OBW

OBW.1 Zeolite framework type and topology

The designation of the FTC refers to the type material OSB-2 (Universities of **O**slo and Santa **B**arbara, sequence number t**W**o) first synthesized by [2001Che1] who also solved the crystal structure. However, atomic parameters have not been published yet, they are taken from the *Collection of Simulated XRD Powder Diffraction Patterns for Zeolites* [2006Tre1]. The framework structure (Fig. OBW.1.1) can be described as being built from *bb47* ($3^4 3^4 3^4 4^1 8^4 8^1 10^4$) and *trc* ($3^8 8^6$) units in a body centered arrangement as shown in Fig. OBW.1.2.

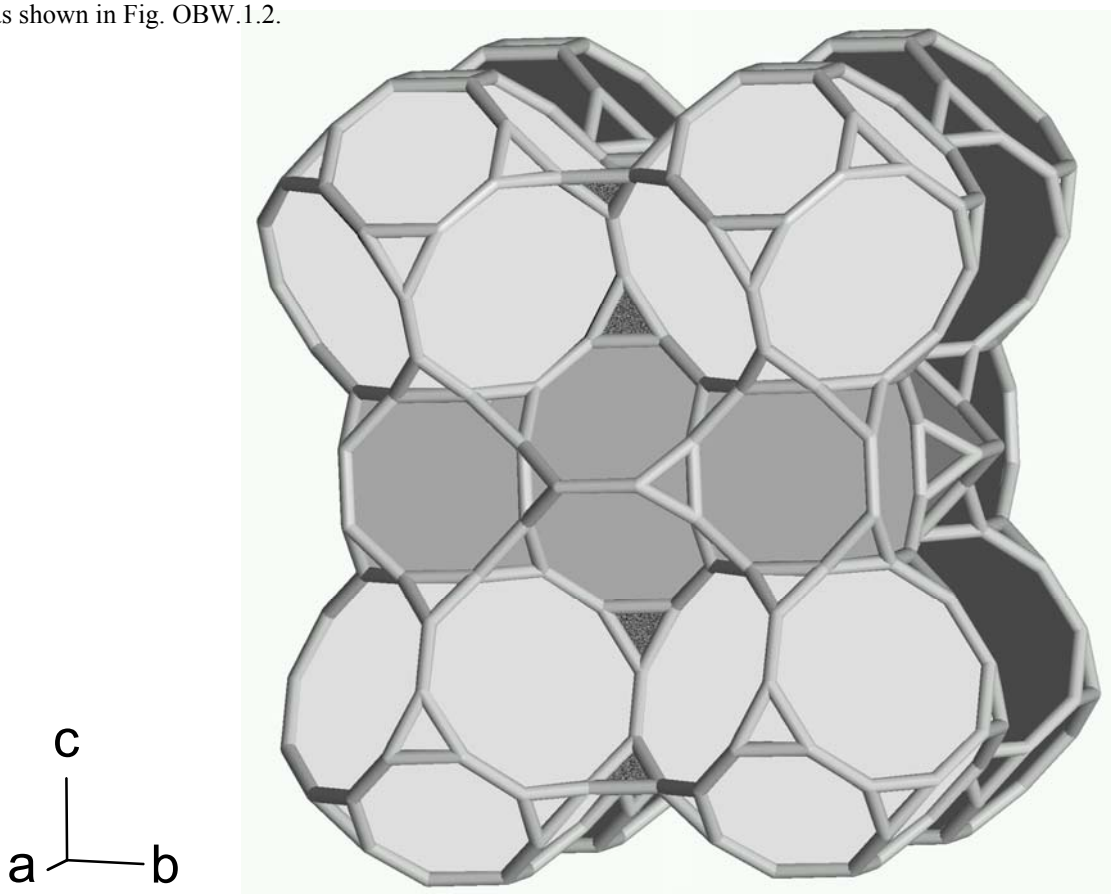
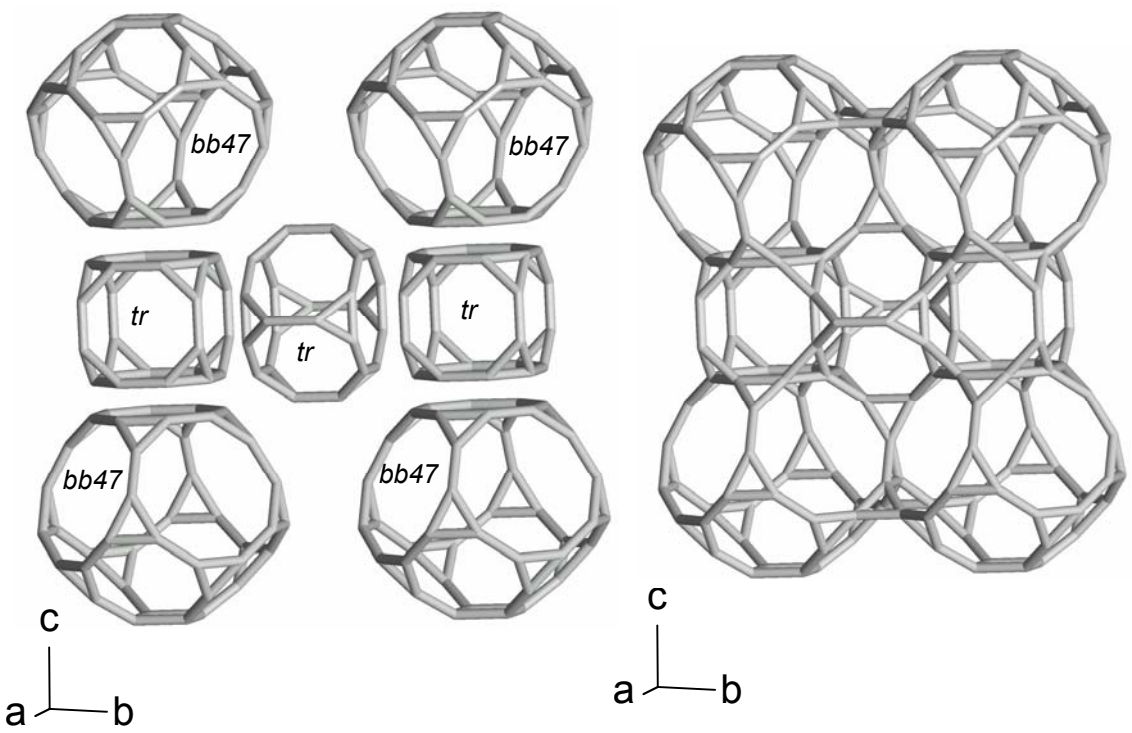


Fig. OBW.1.1. The framework structure of OBW-type compounds in the highest possible topological symmetry *I* 4/*m m m*. View parallel **a** rotated by 5° about **b** and 15° about **c**.



a Linakge of *bb47* and *trc* units.

b The complete assemblage shown in a).

Fig. OBW.1.2 Building scheme of OBW-type compounds. View of 0*yz*-layer parallel **a** rotated by 5° about **b** and 15° about **c**. The next layer in ½, *y*, *z* is shifted by ½, ½, ½ according to the body centered symmetry.

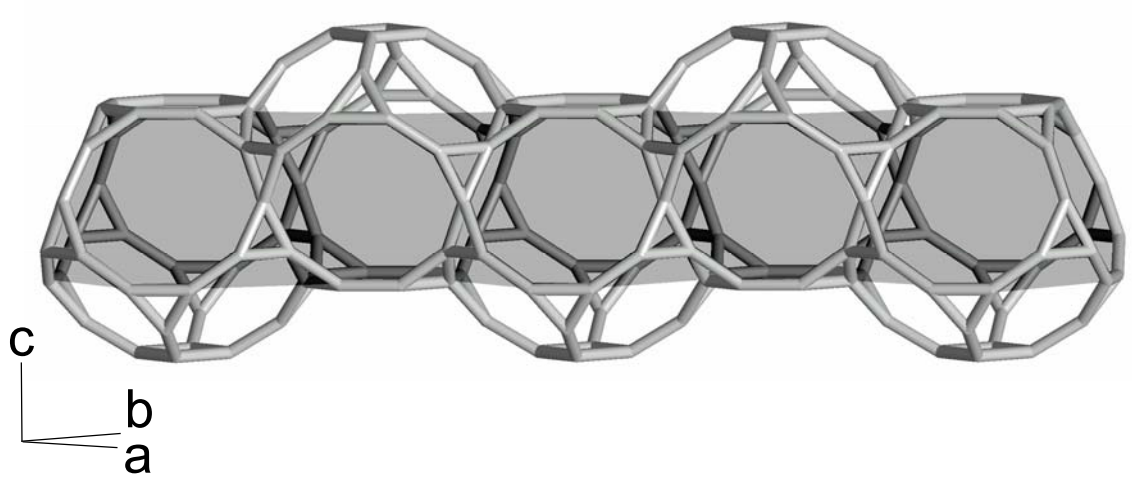


Fig. OBW.1.3 The 10-ring channel parallel [110]. View parallel [$1\,\bar{1}\,0$] rotated by 5° about [110] and 10° about [001]. The pathway of the straight channel is indicated by the dark shading.

OBW.2 Compounds and crystal data

Table OBW.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	FD	SM	CE	SR	TT	T	REF
OBW-I ***I*** **4/*m m m***								
OBW2004a02	$K_{48} \cdot Be_{24}Si_{52}O_{152} \cdot 96H_2O$	13.1	S	-	-	-	-	2001Che1

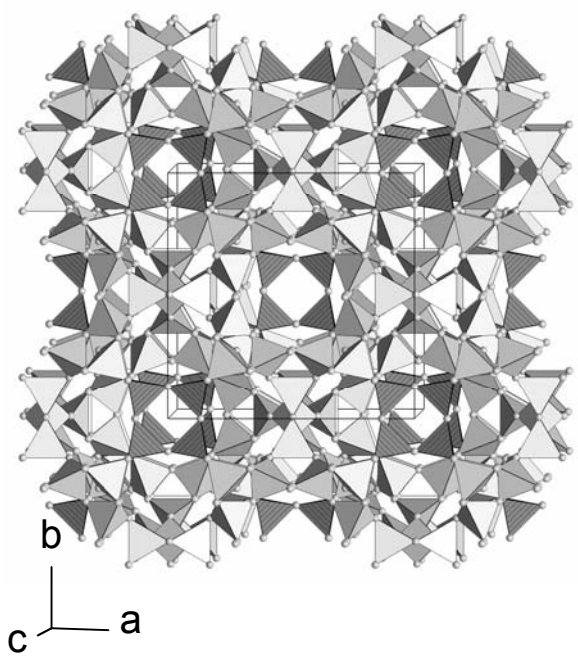
Table OBW.2.2 Structural parameters of OBW-type compound.

code	*a* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
OBW-I ***I*** **4/*m m m***					
OBW2004a02	13.7452(9)	30.654(3)	5791	150	2001Che1, 2006Tre1

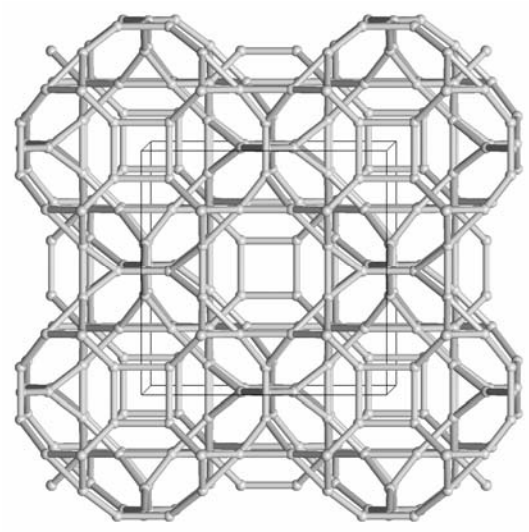
OBW.3 Framework structure of OBW-I compound (*I* 4/*m m m*, IT #139)

Table OBW.3.2 Selected interatomic distances and angles for OSB-2, $K_{48} \cdot Be_{24}Si_{52}O_{152} \cdot 96H_2O$ (OBW1994a02, 2001Che1, 2006Tre1).

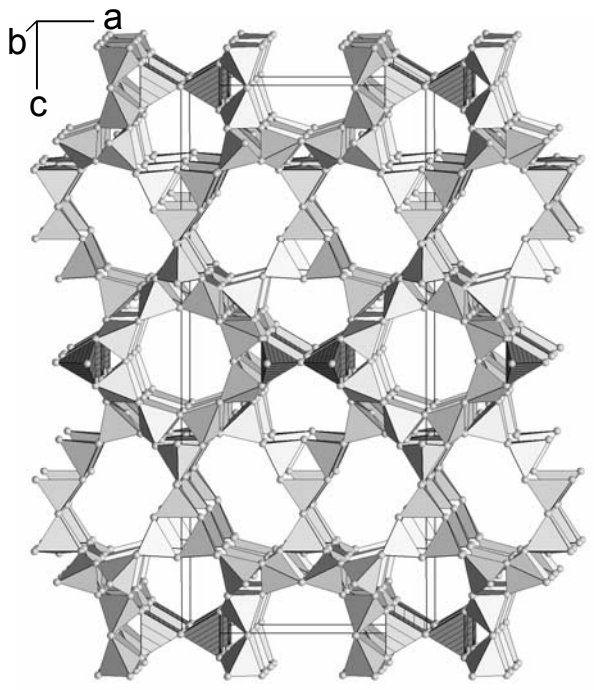
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Be)1 - O2	1.60	129	(Si,Be)2 - O3	1.60	130
(Si,Be)1 - O6	1.60	130	(Si,Be)2 - O9	1.60	130
(Si,Be)1 - O1	1.61	130	(Si,Be)2 - O1	1.61	130
(Si,Be)1 - O4	1.62	130	(Si,Be)2 - O1	1.61	130
mean	1.61	130	mean	1.61	130
(Si,Be)3 - O8	1.61	129	Si4 - O7	1.58	161
(Si,Be)3 - O2	1.61	129	Si4 - O7	1.58	161
(Si,Be)3 - O2	1.61	129	Si4 - O5	1.60	131
(Si,Be)3 - O5	1.63	131	Si4 - O5	1.60	131
mean	1.62	130	mean	1.59	146
(Si,Be)5 - O3	1.61	130			
(Si,Be)5 - O3	1.61	130			
(Si,Be)5 - O3	1.61	130			
(Si,Be)5 - O3	1.61	130			
Mean	1.61	130			



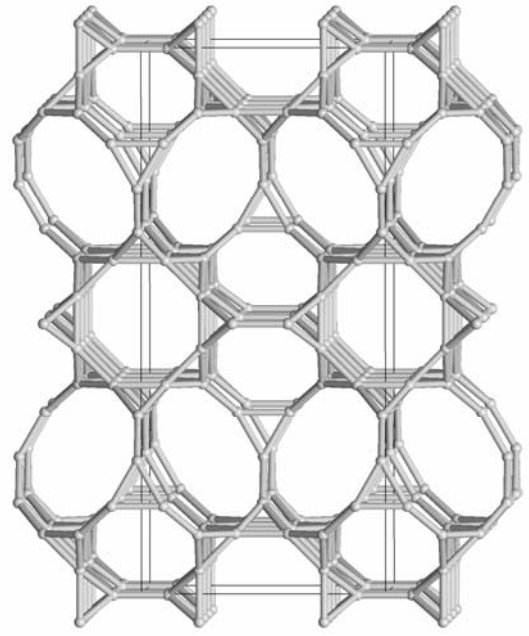
a View parallel **c** rotated by 1° about **a** and **b**.



b Ball and stick model corresponding to a).



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



d Ball and stick model corresponding to c).

Fig. OBW.3.1 Projections of the OBW-I crystal structure of OSB-2, $K_{48} \cdot Be_{24}Si_{52}O_{152} \cdot 96H_2O$ (OBW1994a02, 2001Che1, 2006Tre1). SiO_4-tetrahedra not occupied by Be atoms are hatched.

Table OBW.3.1 Atomic coordinates and site definitions for OSB-2, $K_{48} \cdot Be_{24}Si_{52}O_{152} \cdot 96H_2O$ (OBW1994a02, 2001Che1, 2006Tre1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Be)1	0.25592	0.10666	0.38612	3.55	1	32(o)	21.86/10.14
(Si,Be)2	0	0.3942	0.3322	3.47	. *m* .	16(n)	11.07/4.93
(Si,Be)3	0.2442	0.2442	0.04727	3.94	. . *m*	16(m)	8.99/7.01
Si4	0.1133	0.1133	0	3.86	*m*. 2 *m*	8(h)	8
(Si,Be)5	0	½	¼	3.71	$\bar{4}$ *m* 2	4(d)	1.64/2.36
O1	0.3358	0.0948	0.3481	6.39	1	32(o)	32
O2	0.33460	0.1993	0.07377	6.00	1	32(o)	32
O3	0	0.4041	0.28027	5.92	. *m* .	16(n)	16
O4	0	0.2222	0.4026	5.76	. *m* .	16(n)	16
O5	0.1609	0.1609	0.0425	6.47	. . *m*	16(m)	16
O6	0.1620	0.1620	0.3675	6.23	. . *m*	16(m)	16
O7	0.1325	0	0	7.50	*m* 2 *m*.	8(i)	8
O8	0.2798	0.2798	0	6.15	*m*. 2 *m*	8(h)	8
O9	0	½	0.3541	7.10	2*m m* .	8(g)	8
K1	0	0	0.3914	7.73	4 *m m*	4(e)	3.36
K2	0.2552	0	½	11.3	*m* 2 *m*.	8(j)	7.82
K3	0.3151	0	0.0798	11.6	. *m* .	16(n)	10.64
K4	0.2930	0.8590	0.2276	26.8	1	32(o)	7.47
K18	0.1120	0.1120	0.1232	71.8	. . *m*	16(m)	6.64
OW1	½	-0.0300	½	30.7	*m* 2 *m*.	8(i)	4.72
OW2	0	0	½	16.5	4/*m m m*	2(b)	2.16
OW3	0.061	0.061	0.4773	18.9	. . *m*	16(m)	4.06
OW4	½	0.894	½	41.0	*m* 2 *m*.	8(i)	8.40
OW5	0.462	0	0.5570	22.8	. *m* .	16(n)	2.22
OW6	0.138	0.138	0.2803	38.6	. . *m*	16(m)	17.28
OW7	0	0.226	0.2441	29.2	. *m* .	16(n)	8.16
OW8	0.131	0.226	0.1822	49.7	1	32(o)	17.28
OW11	0.088	0.088	0.3043	34.7	. . *m*	16(m)	4.06
OW12	0.257	0	0.1015	9.86	. *m* .	16(n)	8.00
OW13	0	0	0.3620	9.47	4 *m m*	4(e)	1.40
OW14	0.219	0.405	0.2660	33.9	1	32(o)	8.16

High displacement factors and inappropriate sums of occupancies of mutually exclusive pairs of atoms indicate some problems in the crystal structure refinement. However, these are the only data available and therefore represent the reference data for this framework type.

OBW.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. OBW.4.1 Chemical elements (highlighted) occurring in the OBW-type compound. Framework cations are in grey fields.

OBW.5 Flexibility and apertures

There is not sufficient information available about the OBW-type to judge its flexibility.

The 10-ring openings in the framework of the OBW-type have diameters of approximately 5 Å by 5 Å, that means they are slightly more buckled than the 10-rings in the MFI-type framework.

OBW.6 Other information

No useful properties have been reported for OBW-type compounds. The framework density of the OBW-type is about the same as for the FAU-type, but its thermal stability is low [2001Che1].

OBW.7 References

2001Che1 Cheetham, T., Fjellvåg, H., Gier, T.E., Kongshaug, K.O., Lillerud, K.P., Stucky, G.D. in: Zeolites and mesoporous materials at the dawn of the 21st century. Stud. Surf. Sci. Catal. **135**. Galarneau, A., Di Renzo, F., Fajula, F., Vedrine, J. (eds.), Amsterdam: Elsevier (2001) 158, and Proceedings of the 13th International Conference, Montpellier, France 2001, contribution 05-O-05.

2006Tre1 Treacy, M.M.J., Higgins, J.B., von Ballmoos, R. in: Baerlocher, C., McCusker, L.B.: Database of zeolite structures, http://topaz.ethz.ch/IZA-SC/XRDpatterns.htm

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