OWE

OWE.1 Zeolite framework type and topology

The designation of the FTC refers to the type material UiO-28 (University of **O**slo, sequence number t**W**enty **E**ight), first synthesized and described by Kongshaug et al. [2001Kon1]. UiO-28 is isostructural with the aluminum cobalt phosphate ACP-2 and the gallium cobalt phosphate GCP-2 [97Fen1]. The framework structure (Fig. OWE.1.1) can be described as being built from *bb49* ($4^2 4^1 4^1 8^2 8^2 8^2$) units forming the 8-ring channels (Fig. OWE.1.3) crosslinked by *bb50* ($6^2 8^2$), *lov* ($4^2 6^2$) and *sti* ($4^2 4^2 6^1$) units as shown in Fig. OWE.1.2.

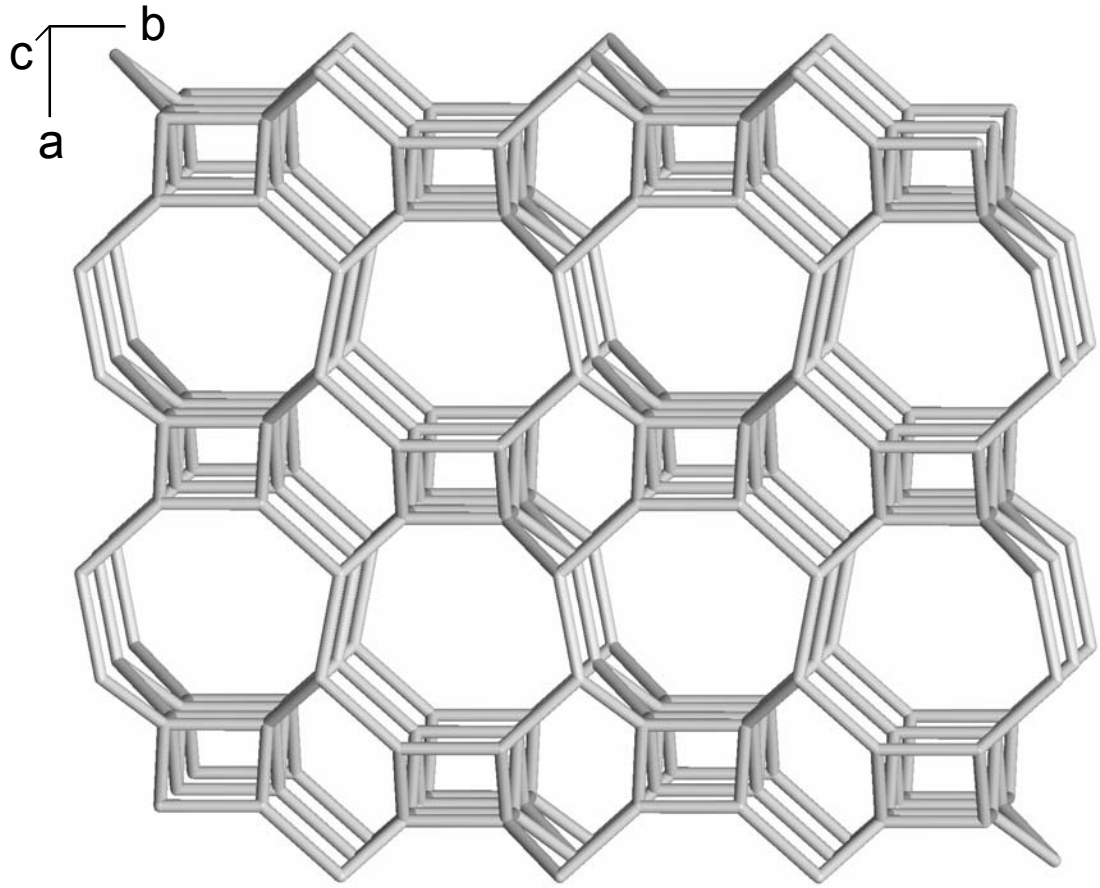
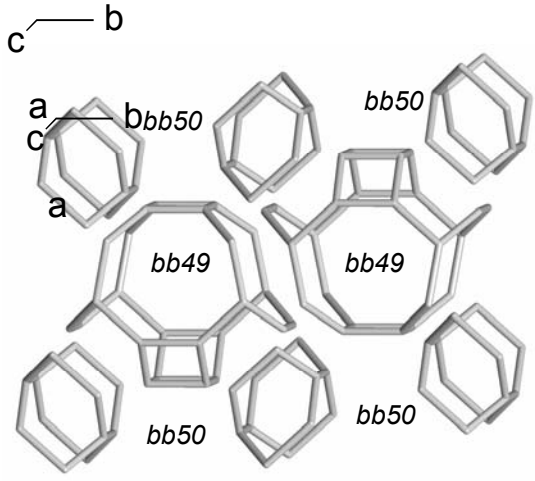
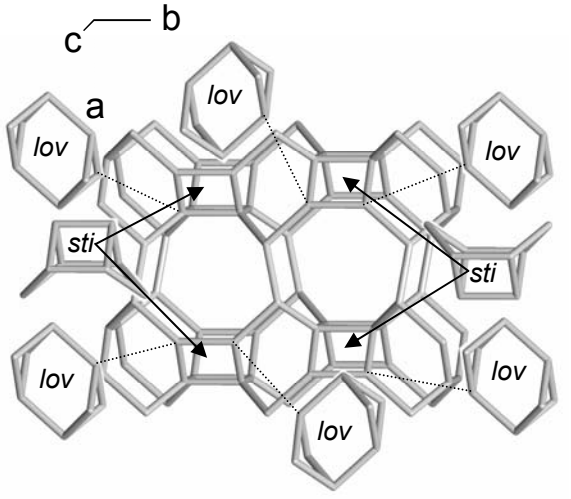


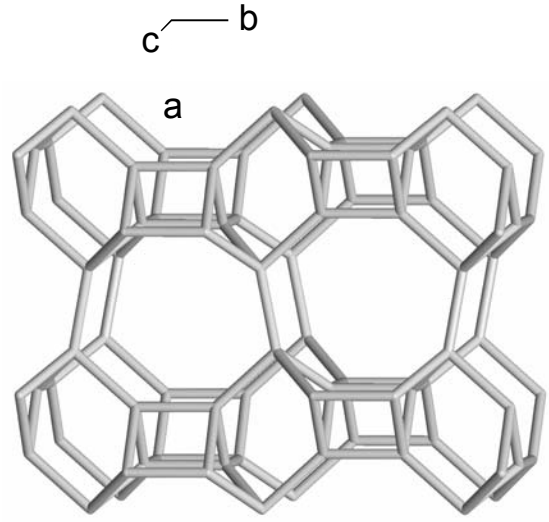
Fig. OWE.1.1. The framework structure of OWE-type compounds in the highest possible topological symmetry *P b m m*. View parallel **c** rotated by 4° about **a** and **b**.



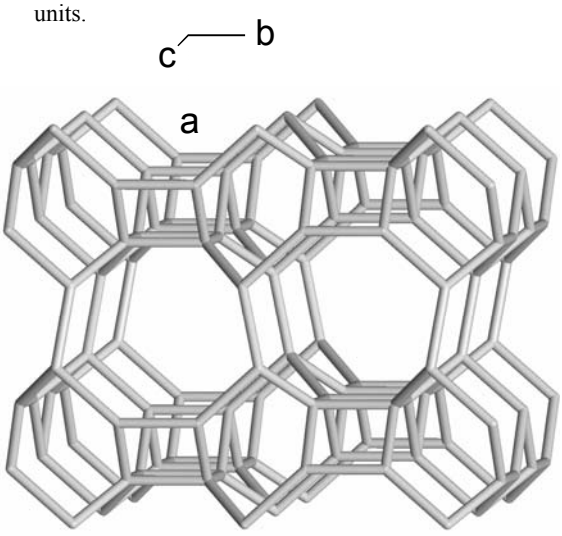
a Linkage of *bb49* and *bb50* units.



b The assemblage shown in a) extended by *lov* and *sti* units.

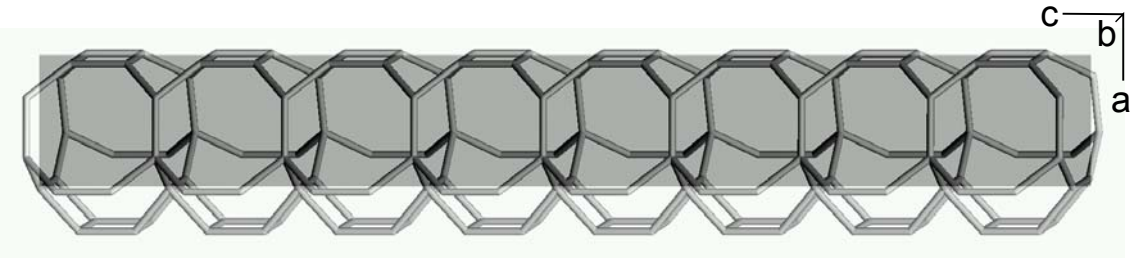


c The complete assemblage shown in b) scaled to 140%.



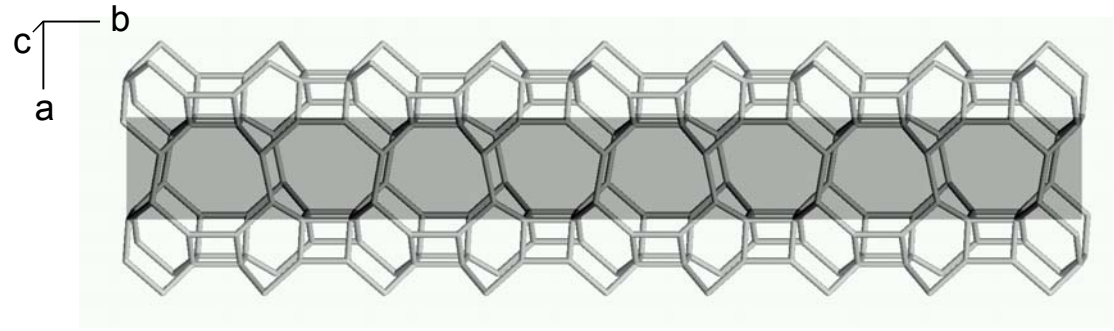
d The assemblage shown in c) extended parallel **c**.

Fig. OWE.1.2. The building scheme of OWE-type compounds. View parallel **c** rotated by 10° about **a** and 4° about **b**.



a The 8-ring channel parallel **c**. View parallel **b** rotated by 16° about **a** and 10° about **c**.

Fig. OWE.1.3. Channels in OWE-type compounds. Channel apertures are indicated by the dark shade.



b The 8-ring channel parallel **b**. View parallel **c** rotated by 6° about **a** and 10° about **b**.

Fig. OWE.1.3 (continued). Channels in OWE-type compounds. Channel apertures are indicated by the dark shade.

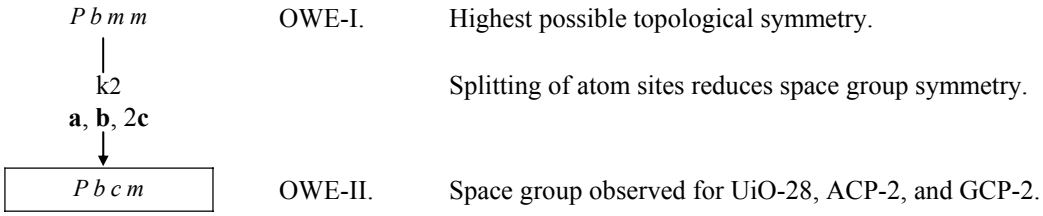


Fig. OWE.1.4 Symmetry relationship of the OWE types.

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

OWE-I *P b m m*		OWE-II *P b c m*	OWE-I *P b m m*		OWE-II *P b c m*
T1 [8(l), 1]	→	T11 [8(e), 1] T12 [8(e), 1]	O3 [4(k), . *m* .]	→	O3 [8(e), 1]
T2 [4(j), . . *m*]	→	T21 [4(d), . . *m*] T22 [4(d), . . *m*]	O4 [4(j), . . *m*]	→	O41 [4(d), . . *m*] O42 [4(d), . . *m*]
T3 [4(j), . . *m*]	→	T31 [4(d), . . *m*] T32 [4(d), . . *m*]	O5 [4(i), . . *m*]	→	O5 [8(e), 1]
O1 [8(l), 1]	→	O11 [8(e), 1] O12 [8(e), 1]	O6 [2(f), 2 *m m*]	→	O6 [4(d), . . *m*]
O2 [8(l), 1]	→	O21 [8(e), 1] O22 [8(e), 1]	O7 [2(d), . . 2/*m*]	→	O7 [4(d), . . *m*]

OWE.2 Compounds and crystal data

Table OWE.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 name	FD	SM	CE	SR	TT	T	REF
OWE-II *P b c m*									
OWE1997a01	$4NH_4$ $4C_4H_{14}N_2$ · $Al_4Co_{12}P_{16}O_{64}$[1])	ACP-2	16.3	S	-	NH_4, HDAB14	-	n.s.	97Fen1
OWE1997a02	$4NH_4$ $4C_4H_{14}N_2$ · $Ga_4Co_{12}P_{16}O_{64}$[1])	GCP-2	16.2	S	-	NH_4, HDAB14	-	n.s.	97Fen1
OWE2001a01	$(C_4N_3H_{14})_4$ · $Mg_4Al_{12}P_{16}O_{64}$	UiO-28	16.0	S	-	HETA	D	448	2001Kon1
OWE2001a02	$(C_4N_3H_{14})_4$ · $Mg_4Al_{12}P_{16}O_{64}$ · $4H_2O$	UiO-28	16.0	S	-	HETA, H_2O	-	-	2001Kon1

[1]) It is assumed here that the 1,4-diaminobutane molecule is diprotonated for charge balance.

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

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
OWE-II *P b c m*						
OWE1997a01	8.910(2)	14.974(3)	14.712(2)	1963	293	97Fen1
OWE1997a02	8.9091(2)	14.9748(5)	14.7891(6)	1973	293	97Fen1
OWE2001a01	9.2186(4)	14.8652(4)	14.5811(4)	1998	448	2001Kon1
OWE2001a02	9.2769(8)	14.798(1)	14.611(1)	2006	150	2001Kon1

OWE.3 Framework structure of OWE-II compound (*P b c m*, IT #57)

Table OWE.3.1 Atomic coordinates and site definitions for OWE-II, UiO-28, $(C_4N_3H_{14})_4$ · $Mg_4Al_{12}P_{16}O_{64}$ · $4H_2O$ (OWE2001a02, 2001Kon1).

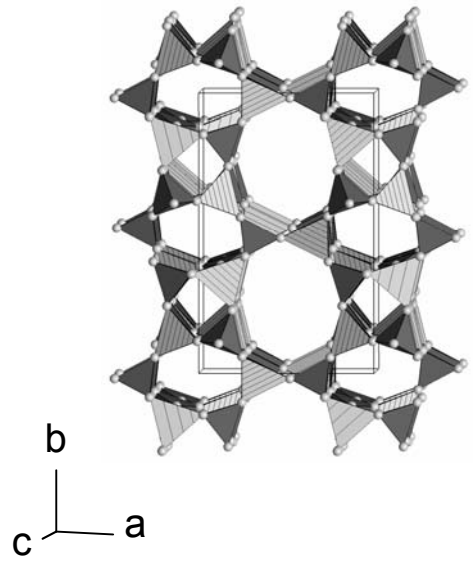
atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
P11	0.8518(3)	0.6334(2)	0.1031(2)	3.98	1	8(e)	8
(Al,Mg)12	0.8574(3)	0.6530(2)	0.6150(2)	3.82	1	8(e)	6.56/1.44
Al21	0.0985(4)	0.6356(2)	¼	3.55	. . *m*	4(d)	4
P22	0.1235(3)	0.6570(2)	¾	3.61	. . *m*	4(d)	4
(Mg,Al)31	0.6677(4)	0.5204(2)	¼	3.34	. . *m*	4(d)	2.80/1.20
P32	0.6820(3)	0.5279(2)	¾	3.26	. . *m*	4(d)	4
O11	0.9974(8)	0.6206(4)	0.1490(5)	5.66	1	8(e)	8

Table OWE.3.1 (continued)

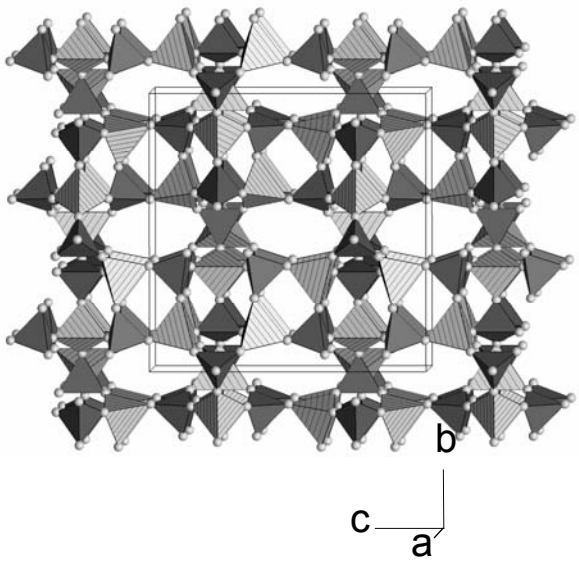
atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
O12	0.0333(8)	0.6408(4)	0.6638(5)	5.58	1	8(e)	8
O21	0.7438(9)	0.5668(5)	0.1397(5)	6.82	1	8(e)	8
O22	0.7279(9)	0.5783(6)	0.6663(6)	7.50	1	8(e)	8
O3	0.1983(7)	0.2308(4)	0.1167(5)	5.00	1	8(e)	8
O41	0.244(1)	0.5616(7)	¼	7.34	. . *m*	4(d)	4
O42	0.253(1)	0.5982(6)	¾	5.90	. . *m*	4(d)	4
O5	0.873(1)	0.6149(5)	0.0007(4)	6.21	1	8(e)	8
O6	0.826(1)	0.2444(5)	¼	4.61	. . *m*	4(d)	4
O7	0.526(1)	-0.0138(8)	¼	7.74	. . *m*	4(d)	4
OW1	0.439(4)	0.158(2)	¼	10.79	. . *m*	4(d)	1.9(2)
OW2	0.502(5)	0.255(4)	¼	27.56	. . *m*	4(d)	2.1(2)
N1	0.213(1)	0.9160(8)	0.0054(7)	6.82	1	8(e)	8
N2	0.625(3)	0.243(1)	0.048(2)	7.82	1	8(e)	4
C1	0.369(2)	0.903(1)	-0.014(1)	10.74	1	8(e)	8
C2	0.436(2)	0.826(1)	0.473(1)	10.32	1	8(e)	8

Table OWE.3.2 Selected interatomic distances and angles for OWE-II, UiO-28, $(C_4N_3H_{14})_4 \cdot Mg_4Al_{12}P_{16}O_{64} \cdot 4H_2O$ (OWE2001a02, 2001Kon1).

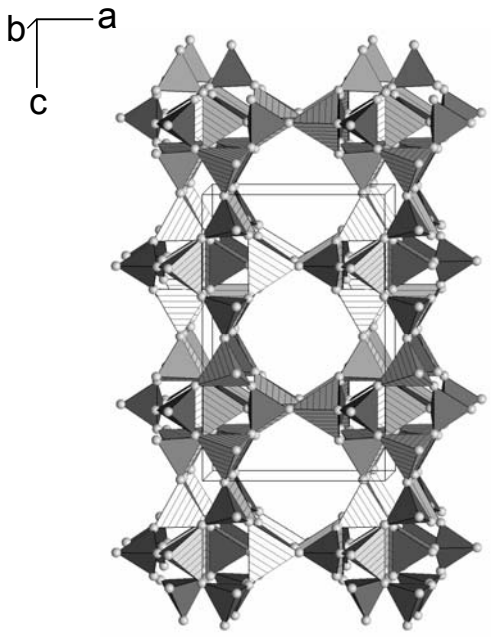
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
P11 - O21	1.504(8)	142.3(5)	(Al,Mg)12 - O5	1.788(7)	148.8(5)
P11 - O11	1.520(8)	145.8(5)	(Al,Mg)12 - O12	1.790(8)	144.1(5)
P11 - O3	1.527(7)	144.5(5)	(Al,Mg)12 - O3	1.796(7)	144.5(5)
P11 - O5	1.534(7)	148.8(5)	(Al,Mg)12 - O22	1.796(9)	147.1(6)
mean	1.521	145.4	mean	1.793	146.1
Al21 - O41	1.739(12)	156.4(8)	P22 - O42	1.483(10)	148.7(7)
Al21 - O6	1.757(8)	138.5(6)	P22 - O12	1.531(7)	144.1(5)
Al21 - O11	1.763(8)	145.8(5)	P22 - O12	1.531(7)	144.1(5)
Al21 - O11	1.763(8)	145.8(5)	P22 - O6	1.534(8)	138.5(6)
mean	1.756	146.6	mean	1.520	143.9
(Mg,Al)31 - O7	1.871(11)	172.5(8)	P32 - O7	1.458(11)	172.5(8)
(Mg,Al)31 - O21	1.889(8)	142.3(5)	P32 - O41	1.491(11)	156.4(8)
(Mg,Al)31 - O21	1.889(8)	142.3(5)	P32 - O22	1.494(9)	147.1(6)
(Mg,Al)31 - O42	1.903(10)	148.7(7)	P32 - O22	1.494(9)	147.1(6)
mean	1.888	151.5	mean	1.484	155.8



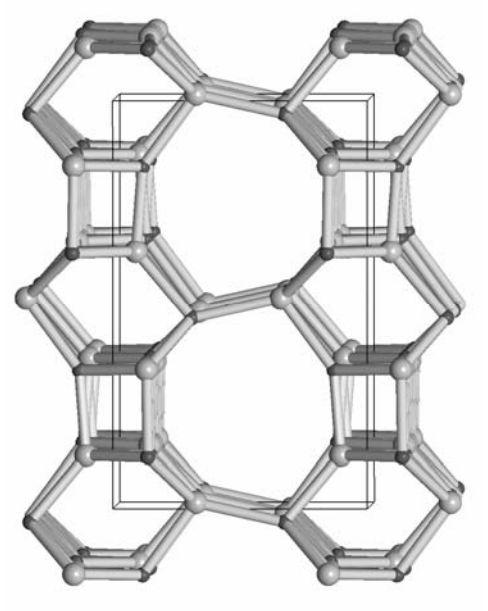
a View parallel **c** rotated by 1° about **a** and **b**.



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



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



d Ball and stick model corresponding to a) scaled to 150%.

Fig. OWE.3.1 Projections of the OWE-II crystal structure of UiO-28, $(C_4N_3H_{14})_4 \cdot Mg_4Al_{12}P_{16}O_{64} \cdot 4H_2O$ (OWE2001a02, 2001Kon1). PO_4 tetrahedra are dark grey, AlO_4 tetrahedra are light grey and hatched.

OWE.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
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

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

OWE.5 Flexibility and apertures

There is insufficient information available about the OWE-type to judge its flexibility.

The 8-ring openings in the OWE-type framework are crooked ovals, with much reduced diameters in one direction compared with the LTA-type, where they are about 4 Å by 4 Å.

OWE.6 Other information

No useful properties have been reported for OWE-type compounds.

OWE.7 References

97Fen1 Feng, P., Bu, X., Stucky, G.D.: Nature **388** (1997) 735.

2001Kon1 Kongshaug, K.O., Fjellvåg, H., Lillerud, K.P.: J. Mater. Chem. **11** (2001) 1242.

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