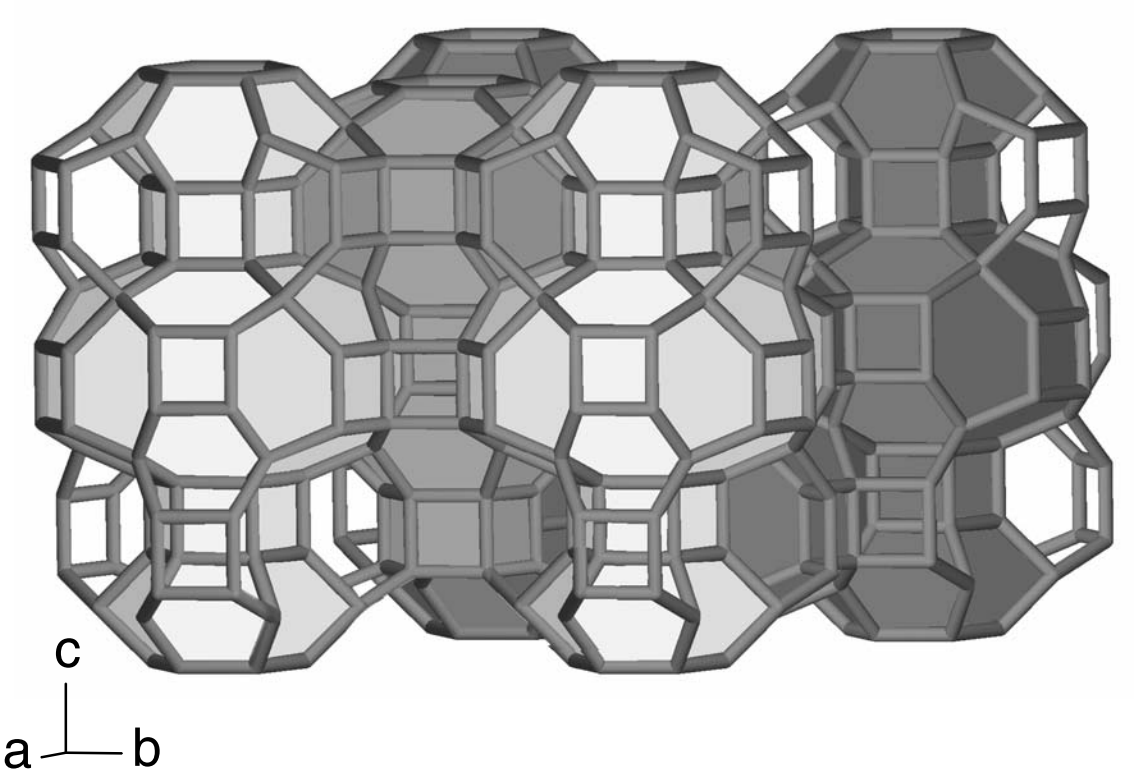
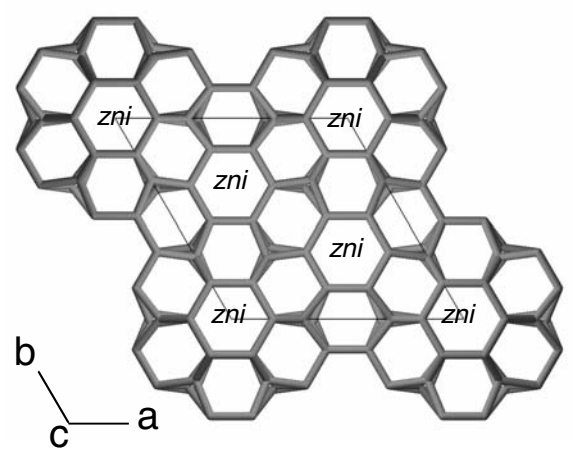
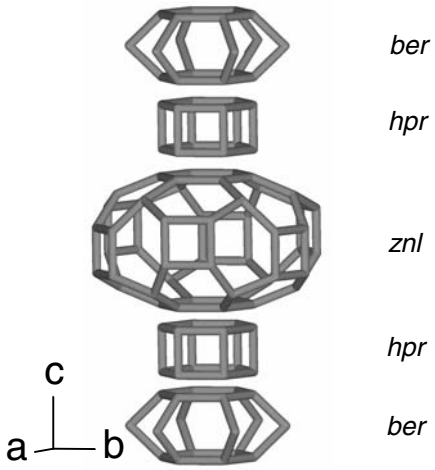


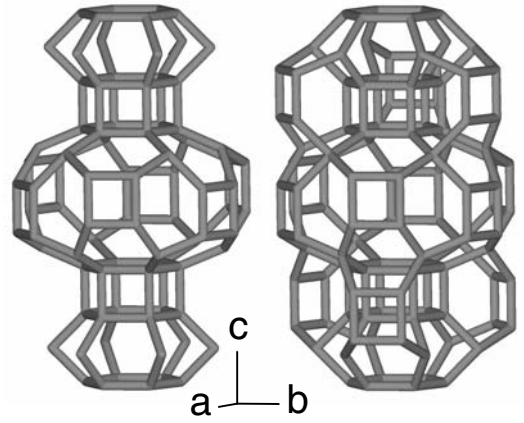
Fig. MSO.1.1. The framework structure of MSO-type compounds in the highest possible topological symmetry $R\,\bar{3}m$ (MSO1999a01, 99Sha1). Units of the **zni** pillars are shown nontransparently. View parallel [210] rotated by 5° about [010] and 10° about [001].



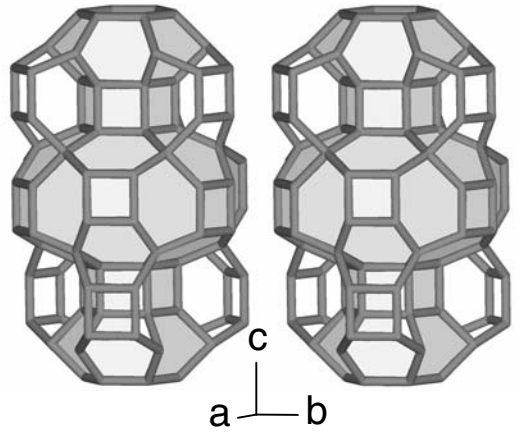
a Stick model projected parallel [001].



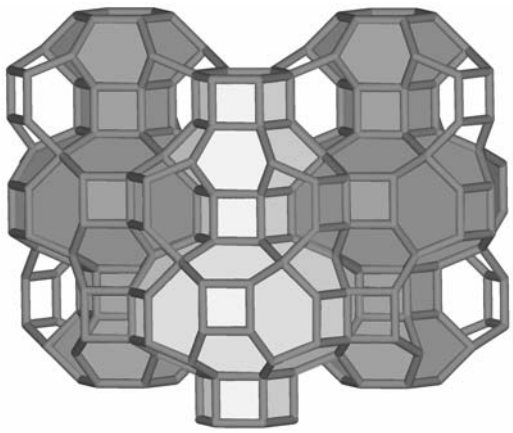
b Units forming the **zni** pillar.



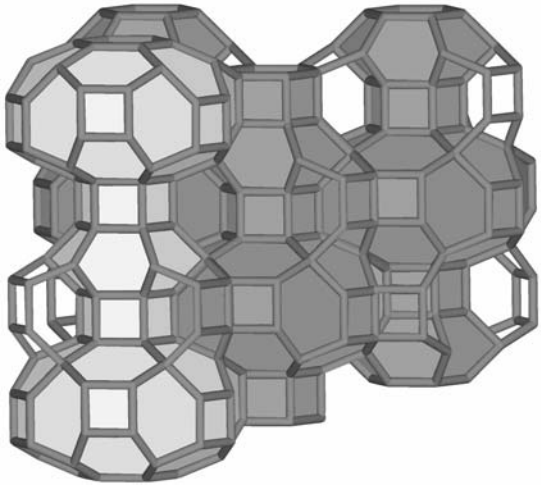
c **zni** pillar (left) completed by *lau* units (right).



d Two pillars in 0, 0, *z* and 0, 1, *z*. The **zni** pillars are shown nontransparently.



e The assemblage shown in d) extended by a **zni** unit in 1/3, 2/3, *z*.



f The assemblage shown in e) extended by a **zni** unit in 2/3, 1/3, *z*.

Fig. MSO.1.2 Building scheme of MSO-type structures. View parallel [210] rotated by 5° about [010] and 10° about [001] in b) to f). The complete assemblage is shown in Fig. MSO.1.1.

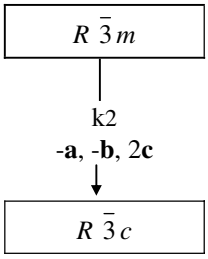


Fig. MSO.1.3 The Bärnighausen tree illustrating the symmetry relationship of the MSO types.

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

MSO-I, $R\,\bar{3}\,m$		MSO-II, $R\,\bar{3}\,c$	MSO-I, $R\,\bar{3}\,m$		MSO-II, $R\,\bar{3}\,c$
T1 [36(i), 1]	→	T11 [36(f), 1] T12 [36(f), 1]	O2 [36(i), 1]	→	O21 [36(f), 1] O22 [36(f), 1]
T2 [36(i), 1]	→	T21 [36(f), 1] T22 [36(f), 1]	O3 [36(i), 1]	→	O31 [36(f), 1] O32 [36(f), 1]
T3 [18(f), . 2]	→	T31 [18(e), . 2] T32 [18(e), . 2]	O4 [18(h), . *m*]	→	O4 [36(f), 1]
			O5 [18(h), . *m*]	→	O5 [36(f), 1]
O1 [36(i), 1]	→	O11 [36(f), 1] O12 [36(f), 1]	O6 [18(h), . *m*]	→	O6 [36(f), 1]
			O7 [18(h), . *m*]	→	O7 [36(f), 1]

MSO.2 Compounds and crystal data

Table MSO.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
MSO-I $R\,\bar{3}\,m$									
MSO1999a01	$K_{6.3} \cdot Si_{83.7}Al_{6.3}O_{180} \cdot 3C_{12}H_{24}O_6$	MCM-61	18.1	S	-	[1])	-	-	99Sha1
MSO-II $R\,\bar{3}\,c$									
MSO2001a01	$P_{90}Al_{90}O_{360} \cdot 6C_{12}H_{28}N_2O_4$ 12OH $11H_2O$	MU-13	17.9	S	-	[2])	-	-	2001Pai1

[1]) 18-Crown-6

[2]) [2.2]cryptand, OH, H_2O

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

code	*a* [Å]	*c* [Å]	*V* [Å^3]	matrix	coord. trans.	shift	*T* [K]	reference
MSO-I $R\bar{3}m$								
MSO1999a01	17.2270(1)	19.3064(2)	4962	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	298	99Sha1
MSO-II $R\bar{3}c$								
MSO2001a01	17.283(2)	38.914(3)	10066	0, 0, ¼	**a**, **b**, **c**	*x*, *y*, *z*-¼	n.s.	2001Pai1

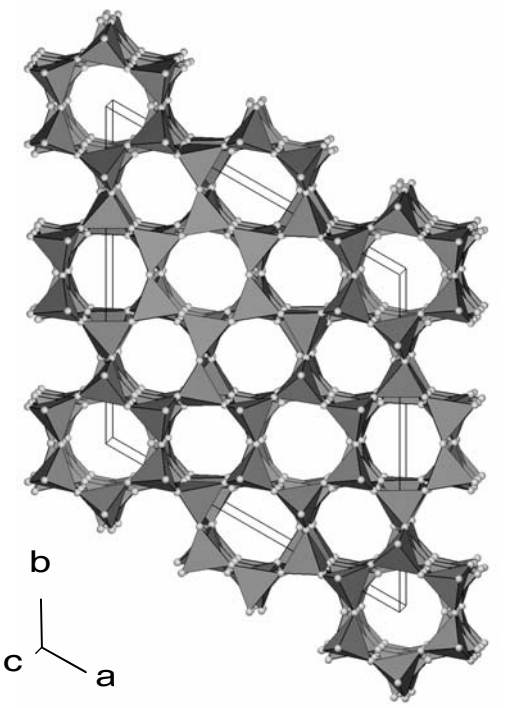
MSO.3 Framework structures

MSO.3.1 MSO-I compound ($R\bar{3}m$, IT #166)

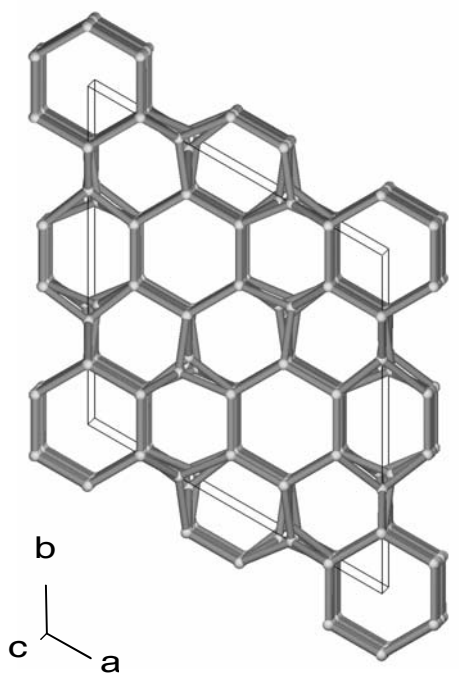
Table MSO.3.1.1 Atomic coordinates and site definitions for MSO-I, MCM-61, $K_{6.3} \cdot Si_{83.7}Al_{6.3}O_{180} \cdot 3C_{12}H_{24}O_6$ (MSO1999a01, 99Sha1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	-0.0002(2)	0.1797(2)	0.2725(1)	0.46	1	36(i)	33.48 / 2.52
(Si,Al)2	0.0002(2)	0.1795(2)	0.1129(1)	0.46	1	36(i)	33.48 / 2.52
(Si,Al)3	0	0.3073(2)	0	0.46	. 2	18(f)	16.74 / 1.26
O1	0.9845(3)	0.2469(3)	0.3200(3)	1.13	1	36(i)	36
O2	-0.0012(2)	0.2058(3)	0.1927(2)	1.13	1	36(i)	36
O3	0.0205(4)	0.2647(3)[1]	0.0667(2)[2]	1.13	1	36(i)	36
O4	0.0930(7)	-*x*	0.2950(4)	1.13	. *m*	18(h)	18
O5	0.9231(2)	-*x*	0.2889(5)	1.13	. *m*	18(h)	18
O6	0.0755(5)	-*x*	0.1005(5)	1.13	. *m*	18(h)	18
O7	0.9044(3)	-*x*	0.0900(5)	1.13	. *m*	18(h)	18
K1	1/3	2/3	0.2355(6)	5.20	3 *m*	6(c)	3.00
K2	0	0	0.0057(3)	5.45	3 *m*	6(c)	2.06
K3	1/3	2/3	0.283(1)	1.34	3 *m*	6(c)	1.00
C1	0.5504(3)	-0.2694(1)	0.1662(4)	7.90	1	36(i)	36
OC1	-0.5198(5)	-0.3338(4)	0.1231(2)	7.79	1	36(i)	18
H1	-0.5346(7)	-*x*	0.1486(2)	9.47	. *m*	18(h)	72

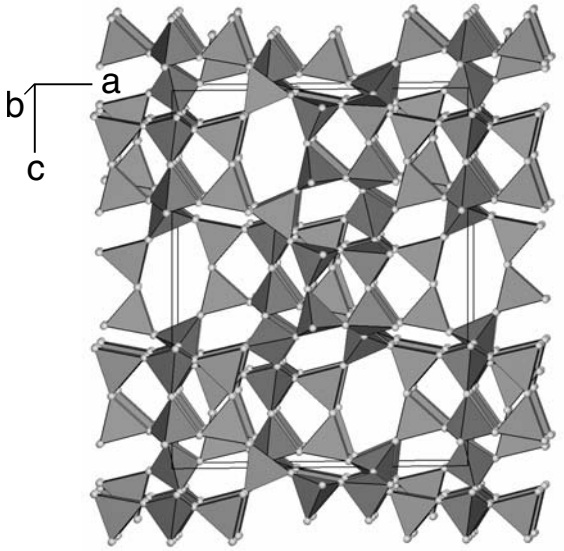
[1]) corrected from 0.0205 [99Sha1] to 0.2647
[2]) corrected from 0.2647 [99Sha1] to 0.0667



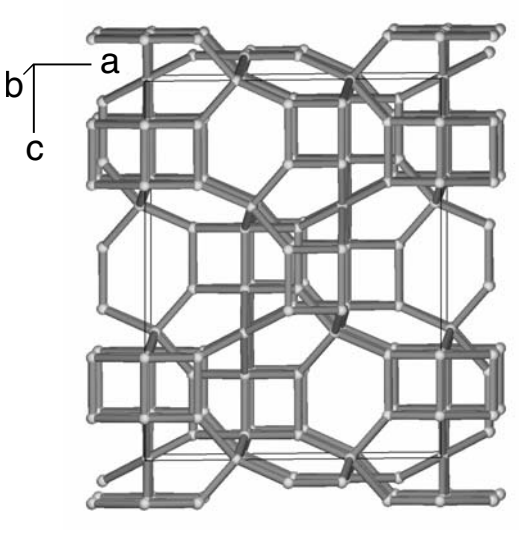
a Polyhedral representation. View parallel [001] rotated by 1° about [210] and [010].



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel [010] rotated by 1° about [210] and [001].



d Ball and stick model corresponding to c).

Fig. MSO.3.1.1 Projections of the MSO-I crystal structure of MCM-61, $K_{6.3} \cdot Si_{83.7}Al_{6.3}O_{180} \cdot 3C_{12}H_{24}O_6$ (MSO1999a01, 99Sha1).

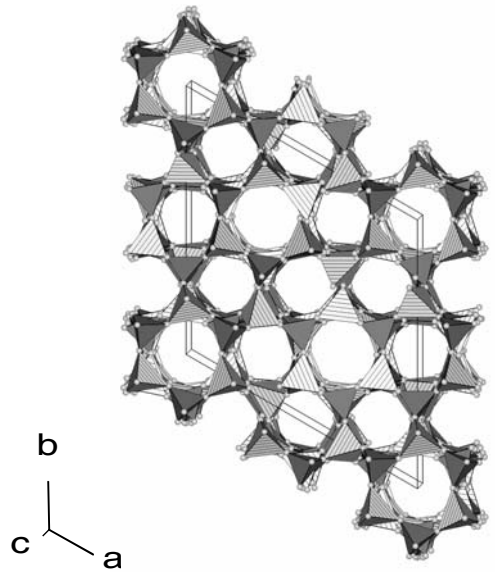
Table MSO.3.1.2 Selected interatomic distances and angles for MSO-I, MCM-61, $K_{6.3} \cdot Si_{83.7}Al_{6.3}O_{180} \cdot 3C_{12}H_{24}O_6$ (MSO1999a01, 99Sha1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)1 - O1	1.599(4)	153.9(4)	(Si,Al)2 - O3	1.600(3)	150.3(4)
(Si,Al)1 - O2	1.607(4)	146.6(3)	(Si,Al)2 - O2	1.609(4)	146.6(3)
(Si.Al)1 - O4	1.614(6)	148.0(6)	(Si.Al)2 - O6	1.618(6)	144.9(5)
(Si,Al)1 - O5	1.626(4)	144.0(4)	(Si,Al)2 - O7	1.619(6)	145.8(6)
Mean	1.611	148.1	mean	1.612	146.9
(Si,Al)3 - O3	1.606(4)	150.3(4)			
(Si,Al)3 - O3	1.606(4)	150.3(4)			
(Si.Al)3 - O1	1.608(4)	153.9(4)			
(Si,Al)3 - O1	1.608(6)	153.9(4)			
Mean	1.607	152.1			

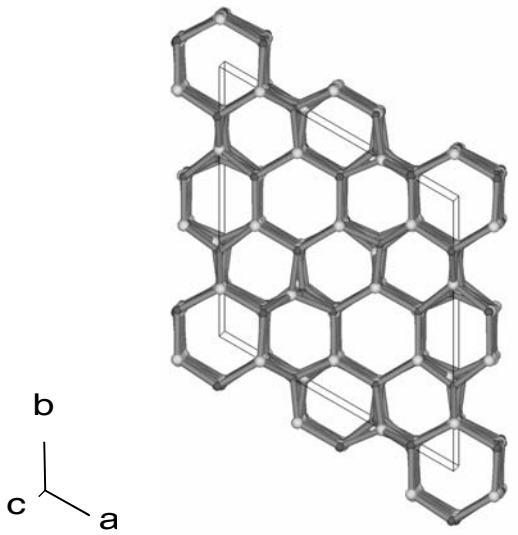
MSO.3.2 MSO-II compound ($R\bar{3}c$, IT #167)

Table MSO.3.2.2 Selected interatomic distances and angles for MSO-II, Mu-13, $P_{90}Al_{90}O_{360} \cdot 6C_{12}H_{28}N_2O_4$ 12OH $11H_2O$ (MSO2001a01, 2001Pai1).

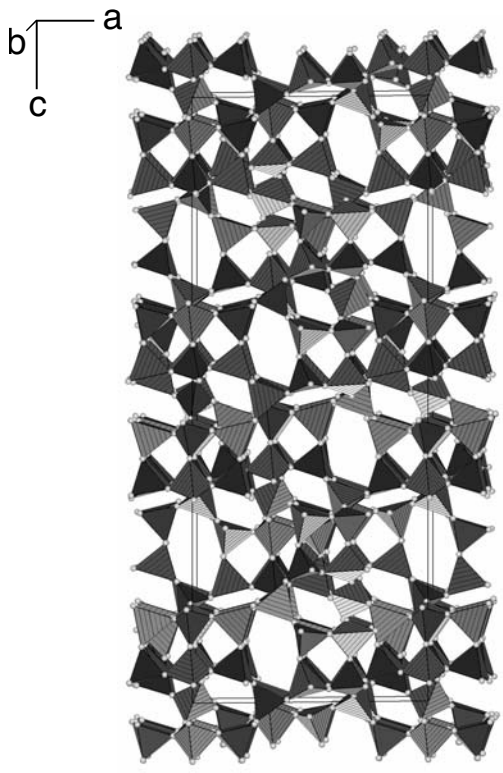
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al1 1 - O21	1.696(9)	140.9(5)	P1 2 - O4	1.497(8)	148.8(4)
Al1 1 - O11	1.720(8)	148.0(5)	P1 2 - O5	1.518(7)	150.4(5)
Al1 1 - O5	1.721(8)	150.4(5)	P1 2 - O12	1.521(6)	155.2(5)
Al1 1 - O4	1.736(13)	148.8(4)	P1 2 - O22	1.535(8)	144.6(3)
mean	1.718	147.0	mean	1.518	149.8
P2 1 - O21	1.499(9)	140.9(5)	Al2 2 - O6	1.688(12)	149.7(5)
P2 1 - O6	1.518(7)	149.7(5)	Al2 2 - O32	1.718(11)	146.3(3)
P2 1 - O7	1.522(6)	151.3(4)	Al2 2 - O7	1.744(7)	151.3(4)
P2 1 - O31	1.525(12)	143.2(5)	Al2 2 - O22	1.832(8)	144.6(3)
mean	1.516	146.3	mean	1.745	148.0
Al3 1 - O12	1.720(4)	155.2(5)	P3 2 - O32	1.496(6)	146.3(3)
Al3 1 - O12	1.720(13)	155.2(5)	P3 2 - O32	1.496(6)	146.3(3)
Al3 1 - O31	1.732(8)	143.2(5)	P3 2 - O11	1.502(7)	148.0(5)
Al3 1 - O31	1.732(8)	143.2(5)	P3 2 - O11	1.502(7)	148.0(5)
mean	1.726	149.2	mean	1.499	147.2



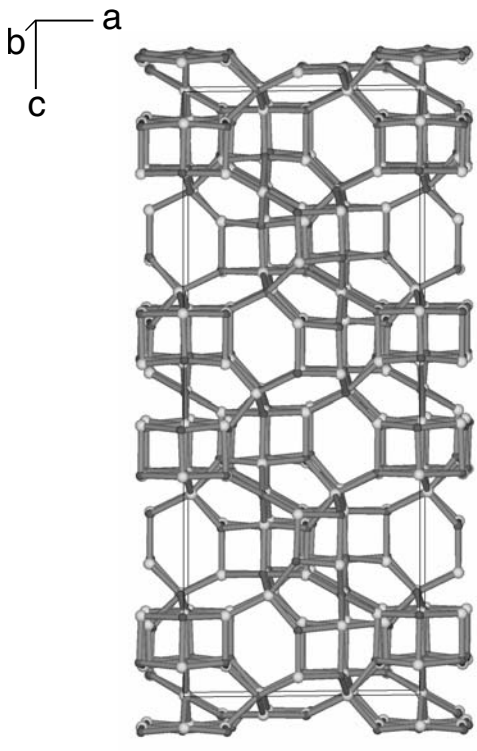
a Polyhedral representation. View parallel [001] rotated by 0.5° about [210] and [010].



b Ball and stick model corresponding to a).



c Polyhedral representation. View parallel [010] rotated by 1° about [210] and [001].



d Ball and stick model corresponding to c).

Fig. MSO.3.2.1 Projections of the MSO-II crystal structure of Mu-13, $P_{90}Al_{90}O_{360} \cdot 6C_{12}H_{28}N_2O_4$ 12OH $11H_2O$ (MSO2001a01, 2001Pai1).

Table MSO..3.2.1 Atomic coordinates and site definitions for MSO-II, Mu-13, $P_{90}Al_{90}O_{360} \cdot 6C_{12}H_{28}N_2O_4$ 12OH $11H_2O$ (MSO2001a01,2001Pai1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Al 11	-0.0005(4)	0.8200(3)	0.1347(1)	2.53(8)	1	36(f)	36
P12	-0.0002(3)	0.8183(3)	0.6328(1)	1.66(8)	1	36(f)	36
P21	-0.0079(3)	0.8125(3)	0.0574(1)	2.05(8)	1	36(f)	36
Al22	0.0050(3)	0.8256(3)	0.5504(1)	2.4(2)	1	36(f)	36
Al31	0	0.6930(3)[1])	0[2])	1.5(2)	. 2	18(e)	18
P32	0	0.6860(3)[3])	½	2.1(2)	. 2	18(e)	18
O11	0.0120(5)	0.7491(4)	0.1622(2)	1.4(2)	1	36(f)	36
O12	0.0199(5)	0.7599(4)	0.6561(2)	3.7(3)	1	36(f)	36
O21	-0.0068(5)	0.7841(4)	0.0937(2)	1.2(2)	1	36(f)	36
O22	0.0046(5)	0.7935(5)	0.5953(2)	3.1(3)	1	36(f)	36
O31	-0.0352(5)	0.7317(6)	0.0342(2)	1.9(2)	1	36(f)	36
O32	-0.0112(5)	0.7286(6)	0.5316(1)	1.6(2)	1	36(f)	36
O4	0.9153(5)	0.1013(6)	0.1446(1)	2.5(2)	1	36(f)	36
O5	0.0865(5)	0.9274(5)	0.1403(2)	2.1(2)	1	36(f)	36
O6	0.9196(7)	0.0732(6)	0.0532(1)	4.7(2)	1	36(f)	36
O7	0.0864(4)	0.8851(4)	0.0481(1)	1.1(2)	1	36(f)	36
OW1	0	0.1259(9)	0	10.4(6)	. 2	18(e)	10.80(2)
OH1	0	0	-0.2029(2)	3.6(2)	3 .	12(c)	12
Oa	0.141(2)	-0.002(2)	-0.2324(8)	3.2(6)	1	36(f)	7.20(4)
C1	0.213(3)	0.056(2)	-0.253(1)	3.2(6)	1	36(f)	7.20(4)
C2	0.242(2)	0.151(2)	-0.245(1)	3.2(6)	1	36(f)	7.20(4)
N1	0.171(2)	0.170(2)	-0.251(1)	3.2(6)	1	36(f)	7.20(4)
C3	0.179(2)	0.248(2)	-0.234(1)	3.2(6)	1	36(f)	7.20(4)
C4	0.108(2)	0.267(2)	-0.247(1)	3.2(6)	1	36(f)	7.20(4)
Ob	0.023(2)	0.197(1)	-0.2364(9)	3.2(6)	1	36(f)	7.20(4)
C5	-0.033(3)	0.151(3)	-0.2650(8)	3.2(6)	1	36(f)	7.20(4)
C6	-0.129(2)	0.121(2)	-0.255(1)	3.2(6)	1	36(f)	7.20(4)
Oc	-0.158(2)	0.044(2)	-0.234(1)	3.2(6)	1	36(f)	7.20(4)
C7	-0.245(2)	-0.026(2)	-0.243(1)	3.2(6)	1	36(f)	7.20(4)
C8	-0.239(3)	-0.102(2)	-0.259(1)	3.2(6)	1	36(f)	7.20(4)
N2	-0.192(2)	-0.133(1)	-0.238(1)	3.2(6)	1	36(f)	7.20(4)
C9	-0.197(2)	-0.214(2)	-0.249(1)	3.2(6)	1	36(f)	7.20(4)
C10	-0.126(2)	-0.228(2)	-0.233(1)	3.2(6)	1	36(f)	7.20(4)
Od	-0.040(2)	-0.156(1)	-0.242(1)	3.2(6)	1	36(f)	7.20(4)
C11	0.027(2)	-0.149(2)	-0.219(1)	3.2(6)	1	36(f)	7.20(4)
C12	0.117(2)	-0.095(2)	-0.237(1)	3.2(6)	1	36(f)	7.20(4)

[1]) corrected from -0.0263 [2001Pai1] to 0.3070 (original setting)

[2]) corrected from 0.25 [2001Pai1] to 0.75 (original setting)

[3]) corrected from 0.0193 [2001Pai1] to 0.3140 (original setting)

Nonstandard setting, origin at 3 2, at 0, 0, ¼ from $\bar{3}$.

Symmetry operators: *x*, *y* ,*z* -*y*, *x*-*y*, *z* -*x*+*y*, -*x*, *z* -*y*, -*x*, *z*+½
-*x*+*y*, *y*, *z*+½ *x*, *x*-*y*, *z*+½ -*x*, -*y*, -*z*+½ *y*, -*x*+*y*, -*z*+½
x-*y*, *x*, -*z*+½ *y*, *x*, -*z* *x*-*y*, -*y*, -*z* -*x*, -*x*+*y*, -*z*

and equivalent positions related by R-centering (1/3, 2/3, 2/3)+, (2/3, 1/3, 1/3)+

MSO.4 Chemical composition

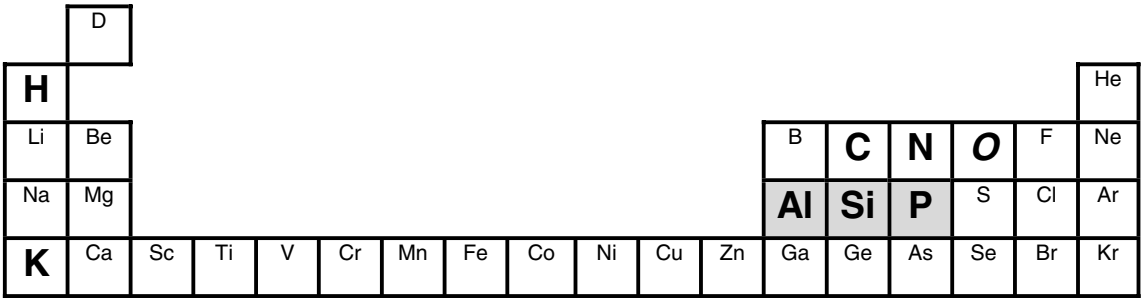


Fig. MSO.4.1 Chemical elements (highlighted) occurring in MSO-type compounds. Framework cations are in grey fields.

MSO.5 Flexibility and apertures

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

The largest openings in the MSO-type framework are 6-rings. Actually the framework is made up entirely of 6- and 4-rings. Nevertheless, the znl-cage itself is large since it contains 18-rings, but of course it is not accessible.

MSO.6 Other Information

Aluminosilicates with the MSO 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 alkene epoxidation [2001Che1].

MSO.7 References

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