NSI

NSI.1 Zeolite framework type and topology

The designation of the FTC refers to the type material Nu-6(2) (**N**ew (ICI, Imperial Chemical Industries) with sequence number **SI**x), first synthesized by [82Whi1]. The crystal structure was solved by Zanardi et al. [2004Zan1] in space group $P\,2_1/a$. The framework structure (Fig. NSI.1.1) can be described as being built from *bb48* ($5^2 5^2 6^4 8^2$) units forming the 8-ring channels (Fig. NSI.1.3) parallel **b**. The *bb48* units are crosslinked by *pes* ($5^2 6^2$) units in the **ab**-plane as shown in Fig. NSI.1.2.

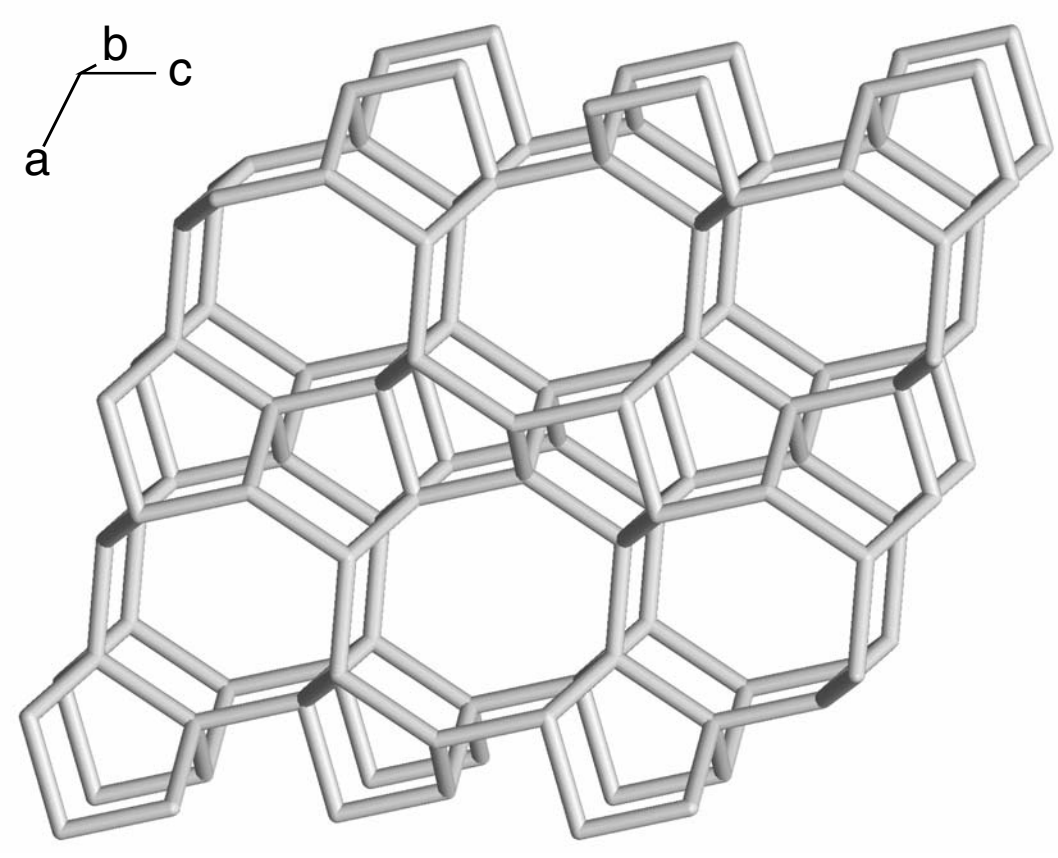
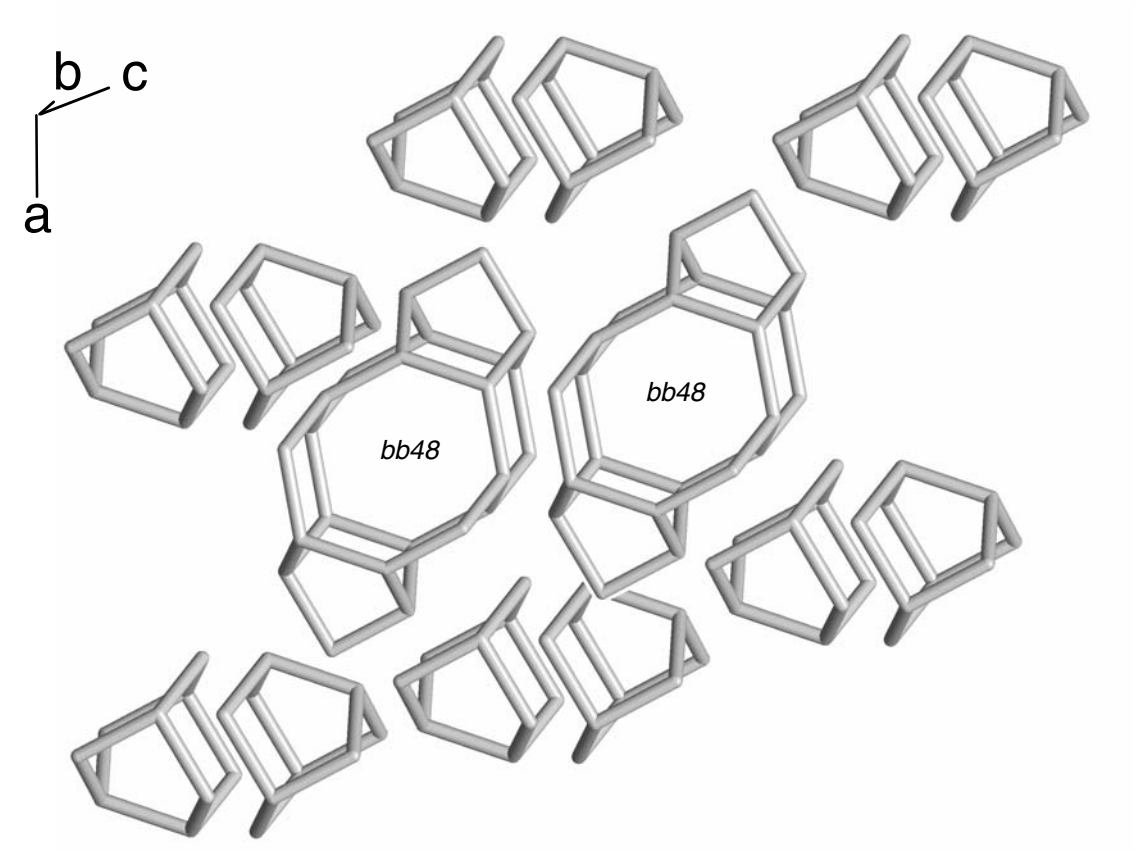
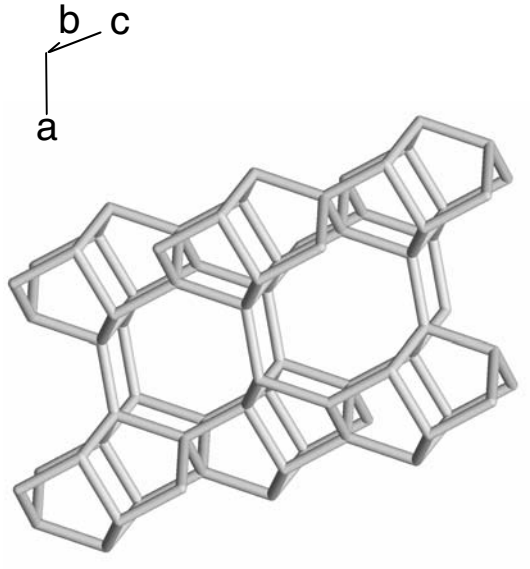


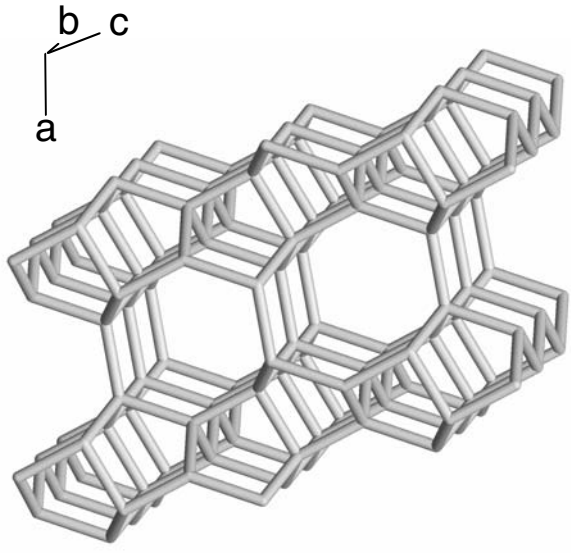
Fig.NSI.1.1. The framework structure of NSI-type compounds in the highest possible topological symmetry *A* 2/*m*. View parallel -**b** rotated by 10° about **b**×**c** and **c**.



a Linkage of *bb48* and *pes* (not labeled) units.



b The complete assemblage shown in a).



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

Fig. NSI.1.2. The building scheme of NSI-type compounds. View parallel -**b** rotated by 10° about **c** and 8° about **a**×**b**.

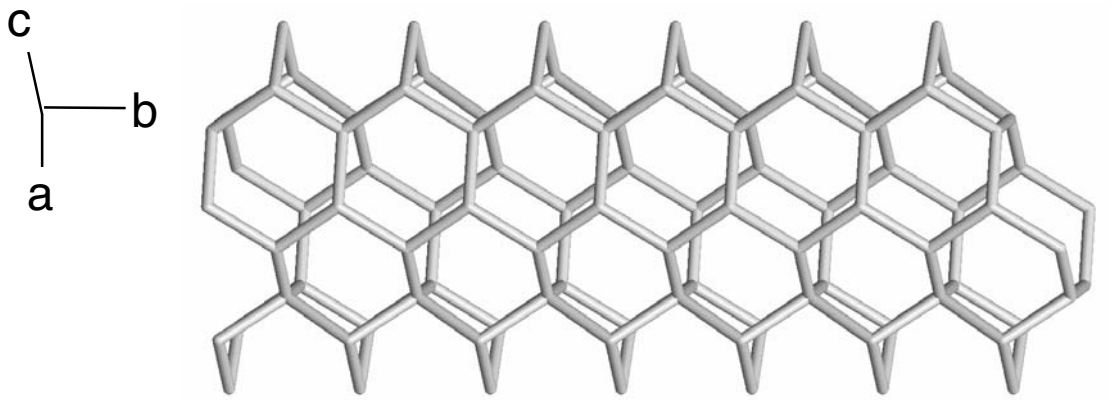


Fig. NSI.1.3. The 8-ring channel parallel **b** formed by *bb48* units. View parallel [101] rotated by 10° about [010] and [101] × [010].

A 1 2/*m* 1	NSI-I.	Highest possible topological symmetry.
k2 2**a**, **b**, **c**		Splitting of atom sites reduces space group symmetry.
A 1 2/*a* 1	NSI-II.	Intermediate step to describe the transformation
k2 **a**, **b**, **c**		Further splitting of atom sites reduces space group symmetry.
P 1 2_1/*a* 1	NSI-IV.	Space group observed for Nu-6(2).

Fig. NSI.1.4 Symmetry relationships of the NSI types.

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

NSI-I *A* 1 2/*m* 1		NSI-II *A* 1 2/*a* 1		NSI-IV *P* 1 2_1/*a* 1	
T1	[4(i), *m*]	T1	[8(f), 1]	T11	[4(e), 1]
				T12	[4(e), 1]
T2	[4(i), *m*]	T2	[8(f), 1]	T21	[4(e), 1]
				T22	[4(e), 1]
T3	[4(i), *m*]	T3	[8(f), 1]	T31	[4(e), 1]
				T32	[4(e), 1]

Table NSI.1.1 (continued).

NSI-I *A* 1 2/*m* 1		NSI-II *A* 1 2/*a* 1		NSI-IV *P* 1 2_1/*a* 1	
O1	[8(j), 1]	O11	[8(f), 1]	O11a	[4(e), 1]
				O11b	[4(e), 1]
		O12	[8(f), 1]	O12a	[4(e), 1]
				O12b	[4(e), 1]
O2	[4(i), *m*]	O2	[8(f), 1]	O21	[4(e), 1]
				O22	[4(e), 1]
O3	[4(i), *m*]	O3	[8(f), 1]	O31	[4(e), 1]
				O32	[4(e), 1]
O4	[4(f), $\bar{1}$]	O4	[8(f), 1]	O41	[4(e), 1]
				O42	[4(e), 1]
O5	[2(b), 2/*m*]	O5	[4(d), $\bar{1}$]	O5	[4(e), 1]
O6	[2(d), 2/*m*]	O6	[4(e), 2]	O6	[4(e), 1]

NSI.2 Compounds and crystal data

Table NSI.2.1 Chemical data.

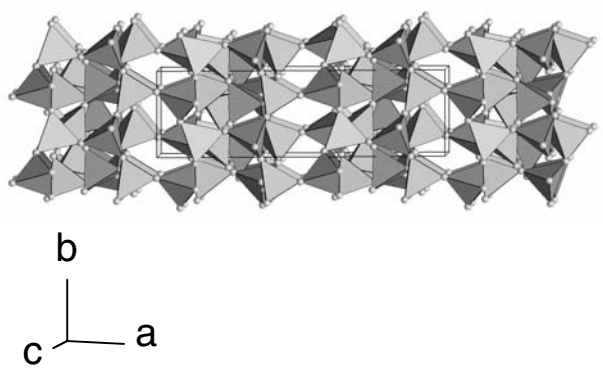
FD = framework density CE = cation exchange TT = thermal treatment REF = reference
SM = source of material SR = sorbate T = temperature of thermal treatment [K]

code	chemical composition	FD	SM	CE	SR	TT	T	REF
NSI-IV *P* 1 2_1/*a* 1								
NSI2004a01	$Si_{24}O_{48}$	21.0	S	-	-	C	473	2004Zan1

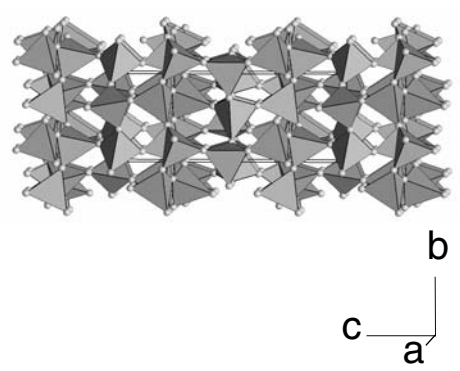
Table NSI.2.2 Structural parameters of the NSI-type compound.

code	*a* [Å]	*b* [Å]	*c* [Å]	β [°]	*V* [Å^3]	*T* [K]	reference
NSI-IV *P* 1 2_1/*a* 1							
NSI2004a01	17.257(2)	4.9881(4)	13.848(1)	106.09(1)	1145	RT	2004Zan1

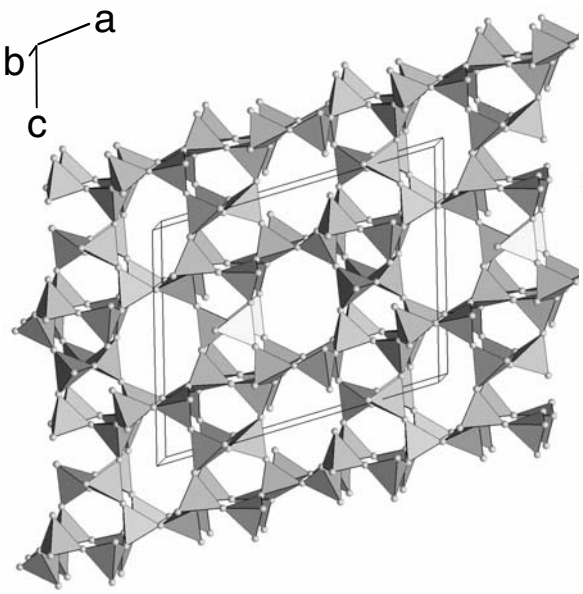
NSI.3 Framework structure of NSI-IV compound ($P\,1\,2_1/a\,1$, IT #14)



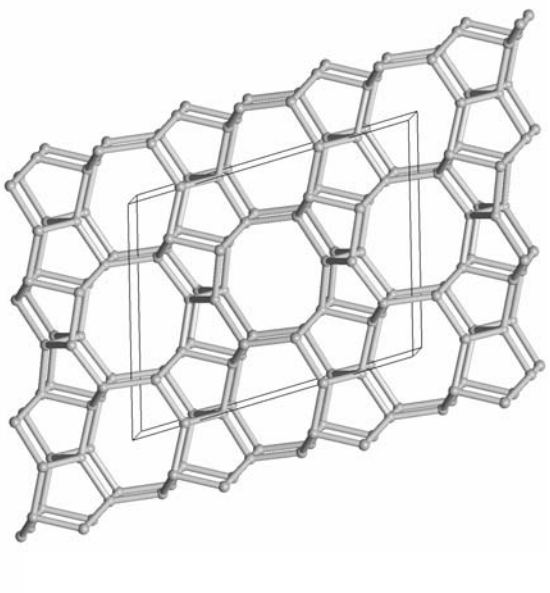
a View parallel **c** rotated by 1° about **b** and **b**×**c**.



b View parallel **a** rotated by 0.5° about **b** and **a**×**b**.



c View parallel **b** rotated by 6° about **c** and **b**×**c**.



d Ball and stick model corresponding to c).

Fig. NSI.3.1 Projections of the NSI-IV crystal structure of Nu-6(2) $Si_{24}O_{48}$ (NSI2004a01, 2004Zan1).

Table NSI.3.1 Atomic coordinates and site definitions for NSI-IV, Nu-6(2) $Si_{24}O_{48}$ (NSI2004a01, 2004Zan1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si11	0.3286(6)	0.234(2)	0.3038(6)	1.06(7)	1	4(e)	4
Si12	0.3501(6)	0.729(2)	0.8094(6)	1.06(7)	1	4(e)	4
Si21	0.0932(6)	0.225(2)	0.7677(6)	1.06(7)	1	4(e)	4
Si22	0.0921(6)	0.703(2)	0.2688(6)	1.06(7)	1	4(e)	4
Si31	0.1907(4)	0.142(2)	0.9891(6)	1.06(7)	1	4(e)	4
Si32	0.1973(4)	0.548(2)	0.4901(6)	1.06(7)	1	4(e)	4
O11a	0.3852(8)	0.482(3)	0.2984(8)	1.3(2)	1	4(e)	4
O11b	0.4167(7)	0.925(3)	0.793(1)	1.3(2)	1	4(e)	4
O12a	0.864(1)	0.511(3)	0.2527(8)	1.3(2)	1	4(e)	4
O12b	0.8639(9)	0.067(3)	0.771(1)	1.3(2)	1	4(e)	4
O21	0.3462(7)	0.140(3)	0.4236(6)	1.3(2)	1	4(e)	4
O22	0.3612(6)	0.709(3)	0.9312(6)	1.3(2)	1	4(e)	4
O31	0.1263(5)	0.125(2)	0.8825(5)	1.3(2)	1	4(e)	4
O32	0.1402(6)	0.645(3)	0.3845(5)	1.3(2)	1	4(e)	4
O41	0.2481(9)	0.885(4)	0.0176(8)	1.3(2)	1	4(e)	4
O42	0.2780(4)	0.736(2)	0.505(1)	1.3(2)	1	4(e)	4
O5	-0.0013(5)	0.226(2)	0.740(1)	1.3(2)	1	4(e)	4
O6	0.2608(6)	0.815(2)	0.750(1)	1.3(2)	1	4(e)	4

Table NSI.3.2 Selected interatomic distances and angles for NSI-IV, Nu-6(2) $Si_{24}O_{48}$ (NSI2004a01, 2004Zan1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si11 - O6	1.57(1)	149(1)	Si12 - O11b	1.57(2)	130(1)
Si11 - O11a	1.59(2)	148(1)	Si12 - O6	1.59(1)	149(1)
Si11 - O12a	1.61(2)	165(1)	Si12 - O12b	1.61(2)	157(1)
Si11 - O21	1.67(1)	144(1)	Si12 - O22	1.65(1)	141(1)
mean	1.61	152	mean	1.61	144
Si21 - O5	1.57(1)	165(1)	Si22 - O12b	1.56(2)	157(1)
Si21 - O12a	1.58(2)	165(1)	Si22 - O5	1.58(1)	165(1)
Si21 - O31	1.61(1)	150(1)	Si22 - O32	1.61(1)	169(1)
Si21 - O11a	1.62(1)	148(1)	Si22 - O11b	1.62(2)	130(1)
mean	1.60	157	mean	1.59	155
Si31 - O31	1.59(1)	150(1)	Si32 - O32	1.60(1)	169(1)
Si31 - O41	1.60(2)	162(1)	Si32 - O42	1.61(2)	140(1)
Si31 - O41	1.63(2)	162(1)	Si32 - O21	1.64(1)	144(1)
Si31 - O22	1.64(1)	141(1)	Si32 - O42	1.65(1)	140(1)
mean	1.62	154	mean	1.63	148

NSI.4 Chemical composition

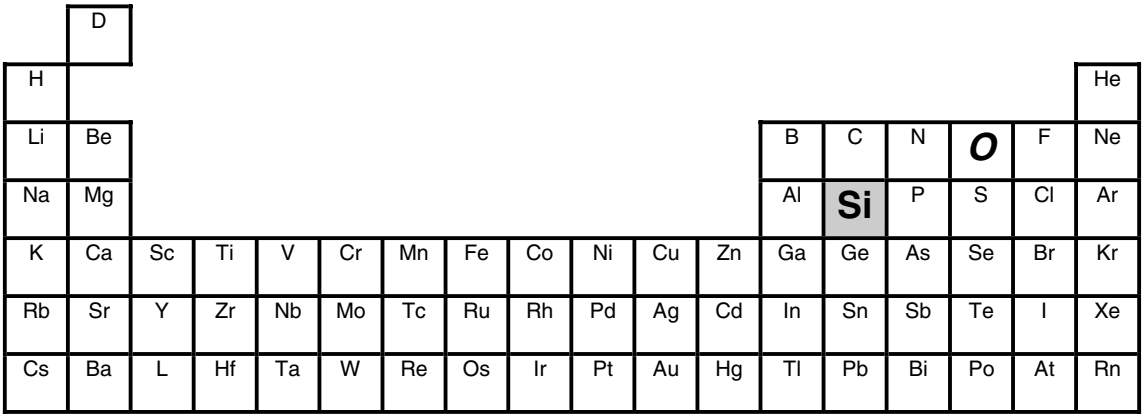


Fig. NSI.4.1 Chemical elements (highlighted) occurring in NSI-type compounds. Framework cations are in grey fields.

NSI.5 Flexibility and apertures

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

The 8-rings in NU-6(2) are severely distorted wit diameters of about 2.5 Å by 4.5 Å as compared to the LTA-type where they measure more than 4 Å by 4 Å.

NSI.6 Other information

Catalytic properties for NU-6(2) have been claimed in the original patent [82Whi1]. Compare also [2001Cor1].

NSI.7 References

82Whi1 Whittam, T.V.: European Patent EP 54364 (1882).

2001Cor1 Corma, A., Fornés, V., Díaz, U.: Chem. Commun. (2001) 2642.

2004Zan1 Zanardi, S., Alberti, A., Cruciani, G., Corma, A., Fornés, V., Brunelli, M.: Angew. Chem. int. Ed. **43** (2004) 4933.

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