NAB

NAB.1 Zeolite framework type and topology

The framework type code is named after the mineral **NAB**esite $Na_2BeSi_4O_{10} \cdot 4H_2O$, first found in South Greenland and described in [2002Pet1]. The name is derived from the chemical composition containing Na, Be, and Si. The crystal structure was first described by Petersen et al. [2002Pet2]. The framework structure (Fig. NAB.1.1) can be built from *bb29* ($3^2 4^1 8^1 9^2$) units (Fig. NAB.1.2) forming the 9-ring channels parallel **a** and and **b** as shown in Fig. NAB.1.3. Parallel **c** there is a sinuous channel limited by an 8-ring intersecting the channels composed of 9-rings. The channel system is three-dimensional.

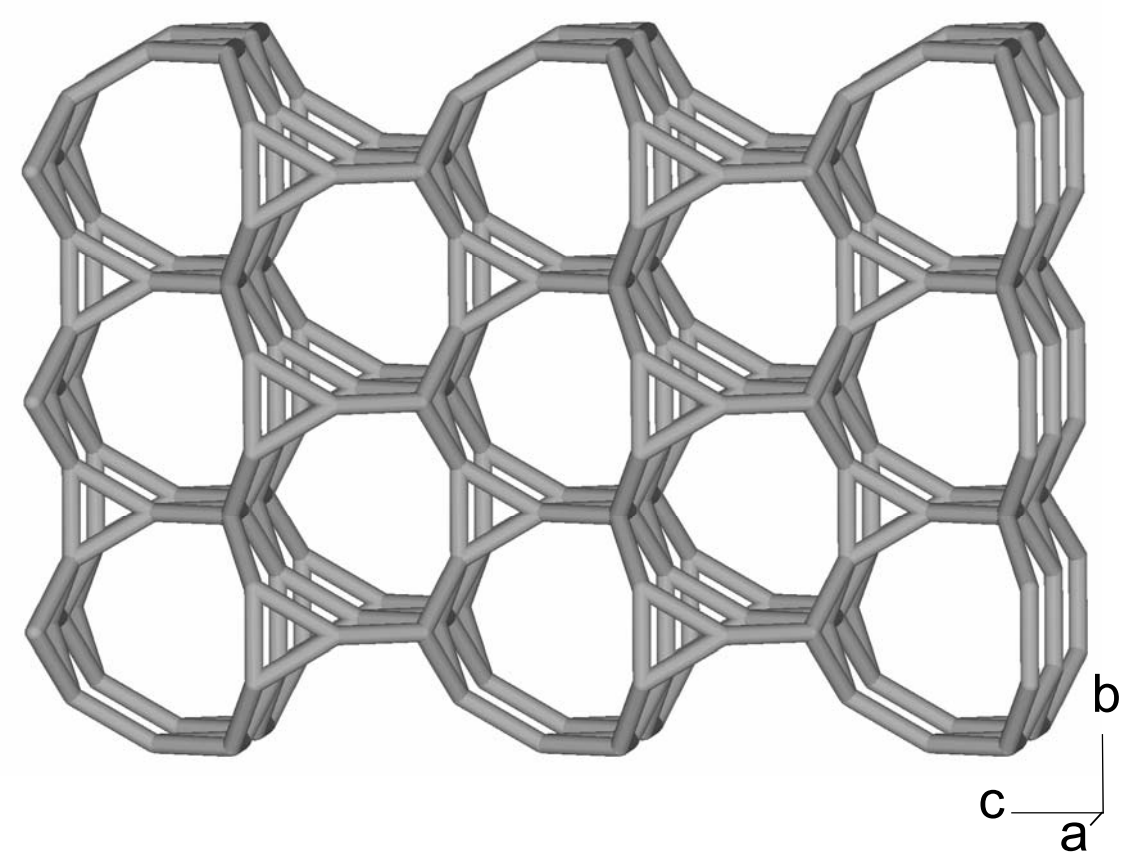
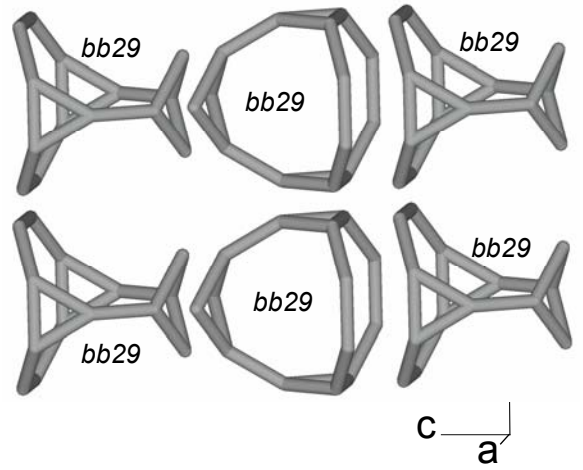
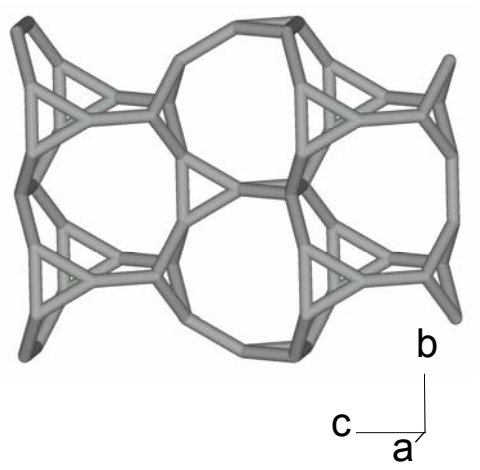


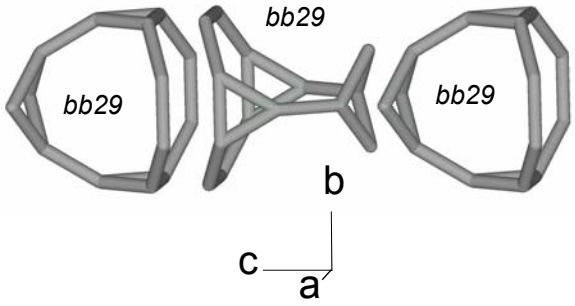
Fig. NAB.1.1 The framework structure of NAB-type zeolites in space group $I\,\bar{4}\,m\,2$. Projection parallel **a** rotated by 6° about **b** and 4° about **c**.



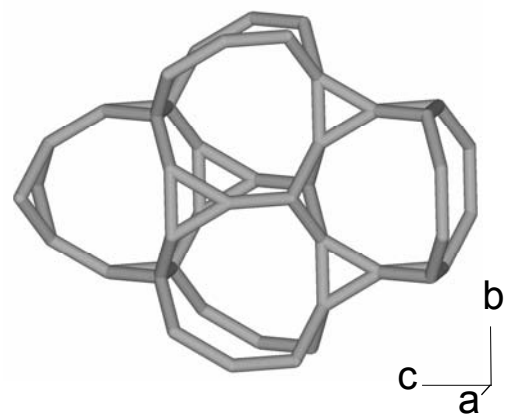
a Linkage of *bb29* units in the (100) plane.



b The complete assemblage shown in a).



c Linkage of *bb29* units in the front and rear of the layer shown in a) according to I-centering.



d The assemblage shown in c) with additional links to the rear and front layer shown in b).

Fig. NAB.1.2 The linkage of building units in NAB-type zeolites. View parallel **a** rotated by 10° aboaut **b** and 8° about **c**.

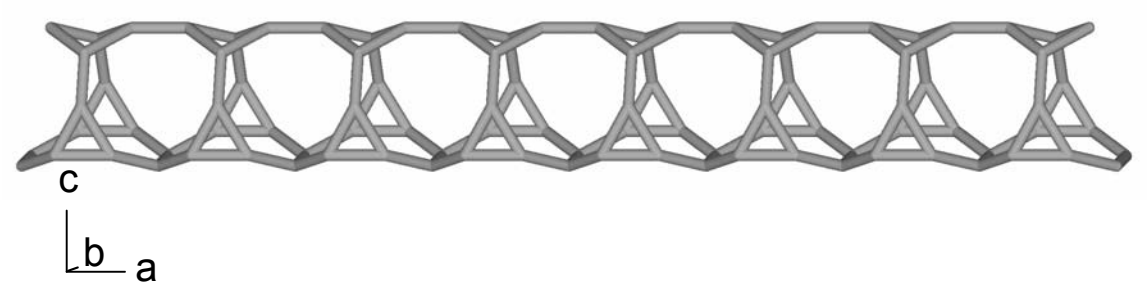


Fig. NAB.1.3 The 9-ring channel built by *bb29* units parallel **a** and **b** forming the two-dimensional channel system crosslinked by the 8-ring windows of the *bb29* units parallel **c**. View parallel **-b** rotated by 10° about **a** and **c**.

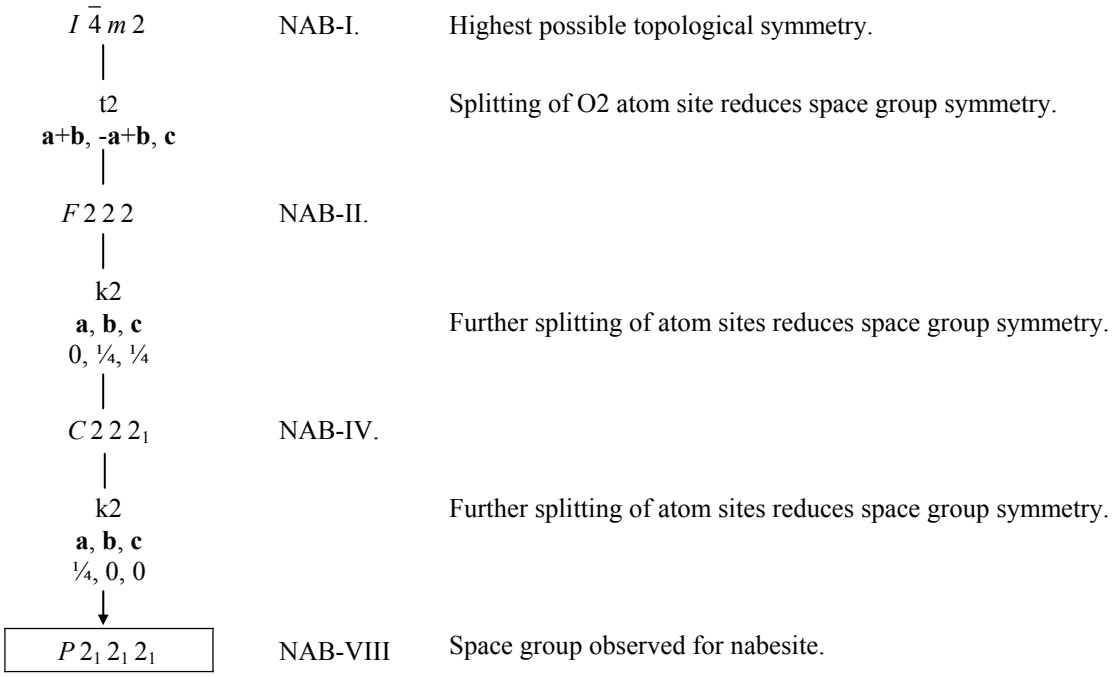


Fig. NAB.1.3 Symmetry relationship of the NAB types.

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

NAB-I $I\bar{4}m2$	NAB-II $F222$	NAB-IV $C222_1$	NAB-VIII $P2_12_12_1$
T1 [2(a), $\bar{4}m2$]	→ T1 [4(a), 2 2 2]	→ T1 [4(b), . 2 .]	→ T1 [4(a), 1]
T2 [8(i), . *m* .]	→ T2 [16(k), 1]	→ T21 [8(c), 1]	→ T21a [4(a), 1]
			T21b [4(a), 1]
		T22 [8(c), 1]	→ T22a [4(a), 1]
			T22b [4(a), 1]
O1 [8(i), . *m* .]	→ O1 [16(k), 1]	→ O11 [8(c), 1]	→ O11a [4(a), 1]
			O11b [4(a), 1]
		O12 [8(c), 1]	→ O12a [4(a), 1]
			O12b [4(a), 1]
O2 [8(h), . . 2]	→ O21 [8(j), 2 . .]	→ O21a [4(a), 2 . .]	→ O21a [4(a), 1]
		O21b [4(a), 2 . .]	→ O21b [4(a), 1]
	O22 [8(i), 1]	→ O22 [8(c), 1]	→ O22a [4(a), 1]
			O22b [4(a), 1]
O3 [4(e), 2*m* *m* .]	→ O3 [8(g), . . 2]	→ O3 [8(c), 1]	→ O31 [4(a), 1]
			O31 [4(a), 1]

NAB.2 Compounds and crystal data

Table NAB.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
NAB-VIII $P2_12_12_1$								
NAB2002a01	$Na_8 \cdot Be_4Si_{16}O_{40} \cdot 16H_2O$	16.9	M	-	H_2O	-	-	2002Pet2

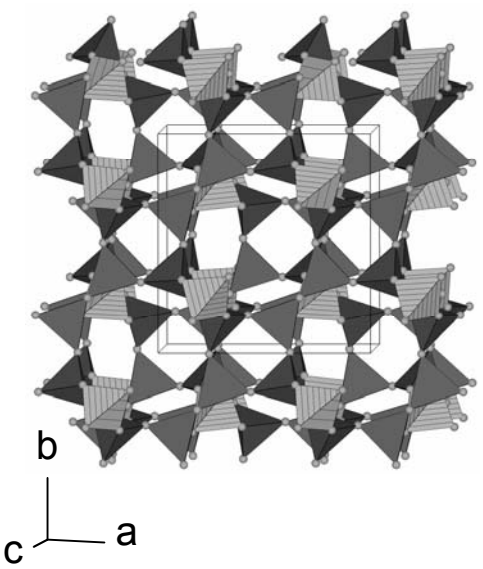
Table NAB.2.2 Structural parameters of the NAB-type compound.

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
NAB-VIII $P2_12_12_1$						
NAB2002a01	9.748(1)	10.133(1)	11.954(2)	1181	293	2002Pet2

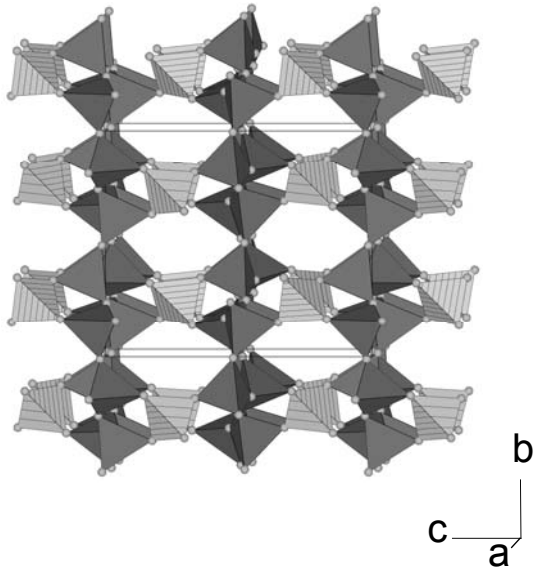
NAB.3 Framework structure of NAB-VIII compound ($P2_12_12_1$, IT #19)

Table NAB.3.2 Selected interatomic distances and angles for nabesite, $Na_8 \cdot Be_4Si_{16}O_{40} \cdot 16H_2O$ (NAB2002a01, 2002Pet2

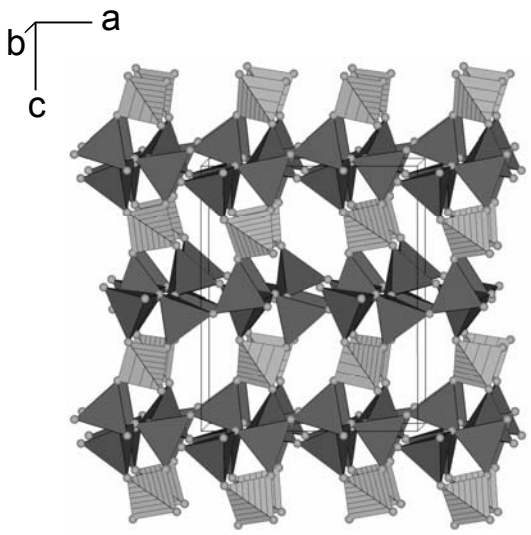
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Be1 - O11b	1.636(2)	129.7(1)	Si21a - O11a	1.587(1)	130.2(1)
Be1 - O12a	1.641(2)	129.8(1)	Si21a - O22b	1.625(1)	143.2(1)
Be1 - O12b	1.642(2)	129.9(1)	Si21a - O31	1.634(1)	127.0(1)
Be1 - O11a	1.653(2)	130.2(1)	Si21a - O21a	1.634(1)	141.3(1)
mean	1.643	129.9	mean	1.620	135.4
Si21b - O11b	1.588(1)	129.7(1)	Si22a - O12a	1.590(1)	129.8(1)
Si21b - O22a	1.622(1)	141.3(1)	Si22a - O21b	1.618(1)	159.7(1)
Si21b - O21a	1.636(1)	141.3(1)	Si22a - O22b	1.627(1)	143.2(1)
Si22b - O32	1.636(1)	127.2(1)	Si22a - O31	1.638(1)	127.0(1)
mean	1.621	134.9	mean	1.618	139.9
Si22b - O12b	1.590(1)	129.9(1)			
Si22b - O21b	1.622(1)	159.7(1)			
Si22b - O22a	1.626(1)	141.3(1)			
Si22b - O32	1.644(1)	127.2(1)			
mean	1.620	139.5			



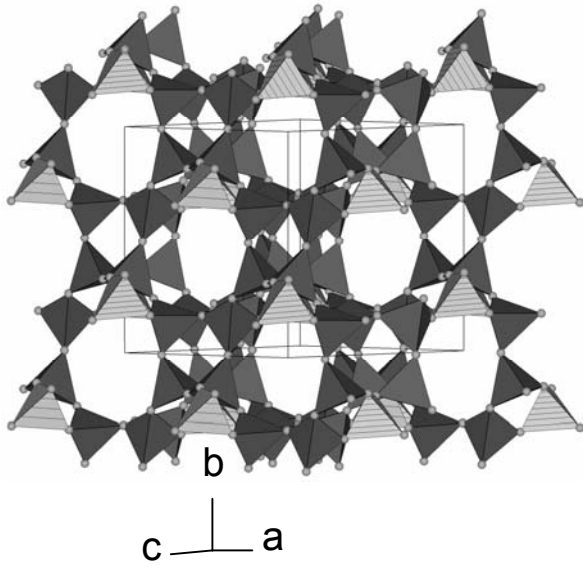
a View parallel [001] rotated by 2° about [100] and [010].



b View parallel [100] rotated by 2° about [010] and [001].



c View parallel [010] rotated by 2° about [100] and [001].



d View parallel [101] rotated by 2° about [010] and [10 $\bar{1}$]

Fig. NAB.3.1 Projections of the NAB-VIII crystal structure of nabesite, $Na_8 \cdot Be_4Si_{16}O_{40} \cdot 16H_2O$ (NAB2002a01, 2002Pet2).

Table NAB.3.1 Atomic coordinates and site definitions for nabesite, $Na_8 \cdot Be_4Si_{16}O_{40} \cdot 16H_2O$ (NAB2002a01, 2002Pet2).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Be1	0.2423(2)	0.2622(2)	0.2568(1)	0.66(2)	1	4(a)	4
Si21a	0.29128(3)	0.14866(3)	0.03408(3)	0.663(5)	1	4(a)	4
Si21b	0.79977(3)	0.64856(3)	0.02158(3)	0.616(5)	1	4(a)	4
Si22a	0.41607(3)	0.64522(3)	0.56419(3)	0.592(5)	1	4(a)	4
Si22b	0.89961(3)	0.13717(3)	0.55278(3)	0.604(5)	1	4(a)	4
O11a	0.3279(1)	0.1782(1)	0.16101(8)	1.02(1)	1	4(a)	4
O11b	0.8239(1)	0.6593(1)	0.15267(8)	1.17(1)	1	4(a)	4
O12a	0.3807(1)	0.6559(1)	0.69374(7)	0.96(1)	1	4(a)	4
O12b	0.8474(1)	0.13647(9)	0.67882(8)	0.96(1)	1	4(a)	4
O21a	0.7591(1)	0.49660(8)	0.48577(9)	1.09(1)	1	4(a)	4
O21b	0.6209(1)	0.00306(9)	-0.01041(9)	1.36(2)	1	4(a)	4
O22a	0.0620(1)	0.1739(1)	0.55085(9)	1.26(1)	1	4(a)	4
O22b	0.5795(1)	0.6727(1)	0.54934(9)	1.13(1)	1	4(a)	4
O31	0.1673(1)	0.24433(9)	0.99072(8)	0.89(1)	1	4(a)	4
O32	0.68420(9)	0.75353(9)	0.97763(7)	0.89(1)	1	4(a)	4
Na1	0.02823(8)	0.19660(8)	0.81506(7)	2.27(1)	1	4(a)	4
Na2	0.3737(1)	0.25369(9)	0.73922(9)	3.53(2)	1	4(a)	4
OW1	0.2206(2)	0.0755(1)	0.7617(1)	2.19(2)	1	4(a)	4
OW2	0.1610(2)	0.3752(1)	0.7381(1)	2.50(2)	1	4(a)	4
OW3	-0.0588(2)	0.0208(2)	0.9493(2)	2.99(2)	1	4(a)	4
OW4	0.4744(2)	0.4444(2)	0.8089(2)	3.11(3)	1	4(a)	4
H1	0.249(4)	0.009(4)	0.807(3)	5.2(8)	1	4(a)	4
H2	0.209(4)	0.049(4)	0.689(3)	5.3(9)	1	4(a)	4
H3	0.171(3)	0.442(3)	0.759(3)	3.6(6)	1	4(a)	4
H4	0.095(4)	0.383(4)	0.699(3)	4.7(8)	1	4(a)	4
H5	-0.077(3)	0.029(3)	0.023(2)	3.7(7)	1	4(a)	4
H6	0.034(2)	0.011(4)	0.959(4)	8(1)	1	4(a)	4
H7	0.446(4)	0.527(4)	0.788(3)	5.8(9)	1	4(a)	4
H8	0.554(4)	0.404(4)	0.765(3)	5.9(9)	1	4(a)	4

NAB.4 Chemical composition

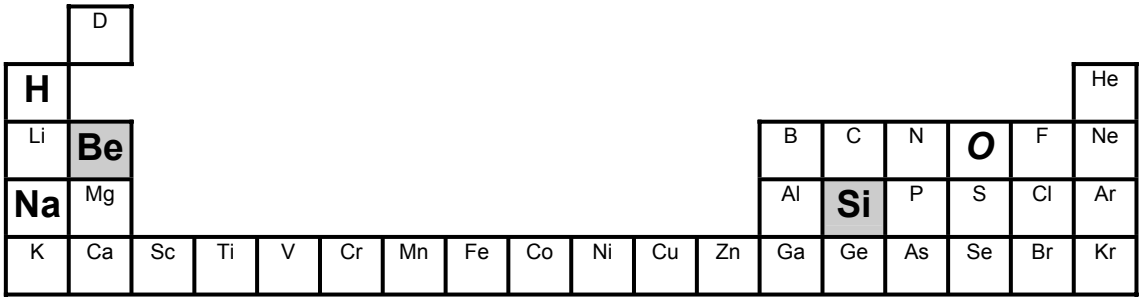


Fig. NAB.4.1 Chemical elements (highlighted) occurring in NAB-type compounds. Framework cations are in grey fields.

NAB.5 Flexibility and apertures

The value of the mean T-O-T angles in NAB2002a01 is about 136°, with values for individual angles ranging from 127° to 160° (Table MTN.3.2). This range of values T-O-T for the NAB-type is smaller than observed for the LTA-type compounds where it varies from 125° to 179° (see the LTA chapter and [92Bau1]). The full range of values displayed by numerous zeolite frameworks of different types is 115° to 180° as observed in a sample of 2436 T-O-T values [95Bau1]. The mean angle in the NAB-type compound is clearly smaller than the maximum of the distribution of T-O-T angles in silicoaluminate zeolites (about 143° [95Bau1]). But NAB2002a01 is a beryllosilicate.

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

The maximal opening for all three channels in the three main directions is about 3.5 Å. Because the 9-ring is severely bent, its effective opening is smaller than in the LTA-type which is limited by 8-rings in all three directions (free opening about 4 Å).

NAB.6 Other information

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

NAB.7 References

92Bau1 Baur, W.H.: J. Solid State Chem. **97** (1992) 243.

95Bau1 Baur, W. H.: Proc. Second Polish-German Zeolite Colloquium, Toruń (1995) 171.

2002Pet1 Petersen, O.V., Niedermayr, G., Johnsen, O., Gault, R.A., Brandstätter, F.: N. Jb. Mineral. Mh. (2002) 23.

2002Pet2 Petersen, O.V., Giester, G., Brandstätter, F., Niedermayr, G.: Canad. Mineral. **40** (2002) 173.

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