OSI

OSI.1 Zeolite framework type and topology

The designation of the FTC refers to the type material UiO-6 (University of **O**slo, sequence number **SI**x), first synthesized by [96Akp1] who also solved and described the crystal structure. However, atomic parameters are not given in the original paper, 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 **osi** channels crosslinked by *lau* ($4^2 6^4$) and *oth* ($4^2 6^2 6^2$) units as shown in Fig. OSI.1.2 and OSI.1.3.

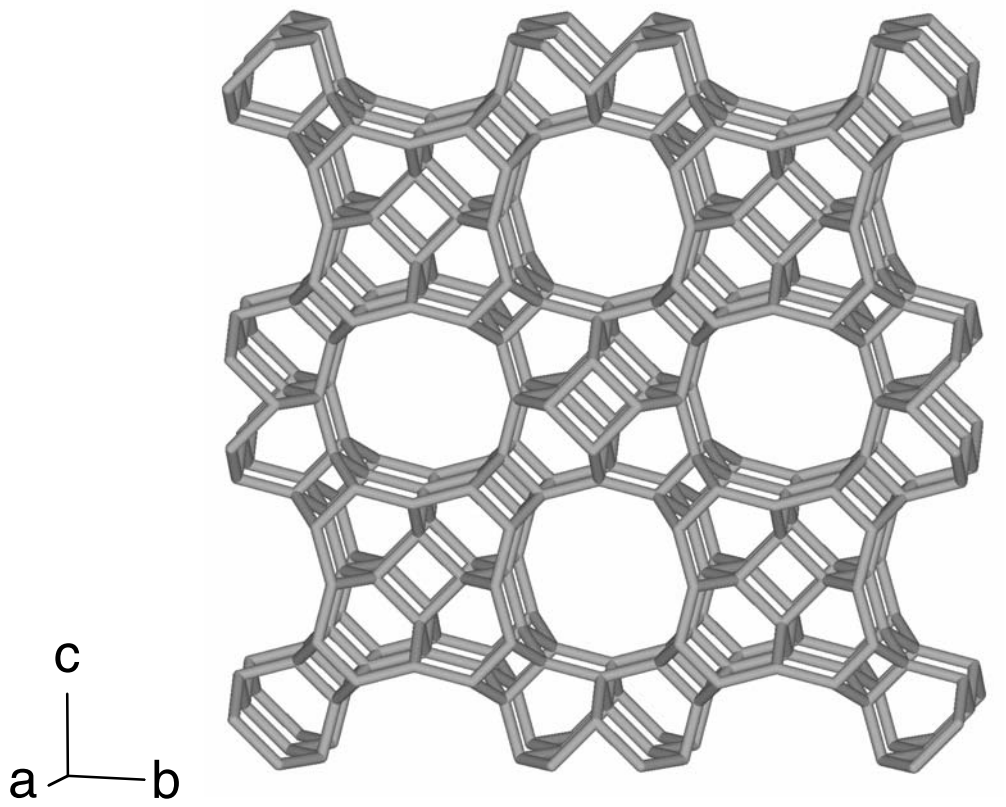


Fig. OSI.1.1. The framework structure of OSI-type compounds in the highest possible topological symmetry *I* 4/*m m m*.

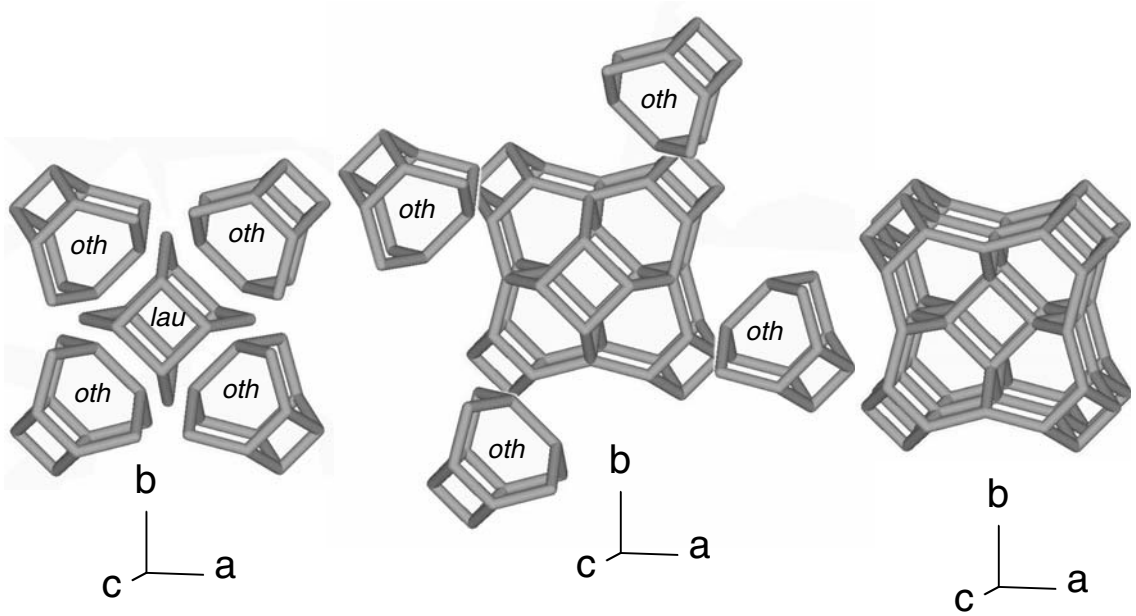


Fig. OSI.1.2 Building scheme of the composite unit formed by *lau* and *oth* units. View parallel **c** rotated by 8° about **a** and 6° about **b**

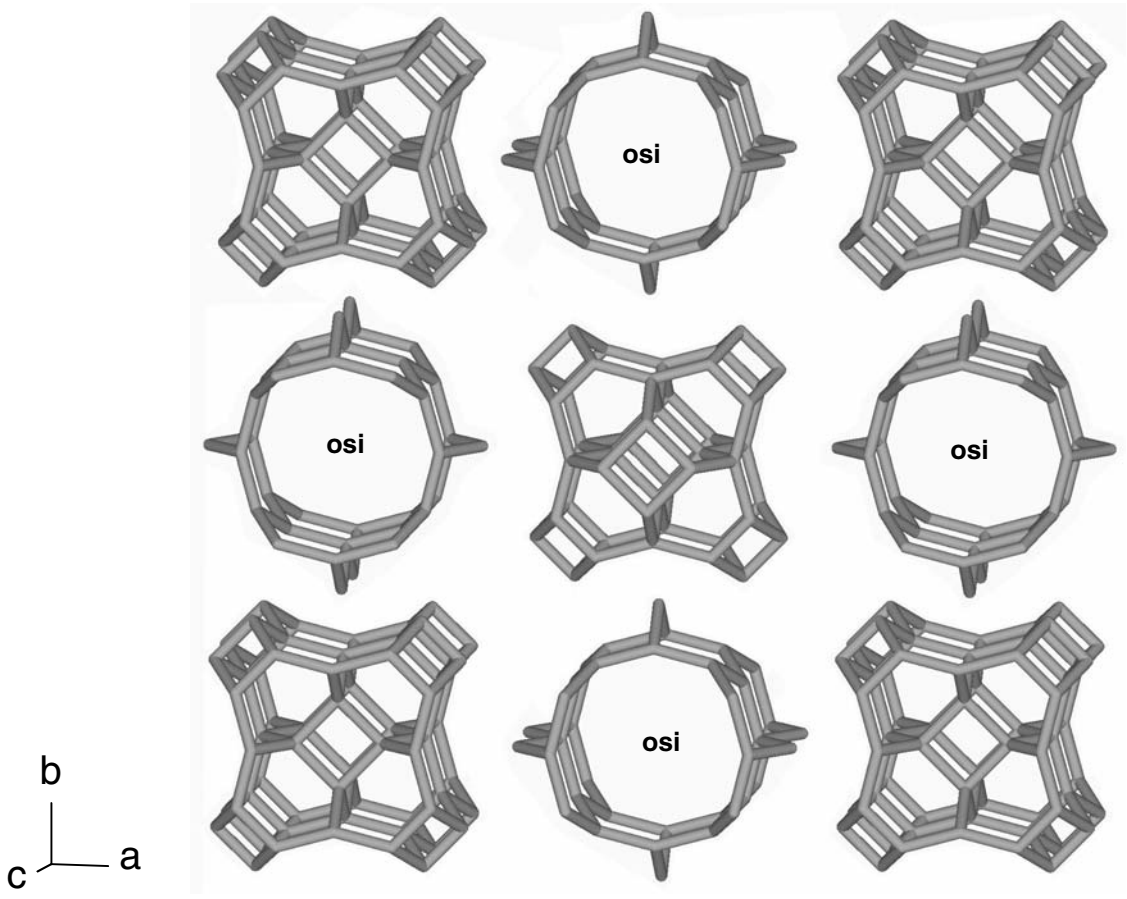


Fig. OSI.1.3 The building scheme of OSI-type compounds. View parallel **c** rotated by 8° about **a** and 6° about **b**.

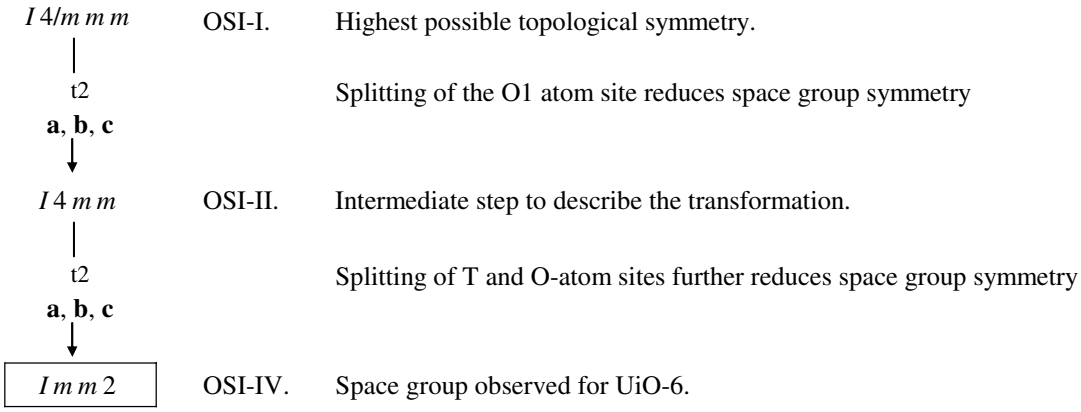


Fig. OSI.1.4 The Bärnighausen tree illustrating the symmetry relationships of the OSI types.

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

OSI-I *I* 4/*m m m*		OSI-II *I* 4 *m m*		OSI-IV *I m m* 2
T1 [16(l), *m* . .]	→	T1 [16(e), 1]	→	T11 [8(e), 1] T12 [8(e), 1]
T2 [8(j), *m* 2*m* .]	→	T2 [8(d), . *m* .]	→	T21 [4(c), . *m* .] T22 [4(d), *m* . .]
T3 [8(i), *m* 2*m* .]	→	T3 [8(d), . *m* .]	→	T31 [4(c), . *m* .] T32 [4(d), *m* . .]
O1 [16(n), . *m* .]	→	O11 [8(d), . *m* .]	→	O11a [4(c), . *m* .] O11b [4(d), *m* . .]
		O12 [8(d), . *m* .]	→	O12a [4(c), . *m* .] O12b [4(d), *m* . .]
O2 [16(l), *m* . .]	→	O2 [16(e), 1]	→	O21 [8(e), 1] O22 [8(e), 1]
O3 [16(k), . . 2]	→	O3 [16(e), 1]	→	O31 [8(e), 1] O32 [8(e), 1]
O4 [8(h), *m* . 2*m*]	→	O4 [8(c), . . *m*]	→	O4 [8(e), 1]
O5 [8(h), *m* . 2*m*]	→	O5 [8(c), . . *m*]	→	O5 [8(e), 1]

OSI.2 Compounds and crystal data

Table OSI.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
OSI-IV ***I m m* 2**								
OSI1996a01	$Al_{16}P_{16}O_{64}$	18.8	S	-	-	C	n.s.	96Akp1

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

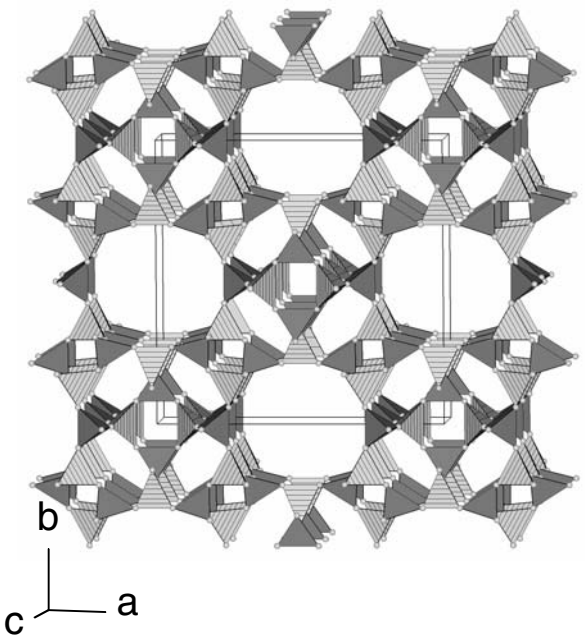
code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
OSI-IV ***I m m* 2**						
OSI1996a01	18.3549	18.3206	5.0530	1699	n.s.	96Akp1, 2006Tre1

OSI.3 Framework structure of the OSI-IV compound (*I m m* 2, IT #44)

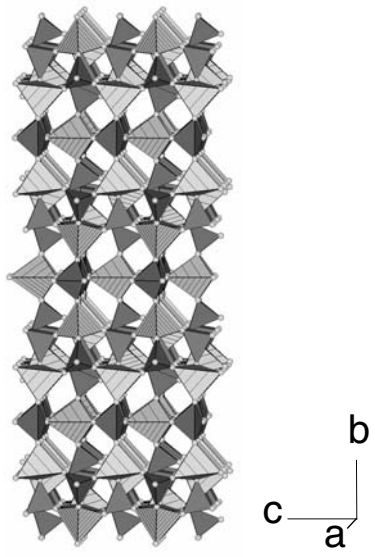
Table OSI.3.1 Atomic coordinates and site definitions for OSI-IV, $Al_{16}P_{16}O_{64}$ (OSI1996a01, 96Akp1, 2006Tre1).

atom	*x*	*y*	*z*	site symmetry	Wyckoff position	no. of atoms in unit cell
Al11	0.7795	0.6659	0.028	1	8(e)	8
P12	0.6446	0.7691	0.068	1	8(e)	8
P21	0.7779	0	0.581	. *m* .	4(c)	4
Al22	0	0.7867	0.500	*m* . .	4(d)	4
Al31	0.1179	0	0.104	. *m* .	4(c)	4
P32	0	0.1205	0.027	*m* . .	4(d)	4
O11a	0.1738	0	0.8272	. *m* .	4(c)	4
O11b	0	0.1444	0.7413	*m* . .	4(d)	4
O12a	0.8509	0	0.4332	. *m* .	4(c)	4
O12b	0	0.8073	0.1602	1	4(d)	4
O21	0.7624	0.5718	0.0281	1	8(e)	8
O22	0.5647	0.7846	0.0247	1	8(e)	8
O31	0.6977	0.1764	0.1912	1	8(e)	8
O32	0.1709	0.6950	0.3099	1	8(e)	8
O4	0.6919	0.7030	0.0110	1	8(e)	8
O5	0.0724	0.0815	0.0300	1	8(e)	8

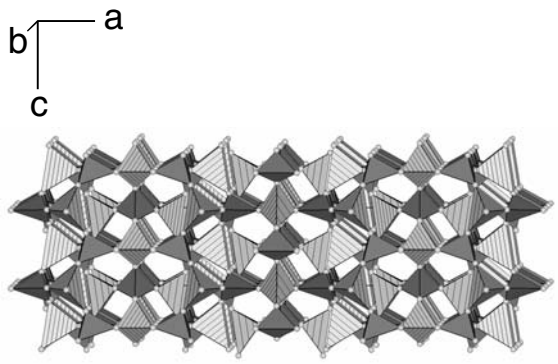
The crystal structure consits of strongly distorted tetrahedra with some cations residing close to the centers of the tetrahedral planes which indicates some problems in the structure refinement. The angles O-T-O vary from 83° to 133°. However, these are the only data available and therefore represent the reference data for this framework type.



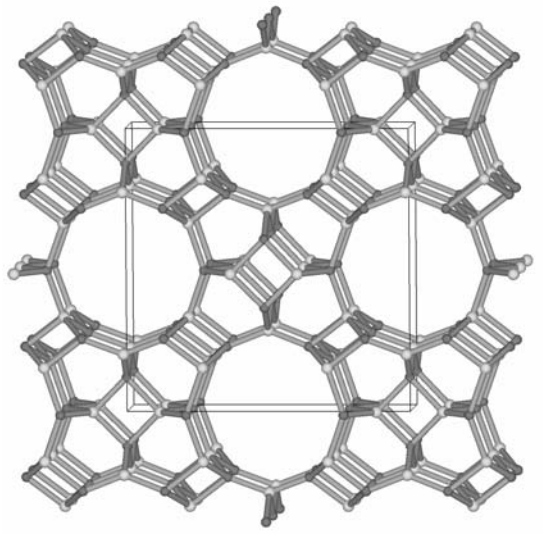
a View parallel **c** rotated by 5° about **a** and **b**.



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



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



d Ball and stick model corresponding to a).

Fig. OSI.3.1 Projections of the OSI-IV crystal structure of $Al_{16}P_{16}O_{64}$ (OSI1996a01, 96Akp1, 2006Tre1).

Table OSI.3.2 Selected interatomic distances and angles OSI-IV, $Al_{16}P_{16}O_{64}$ (OSI1996a01, 96Akp1, 2006Tre1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11 - O4	1.75	146	P12 - O22	1.51	122
Al 11 - O21	1.75	159	P12 - O4	1.52	146
Al 11 - O31	1.76	128	P12 - O31	1.53	128
Al 11 - O32	1.77	166	P12 _ O32	1.54	166
mean	1.76	150	mean	1.53	141
P21 - O11a	1.53	180	Al22 - O11b	1.76	151
P21 - O21	1.53	159	Al22 - O12b	1.76	129
P21 - O21	1.53	159	Al22 - O22	1.77	122
P21 - O12a	1.53	138	Al22 - O22	1.77	122
mean	1.53	159	mean	1.77	131
Al31 - O11a	1.74	180	P32 - O12b	1.48	129
Al31 - O5	1.75	146	P32 - O11b	1.51	151
Al31 - O5	1.75	146	P32 - O5	1.51	146
Al31 - O12a	1.76	138	P32 - O5	1.51	146
mean	1.75	153	mean	1.50	143

OSI.4 Chemical composition

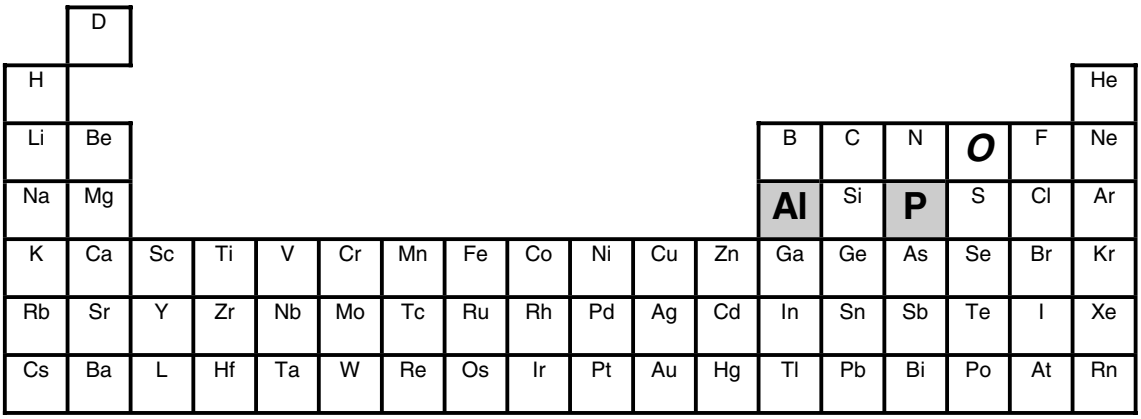


Fig. OSI.4.1 Chemical elements (highlighted) occurring in OSI-type compounds. Framework cations are in grey fields.

OSI.5 Flexibility and apertures

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

The 12-ring openings in the OSI-type framework are buckled. They measure about 5 Å by 6 Å and are therefore smaller than in the FAU-type, where they are about 7.5 Å by 7.5 Å.

OSI.6 Other information

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

OSI.7 References

96Akp1 Akporiaye, D.E., Fjellvag, H., Halvorsen, E.N., Haug, T., Karlsson, A., Lillerud, K.P.: J. Chem. Soc. Chem. Commun. (1996) 1553.

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

Gone to press April 1, 2006