OSO

OSO.1 Zeolite framework type and topology

The designation of the FTC refers to the type material OSB-1 (Universities of **O**slo and **S**anta Barbara, sequence number **O**ne) first synthesized by [2000Kon1] 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. OSI.1.1) can be described as being built from *bb38* ($3^4 3^4 3^4 3^4 8^4 8^4 14^2$) units forming the 14-ring channels as shown in Figs. OSO.1.2 and OSO.1.3.

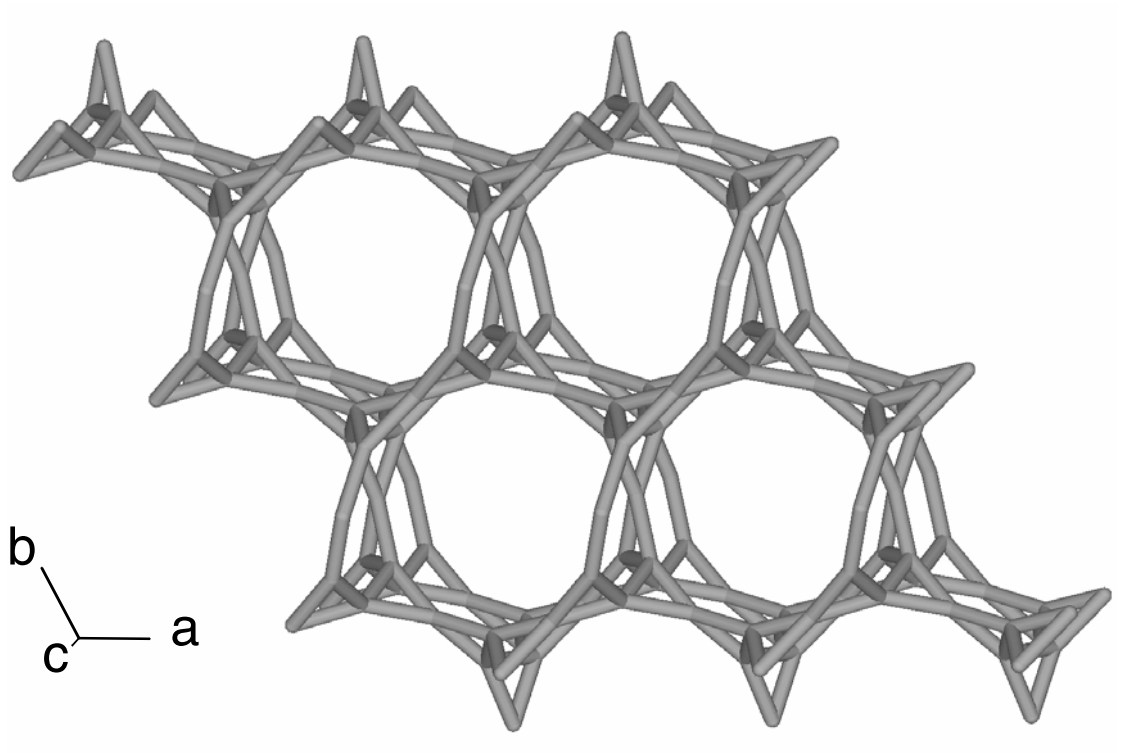
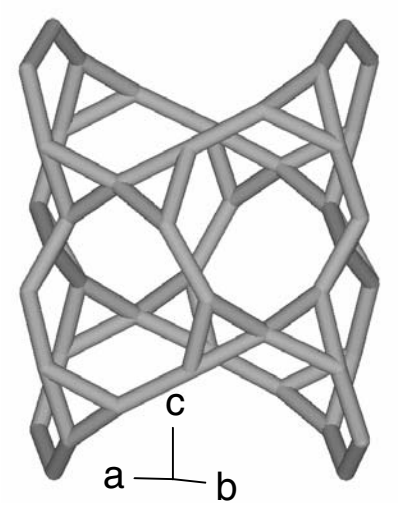
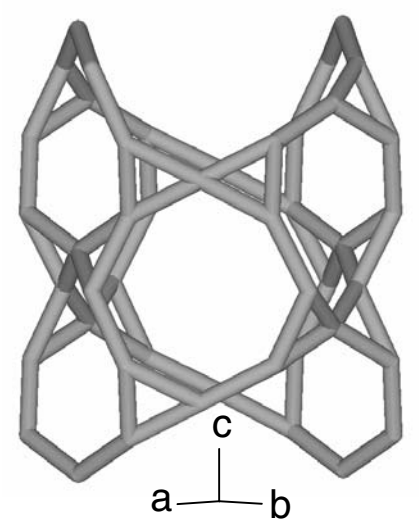


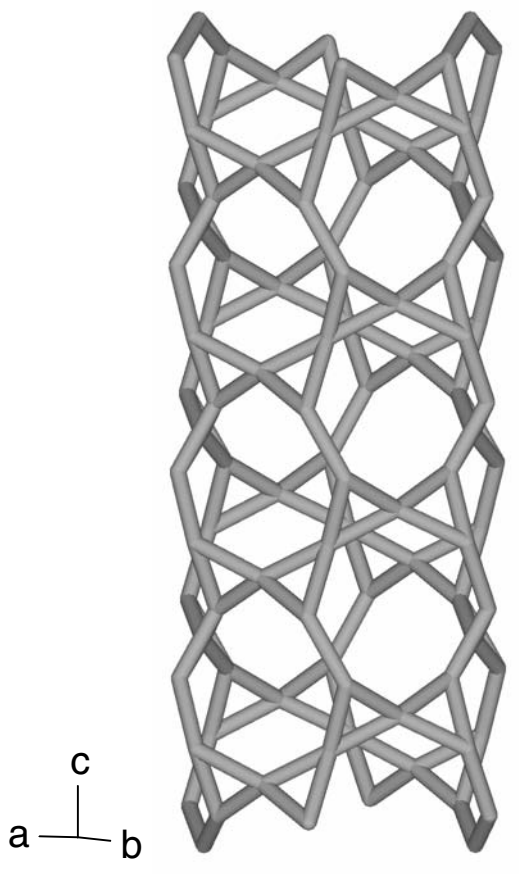
Fig. OSO.1.1. The framework structure of OSO-type compounds in the highest possible topological symmetry $P\,6_2\,2\,2$. View parallel [001] rotated by 5° about [100] and 10° about [120].



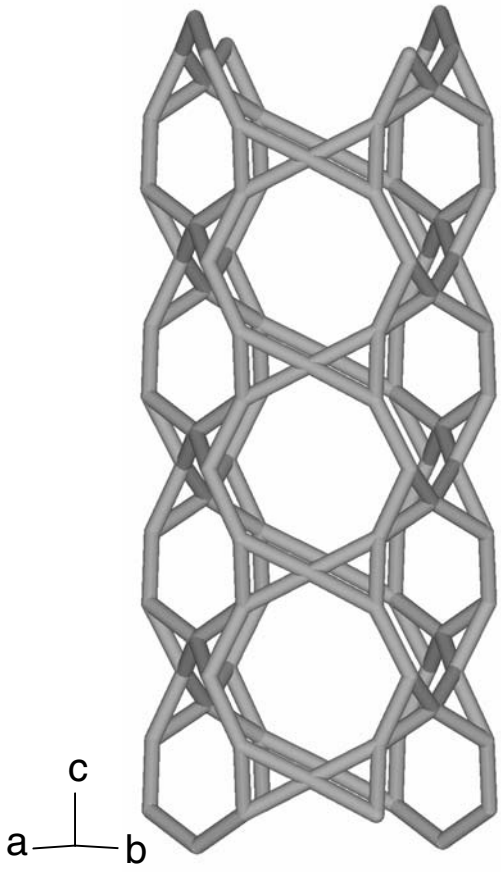
a The *bb38* unit. View parallel [120] rotated by 4° about [100] and [001].



b The *bb38* unit. View parallel [110] rotated by 2° about [$\bar{1}$ 10] and 4° about [001].



c The 14-ring channel. View parallel [120] rotated by 4° about [100] and [001].



d The 14-ring channel. View parallel [110] rotated by 2° about [$\bar{1}$ 10] and 4° about [001].

Fig. OSO.1.2 The *bb38* units forming the 14-ring channels.

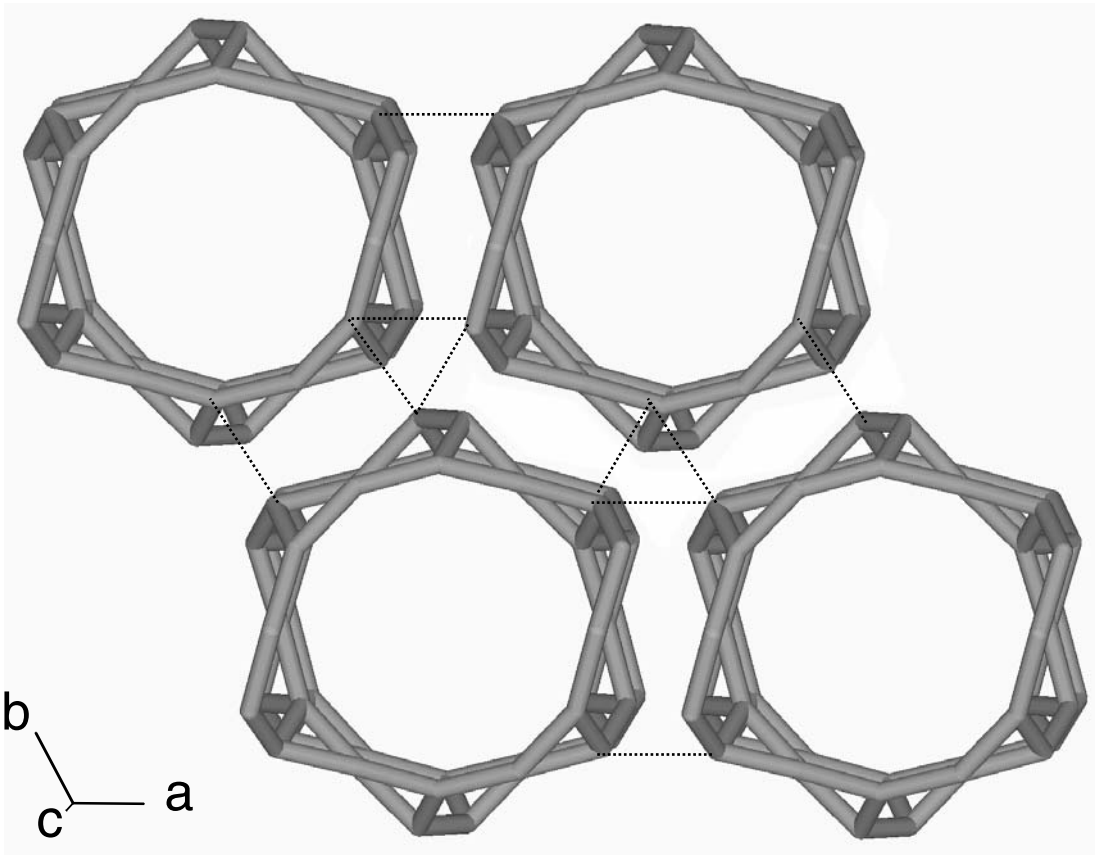


Fig. OSO.1.3 The building scheme of OSO-type compounds formed by *bb38* units. View parallel [001] rotated by 2° about [100] and [120].

$P\,6_2\,2\,2$	OSO-I.	Highest possible topological symmetry.
t2		Splitting of O1 atom site reduces space group symmetry
a, **b**, **c**		
$P\,3_2\,2\,1$	OSO-II.	Intermediate step to describe the transformation.
t2		Splitting of T1 and O atom sites further reduces space group symmetry.
a, **b**, **c**		
$P\,3_2$	OSO-IV.	Space group observed for OSB-1.

Fig. OSO.1.4 The Bärnighausen tree illustrating the symmetry relationships of the OSO types.

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

OSO-I $P6_222$		OSO-II $P3_221$		OSO-IV $P3_2$
T1 [6(j), . . 2]	→	T1 [6(c), 1]	→	T11 [3(a), 1] T12 [3(a), 1]
T2 [3(c), 2 2 2]	→	T2 [3(b), . 2 .]	→	T2 [3(a), 1]
O1 [12(k), 1]	→	O11 [6(c), 1]	→	O11a [3(a), 1] O11b [3(a), 1]
		O12 [6(c), 1]	→	O12a [3(a), 1] O12b [3(a), 1]
O2 [6(i), . . 2]	→	O2 [6(c), 1]	→	O21 [3(a), 1] O22 [3(a), 1]

OSO.2 Compounds and crystal data

Table OSO.2.1 Chemical data.

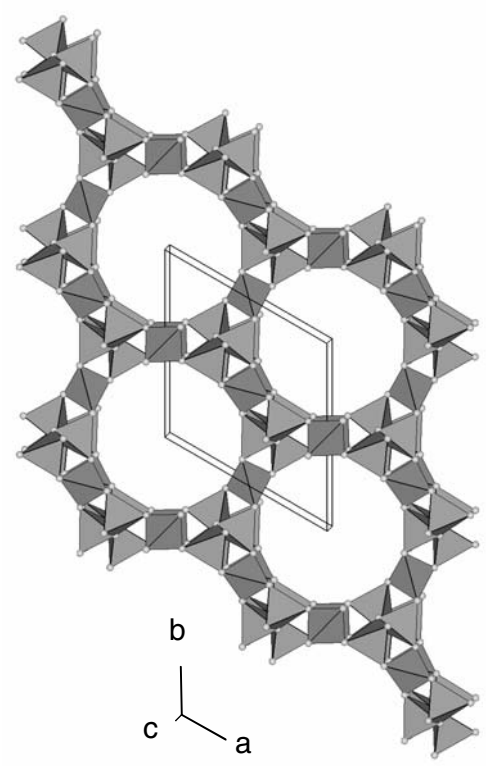
FD = framework density CE = cation exchange TT = thermal treatment REF = reference
SM = source of material SR = sorbate T = temperature of thermal treatment [K]

code	chemical composition	FD	SM	CE	SR	TT	T	REF
OSO-IV $P3_2$								
OSO2000a02	$K_6 \cdot Be_3Si_6O_{18} \cdot 9H_2O$	13.4	S	-	H_2O	-	-	2000Kon1

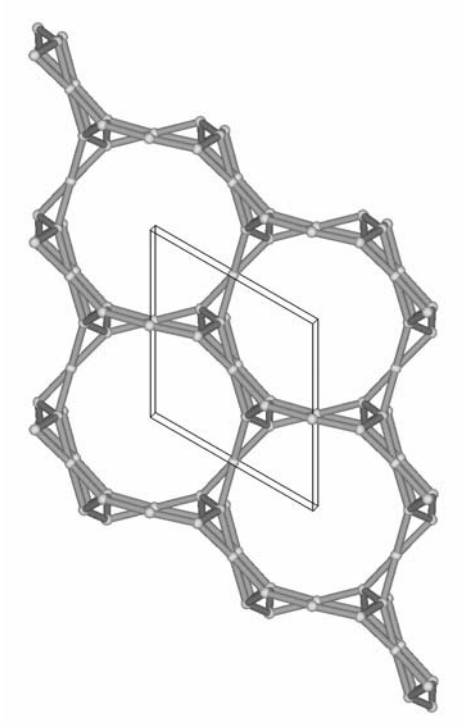
Table OSO.2.2 Structural parameters of OSO-type compound.

code	a [Å]	c [Å]	V [Å^3]	T [K]	reference
OSO-IV $P3_2$					
OSO2000a02	10.0928	7.6264	673	n.s.	2000Kon1, 2006Tre1

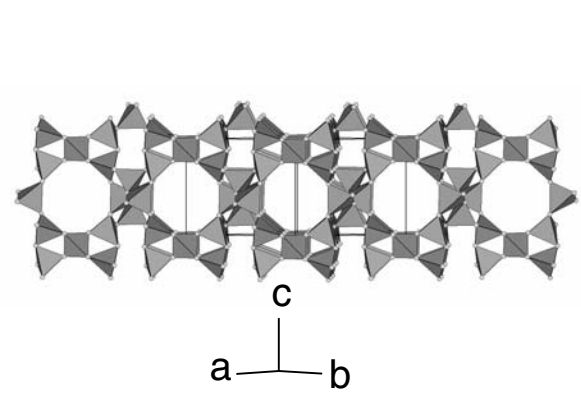
OSO.3 Framework structure of OSO-IV compound ($P3_2$, IT #145)



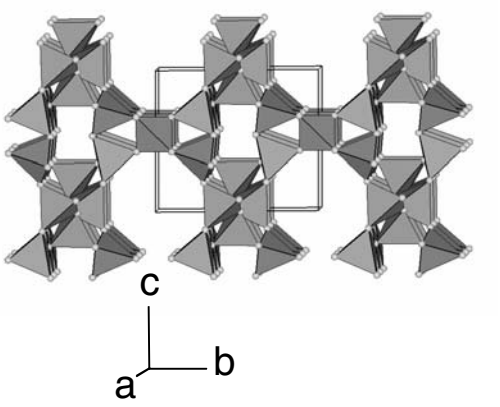
a View parallel [001] rotated by 2° about [210] and [010].



b Ball and stick model corresponding to a).



c View parallel [110] rotated by 1° about [$\bar{1}$ 10] and [001].



d View parallel [100] rotated by 1° about [120] and [001].

Fig. OSO.3.1 Projections of the OSO-IV crystal structure of $K_6 \cdot Be_3Si_6O_{18} \cdot 9H_2O$ (OSO2000a01, 2000Kon1, 2006Tre1).

Table OSO.3.1 Atomic coordinates and site definitions for OSO-IV, $K_6 \cdot Be_3Si_6O_{18} \cdot 9H_2O$ (OSO2000a01, 2006Tre1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Be)11	0.2899	0.5811	0.0599	0.71	1	3(a)	1.59 / 1.41
(Si,Be)12	0.5818	0.2893	0.7241	1.03	1	3(a)	1.74 / 1.26
(Si,Be)2	0.4969	0007	0.5610	1.03	1	3(a)	2.19 / 0.84
O11a	0.469	0.356	0.772	1.74	1	3(a)	3
O11b	0.349	0.456	0.018	2.21	1	3(a)	3
O12a	0.536	0.643	0.769	1.97	1	3(a)	3
O12b	0.642	0.535	0.014	1.66	1	3(a)	3
O21	0.680	0.371	0.554	1.58	1	3(a)	3
O22	0.379	0.688	0.215	2.45	1	3(a)	3
K11	0.005	0.462	0.720	3.95	1	3(a)	1.32
K12	0.006	0.527	0.718	4.50	1	3(a)	1.68
K2	0.185	0.075	0.714	20.53	1	3(a)	2.37
OW1	0.115	0.171	0.051	9.24	1	3(a)	3
OW2	0.136	0.327	0.584	15.00	1	3(a)	3
OW3	0.862	0.189	0.921	14.21	1	3(a)	3

Table OSO.3.2 Selected interatomic distances and angles for OSO-IV, $K_6 \cdot Be_3Si_6O_{18} \cdot 9H_2O$ (OSO2000a01, 2006Tre1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Be)11 - O22	1.55	123	(Si,Be)12 - O21	1.58	128
(Si,Be)11 - O12a	1.65	126	(Si,Be)12 - O21	1.60	128
(Si,Be)11 - O11b	1.68	122	(Si,Be)12 - O11a	1.63	129
(Si,Be)11 - O22	1.70	123	(Si,Be)12 - O12b	1.65	127
Mean	1.65	124	mean	1.62	128
(Si,Be)2 - O12b	1.57	127			
(Si,Be)2 - O12a	1.60	126			
(Si,Be)2 - O11a	1.64	129			
(Si,Be)2 - O11b	1.67	122			
Mean	1.62	126			

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

OSO.5 Flexibility and apertures

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

The 14-ring openings in the framework of the OSO-type are heavily puckered and have effective free diameters of approximately 5.5 Å by 7.5 Å, which means that they are not only smaller than the 14-rings in the DON-type (more than 8 Å by 8 Å), but even smaller than the 12-rings in the FAU-type (about 7.5 Å by 7.5 Å).

OSO.6 Other information

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

OSO.7 References

2000Kon1 Kongshaug, K.O., Fjellvåg, H., Lillerud, K.P., Gier, T.E., Stucky, G.D., Cheetham, A.: Private communication (2000)

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

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