NAT

NAT.1 Zeolite framework type and topology

The framework type code is named after the mineral **NAT**rolite, $Na_2Al_2Si_3O_{10} \cdot 2H_2O$, first found in the Hegau region of Germany and described by Klaproth [1803Kla1, cited after 98Coo1] who also assigned the mineral name. Natrolite belongs to the group of fibrous zeolites. The essential features of its crystal structure have been described by Pauling [30Pau1] and its details were first worked out by Taylor et al. [33Tay1].

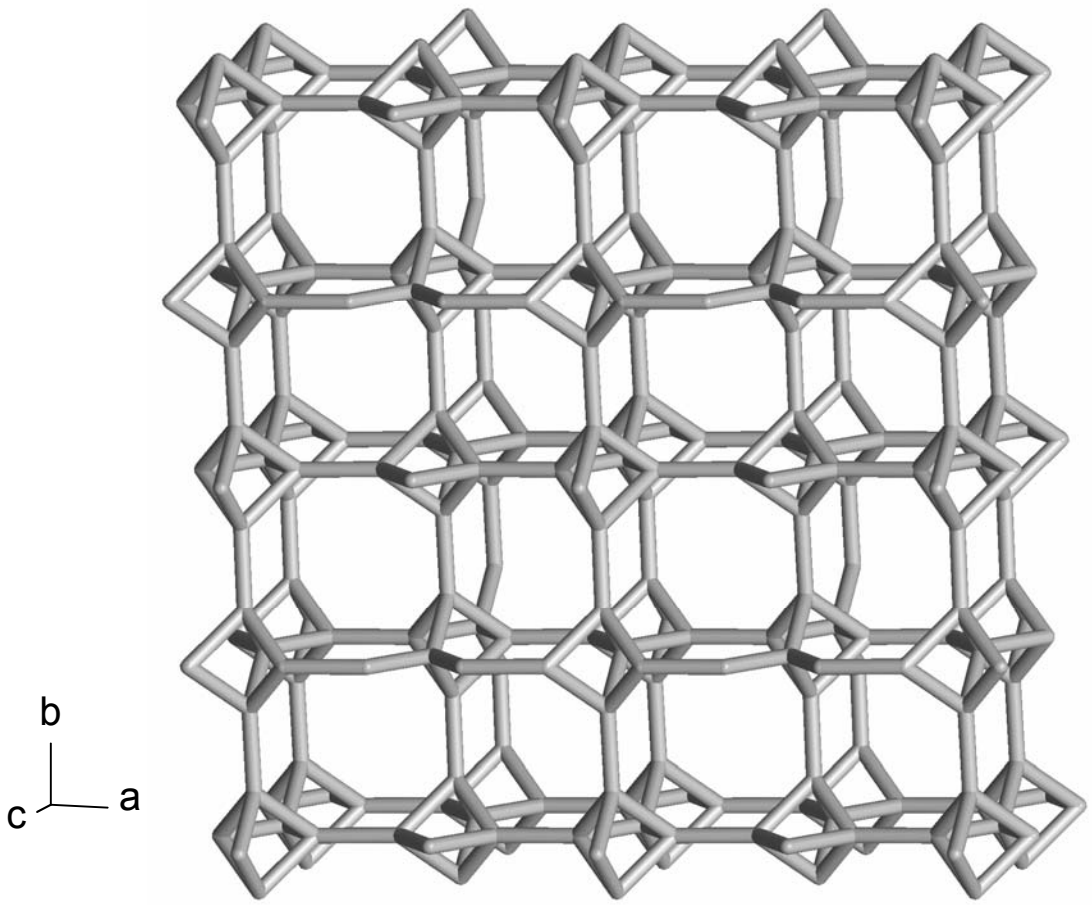
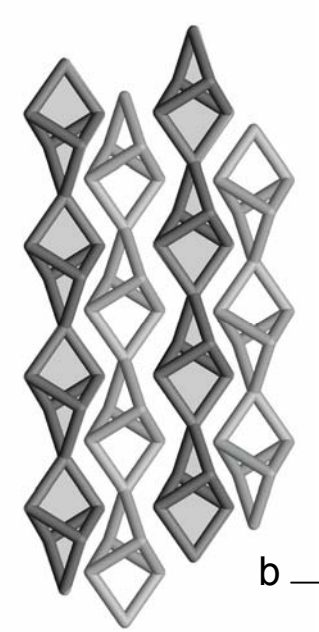
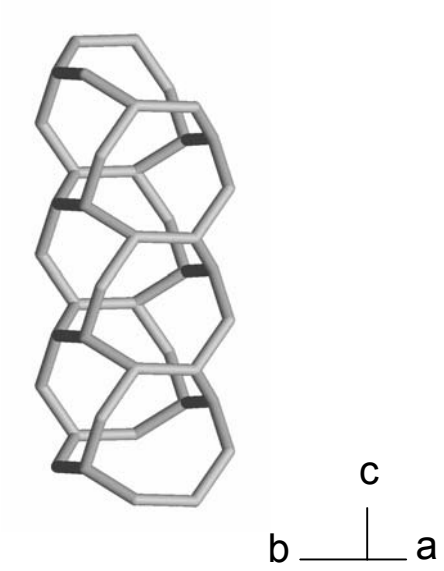


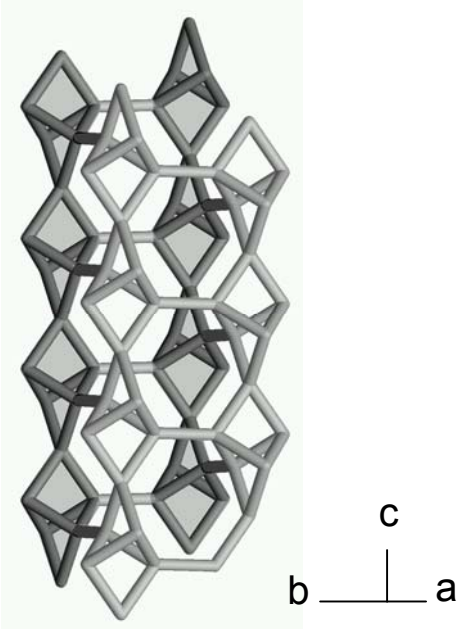
Fig. NAT.1.1. The framework structure of NAT-type compounds in the highest possible topological symmetry $I\,\bar{4}\,\mathbf{2}\,d$. View parallel **c** rotated by 10° about **a** and 16° about **b**.



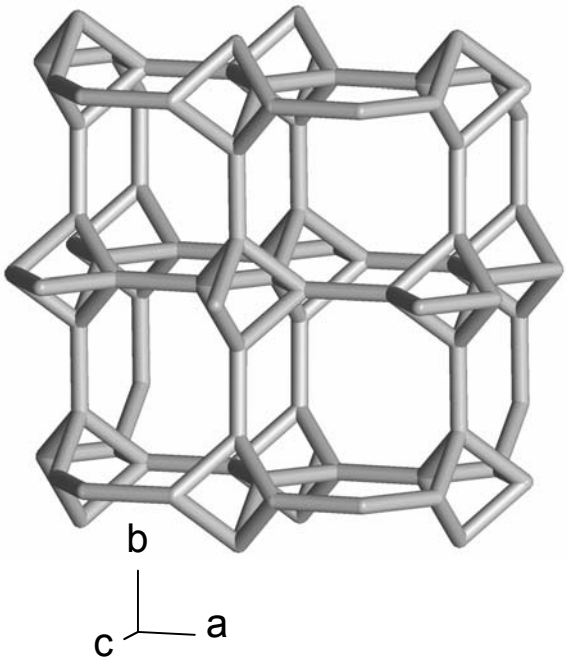
a The **fib** chains parallel [001] consisting of *des* units. Units in the rear are dark grey and semi transparent. View parallel [110] rotated by 20° about [001].



b The **kct** channel enclosed by the **fib** chains shown in a).



a The complete assemblage of **fib** chains around the **kct** channel.



b The unit cell contents (with some extensions) with four **kct** channels shown parallel [001] rotated by 10° about [100] and 16° about [010].

Fig. NAT.1.2. Building scheme of the NAT-type framework.

The structures of the fibrous zeolites contain chains (**fib** units, Fig. NAT.1.2a, and Figs. b in chapter NAT.3) parallel to **c** composed of four-rings of tetrahedra in which opposing tetrahedra are joined by a fifth tetrahedron. These chains mainly determine the fibrous properties of this zeolite. The chains are further connected forming the three-dimensional framework with the **kct** channels as shown in Fig. NAT.1.2.

Minerals with isotypic framework structures are gonnardite ($Na_{6.5}Ca_{1.5}Al_{9.5}Si_{10.5}O_{40} \cdot 12H_2O$), mesolite ($Na_{16}Ca_{16}Al_{48}Si_{72}O_{240} \cdot 64H_2O$), scolecite ($Ca_8Al_{16}Si_{24}O_{80} \cdot 24H_2O$), paranatrolite ($Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 24H_2O$), and tetranatrolite ($(Na,Ca)_8 \cdot Al_9Si_{11}O_{40} \cdot 8H_2O$). Dehydrated natrolite was called metanatrolite by Rinne [1890Rin1]. The names aedelite, apoanalcite, bergmannite, brevicite, crocalite, echellite, epinatrolite, fargite, galactite, hegauit, högauit, hydronatrolite, krokalith, laubanite, lehuntite, mooraboolite, natronite, poonalite, portite, radiolite, ranite, savite, spreustein, verrucite, and weissian, frequently assigned to natrolite or used to describe NAT-type minerals with special compositions or particular habits, are discredited and should not be used anymore [98Coo1]. The crystal structure of gonnardite described by [72Ami1] is actually the structure determination of a thomsonite, THO.

A K-GaSi-NAT in space goup $I\,2_1\,2_1\,2_1$ has been found, but has not been published yet [2006Lee2].

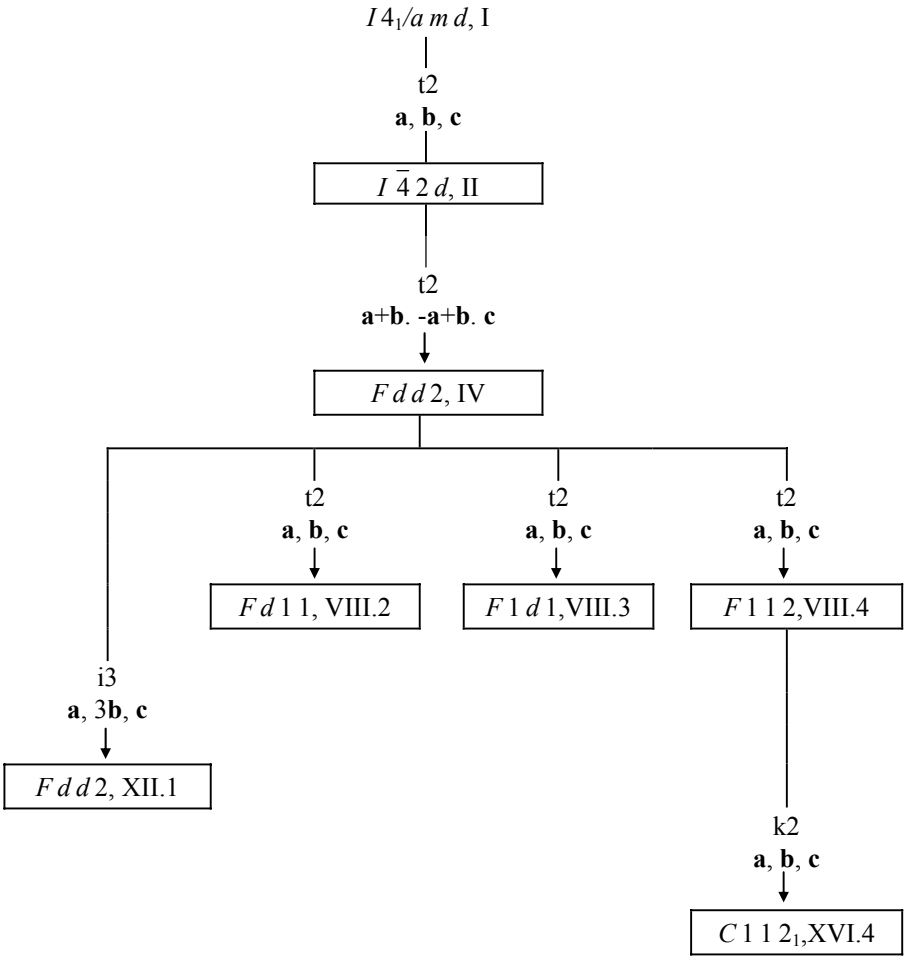


Fig. NAT.1.3 The Bärnighausen tree illustrating the symmetry relationship of the NAT types.

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

NAT-I $I4_1/amd$	NAT-II $I\bar{4}2d$	NAT-IV $Fdd2$	NAT-XII.1 $Fdd2$
T1 [16(h), . *m* .]	T1 [16(e), 1]	T11 [16(b), 1]	T11a [16(b), 1]
			T11b [16(b), 1]
			T11c [16(b), 1]
		T12 [16(b), 1]	T12a [16(b), 1]
			T12b [16(b), 1]
			T12c [16(b), 1]
T2 [4(a), $\bar{4}$ *m* 2]	T2 [4(a), $\bar{4}$ . .]	T2 [8(a), . . 2]	T21 [8(a), . . 2]
			T22 [16(b), 1]
O1 [16(h), . *m* .]	O1 [16(e), 1]	O11 [16(b), 1]	O11a [16(b), 1]
			O11b [16(b), 1]
			O11c [16(b), 1]
		O12 [16(b), 1]	O12a [16(b), 1]
			O12b [16(b), 1]
			O12c [16(b), 1]
O2 [16(g), . . 2]	O2 [16(e), 1]	O21 [16(b), 1]	O21a [16(b), 1]
			O21b [16(b), 1]
			O21c [16(b), 1]
		O22 [16(b), 1]	O22a [16(b), 1]
			O22b [16(b), 1]
			O22c [16(b), 1]
O3 [8(d),. 2/*m* .]	O3 [8(d), . 2 .]	O3 [16(b), 1]	O31 [16(b), 1]
			O32 [16(b), 1]
			O33 [16(b), 1]

NAT-I $I4_1/amd$	NAT-II $I\bar{4}2d$	NAT-IV $Fdd2$	NAT-VIII.2 $Fd11$
T1 [16(h), . *m* .]	T1 [16(e), 1]	T11 [16(b), 1]	T11a [8(a), 1]
			T11b [8(a), 1]
		T12 [16(b), 1]	T12a [8(a), 1]
			T12b [8(a), 1]
T2 [4(a), $\bar{4}$ *m* 2]	T2 [4(a), $\bar{4}$ . .]	T2 [8(a), . . 2]	T2 [8(a), 1]
O1 [16(h), . *m* .]	O1 [16(e), 1]	O11 [16(b), 1]	O11a [8(a), 1]
			O11b [8(a), 1]
		O12 [16(b), 1]	O12a [8(a), 1]
			O12b [8(a), 1]
O2 [16(g), . . 2]	O2 [16(e), 1]	O21 [16(b), 1]	O21a [8(a), 1]
			O21b [8(a), 1]
		O22 [16(b), 1]	O22a [8(a), 1]
			O22b [8(a), 1]
O3 [8(d), . 2/*m*.]	O3 [8(d), . 2 .]	O3 [16(b), 1]	O31 [8(a), 1]
			O32 [8(a), 1]

Table NAT.1.1 (continued).

NAT-I $I4_1/amd$	NAT-II $I\bar{4}2d$	NAT-IV $Fdd2$	NAT-VIII.3 $F1d1$
T1 [16(h), . *m* .]	T1 [16(e), 1]	T11 [16(b), 1]	T11a [8(a), 1]
			T11b [8(a), 1]
		T12 [16(b), 1]	T12a [8(a), 1]
			T12b [8(a), 1]
T2 [4(a), $\bar{4}$ *m* 2]	T2 [4(a), $\bar{4}$ . .]	T2 [8(a), . . 2]	T2 [8(a), . . 2]
O1 [16(h), . *m* .]	O1 [16(e), 1]	O11 [16(b), 1]	O11a [8(a), 1]
			O11b [8(a), 1]
		O12 [16(b), 1]	O12a [8(a), 1]
			O12b [8(a), 1]
O2 [16(g), . . 2]	O2 [16(e), 1]	O21 [16(b), 1]	O21a [8(a), 1]
			O21b [8(a), 1]
		O22 [16(b), 1]	O22a [8(a), 1]
			O22b [8(a), 1]
O3 [8(d), . 2/*m*.]	O3 [8(d), . 2 .]	O3 [16(b), 1]	O31 [8(a), 1]
			O32 [8(a), 1]

NAT-II $I\bar{4}2d$	NAT-IV $Fdd2$	NAT-VIII.4 $F112$	NAT-XVI.4 $C112_1$
T1 [16(e), 1]	T11 [16(b), 1]	T11a [8(c), 1]	T11a1 [4(c), 1]
			T11a2 [4(c), 1]
		T11b [8(c), 1]	T11b1 [4(c), 1]
			T11b2 [4(c), 1]
	T12 [16(b), 1]	T12a [8(c), 1]	T12a1 [4(c), 1]
			T12a2 [4(c), 1]
		T12b [8(c), 1]	T12b1 [4(c), 1]
			T12b2 [4(c), 1]
T2 [4(a), $\bar{4}$ . .]	T2 [8(a), . . 2]	T21 [4(a), 2]	T21 [4(c), 1]
		T22 [4(b), 2]	T22 [4(c), 1]
O1 [16(e), 1]	O11 [16(b), 1]	O11a [8(c), 1]	O11a1 [4(c), 1]
			O11a2 [4(c), 1]
		O11b [8(c), 1]	O11b1 [4(c), 1]
			O11b2 [4(c), 1]
	O12 [16(b), 1]	O12a [8(c), 1]	O12a1 [4(c), 1]
			O12a2 [4(c), 1]
		O12b [8(c), 1]	O12b1 [4(c), 1]
			O12b2 [4(c), 1]

Table NAT.1.1 (continued).

NAT-II $I\bar{4}2d$	NAT-IV $Fdd2$	NAT-VIII.4 $F112$	NAT-XVI.4 $C112_1$
O2 [16(e), 1]	O21 [16(b), 1]	O21a [8(c), 1]	O21a1 [4(c), 1]
			O21a2 [4(c), 1]
		O21b [8(c), 1]	O21b1 [4(c), 1]
			O21b2 [4(c), 1]
	O22 [16(b), 1]	O22a [8(c), 1]	O22a1 [4(c), 1]
			O22a2 [4(c), 1]
		O22b [8(c), 1]	O22b1 [4(c), 1]
			O22b2 [4(c), 1]
O3 [8(d), .2.]	O3 [16(b), 1]	O31 [8(c), 1]	O31a [4(c), 1]
			O31b [4(c), 1]
		O32 [8(c), 1]	O32a [4(c), 1]
			O32b [4(c), 1]

NAT.2 Compounds and crystal data

Table NAT.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	M	FD	SM	CE	SR	TT	T	REF
NAT-II, $I\bar{4}2d$									
NAT1986a01	$Na_8K \cdot Al_9Si_{11}O_{40} \cdot 8H_2O$	tetranatrolite	17.4	M	-	H_2O	-	-	86Mik1
NAT1986b01	$Na_{6.5}Ca_{1.5} \cdot Al_{9.5}Si_{10.5}O_{40} \cdot 12H_2O$	gonnardite	17.3	M	-	H_2O	-	-	86Maz1
NAT1991a01	$Na_{5.6}Ca_{1.6} \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	gonnardite	17.5	M	-	H_2O	-	-	91Art1
NAT1991a02	$Na_{5.6}Ca_{1.6} \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	gonnardite	17.4	M	-	H_2O	-	-	91Art1
NAT1991a03	$Na_{5.6}Ca_{1.6} \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	gonnardite	17.2	M	-	H_2O	-	-	91Art1
NAT1991a04	$Na_{5.6}Ca_{1.6} \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	gonnardite	17.3	M	-	H_2O	-	-	91Art1
NAT1991a05	$K_{8.0} \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	[K-gonnardite]	16.2	M	K	H_2O	-	-	91Art1
NAT1991b01	$Na_8 \cdot Ga_8Si_{12}O_{40} \cdot 8H_2O$	Na-GaSi-NAT	17.2	S	-	H_2O	-	-	91Mal1
NAT1995c01	$Na_8 \cdot Al_8Si_{12}O_{40} \cdot 8H_2O$	tetranatrolite	17.8	M	-	H_2O	-	-	95Ras1
NAT1999b01	$Na_{4.51}Ca_{1.84} \cdot Al_{8.59}Si_{11.50}O_{40} \cdot 12.61H_2O$	gonnardite	17.2	M	-	H_2O	-	-	99Art1
NAT2000a01	$K_8 \cdot Ga_8Si_{12}O_{40} \cdot 6.3H_2O$	K-GaSi-NAT	16.4	S	-	H_2O	-	-	2000Lee1
NAT2000b01	$Na_8 \cdot Al_8Ge_{12}O_{40} \cdot 8H_2O$	Na-AlGe-NAT	16.5	S	-	H_2O	-	-	2000Tri1
NAT2000d01	$Na_{6.25}Ca_{1.47}Sr_{0.06} \cdot Al_{9.55}Si_{10.46}O_{39.87} \cdot 10.9H_2O$	tetranatrolite	17.3	M	-	H_2O	-	-	2000Eva1

Table NAT.2.1 ($I\bar{4}2d$, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT2002c01	$K_{7.9} \cdot Ga_8Si_{12}O_{40} \cdot 12.2H_2O$	K-GaSi-NAT	16.0	S	-	H_2O	-	-	2002Lee2
NAT2002c02	$K_{7.5} \cdot Ga_8Si_{12}O_{40} \cdot 7.2H_2O$	K-GaSi-NAT	16.5	S	-	H_2O	-	-	2002Lee2
NAT2005a01	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40.00} \cdot 10.96H_2O$	tetranatrolite	17.3	M	-	H_2O	-	-	2005Lee1
NAT2005a02	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40.00} \cdot 9.48H_2O$	[tetranatrolite]	17.6	M	-	H_2O	-	-	2005Lee1
NAT2005a03	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40.00} \cdot 8.41H_2O$	[tetranatrolite]	17.8	M	-	H_2O	-	-	2005Lee1
NAT2005a04	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40.00} \cdot 8.00H_2O$	[tetranatrolite]	17.9	M	-	H_2O	-	-	2005Lee1
NAT2005a05	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40.00} \cdot 1.61H_2O$	[tetranatrolite]	18.5	M	-	H_2O	-	-	2005Lee1
NAT2006a01	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40} \cdot 10.96H_2O$	tetranatrolite	17.3	M	-	H_2O	-	-	2006Lee1
NAT2006a02	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40} \cdot 16.0H_2O$	[tetranatrolite]	18.2	M	-	H_2O	-	-	2006Lee1
NAT2006a03	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40} \cdot 16.0H_2O$	[tetranatrolite]	18.9	M	-	H_2O	-	-	2006Lee1
NAT2006a04	$Na_{5.85}Ca_{1.90} \cdot Al_{9.25}Si_{10.75}O_{40} \cdot 16.0H_2O$	[tetranatrolite]	18.3	M	-	H_2O	-	-	2006Lee1
NAT-IV.1，*Fdd*2									
NAT1933a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.9	M	-	H_2O	-	-	33Tay1
NAT1960a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	60Mei1
NAT1963a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	63Gab1
NAT1964a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	64Tor1
NAT1973a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	73Pea1
NAT1973a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	73Pea1
NAT1973a03	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	73Pea1
NAT1973a04	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	73Pea1
NAT1981a01	$Ca_{0.26}K_{0.01}Na_{15.54} \cdot Al_{15.77}Si_{24.16}O_{80} \cdot 20.36H_2O$	natrolite	17.7	M	-	H_2O	-	-	81Alb1
NAT1983a01	$Ca_{0.40}Na_{14.8} \cdot Al_{15.92}Si_{24.08}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	83Hes1
NAT1983b01	$Ca_{1.5}K_{0.5}Na_{14.6} \cdot Al_{16.5}Si_{23.5}O_{80} \cdot 16H_2O$	natrolite	17.7	M	-	H_2O	-	-	83Pec1
NAT1984a01	$Ca_{0.06}Na_{17.12} \cdot Al_{15.76}Si_{24.24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	84Kir1
NAT1984a02	$Ca_{0.06}Na_{17.12} \cdot Al_{15.76}Si_{24.24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	84Kir1
NAT1984a03	$Ca_{0.06}Na_{17.12} \cdot Al_{15.76}Si_{24.24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	84Kir1
NAT1984a04	$Ca_{0.06}Na_{17.12} \cdot Al_{15.76}Si_{24.24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	84Kir1
NAT1984b01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	84Art1
NAT1987b01	$K_{15.8}Na_{0.2} \cdot Al_{15.7}Si_{24.2}O_{80} \cdot 20.6H_2O$	[K-natrolite]	16.2	M	K	H_2O	-	-	87Yam1
NAT1988a01	$Li_{13.3}Na_{2.7} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[Li-natrolite]	18.8	M	Li	H_2O	-	-	88Sie1

Table NAT.2.1 (NAT.IV.1, *F d d* 2, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT1988c01	$Na_{15.5} \cdot Ga_{15.5}Si_{24.5}O_{80} \cdot 16H_2O$	Na-GaSi-NAT	17.3	S	-	H_2O	-	-	88Xie1
NAT1989b01	$Li_{13.3}Na_{2.7} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[Li-natrolite]	18.8	M	Li	H_2O	-	-	89Sie1
NAT1990a01	$Li_{12.8}Na_{3.2} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[Li-natrolite]	18.8	M	Li	H_2O	-	-	90Bau1
NAT1990a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	90Bau1
NAT1990a03	$K_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[K-natrolite]	16.3	M	K	H_2O	-	-	90Bau1
NAT1990b01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	90Kro1
NAT1990b02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	90Kro1
NAT1990b03	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.7	M	-	H_2O	-	-	90Kro1
NAT1990b04	$Li_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[Li-natrolite]	18.8	M	Li	H_2O	-	-	90Kro1
NAT1993b01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	93Stu2
NAT1994a03	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 11.3H_2O$	[mesolite]	18.0	M	-	H_2O	D	523	94Sta1
NAT1994a04	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 14.69H_2O$	[mesolite]	17.8	M	-	H_2O	D	473	94Sta1
NAT1994a05	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 11.15H_2O$	[mesolite]	18.1	M	-	H_2O	D	573	94Sta1
NAT1994a06	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 23.23H_2O$	[mesolite]	17.3	M	-	H_2O	R	523	94Sta1
NAT1994b66	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 7.01H_2O$	[mesolite]	17.8	M	-	H_2O	D	510	94Sta2
NAT1994b67	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 7.22H_2O$	[mesolite]	17.8	M	-	H_2O	D	515	94Sta2
NAT1994b68	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 6.60H_2O$	[mesolite]	17.9	M	-	H_2O	D	521	94Sta2
NAT1994b69	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 6.39H_2O$	[mesolite]	17.9	M	-	H_2O	D	527	94Sta2
NAT1994b70	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 6.13H_2O$	[mesolite]	18.0	M	-	H_2O	D	533	94Sta2
NAT1994b71	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.93H_2O$	[mesolite]	18.0	M	-	H_2O	D	539	94Sta2
NAT1994b72	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.77H_2O$	[mesolite]	18.0	M	-	H_2O	D	545	94Sta2
NAT1994b73	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.74H_2O$	[mesolite]	18.0	M	-	H_2O	D	551	94Sta2
NAT1994b74	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.65H_2O$	[mesolite]	18.1	M	-	H_2O	D	557	94Sta2
NAT1994b75	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.45H_2O$	[mesolite]	18.1	M	-	H_2O	D	563	94Sta2
NAT1994b76	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.42H_2O$	[mesolite]	18.1	M	-	H_2O	D	570	94Sta2
NAT1994b77	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.30H_2O$	[mesolite]	18.1	M	-	H_2O	D	576	94Sta2
NAT1994b78	$Na_{5.33}Ca_{5.33} \cdot Al_{16}Si_{24}O_{80} \cdot 5.31H_2O$	[mesolite]	18.1	M	-	H_2O	D	582	94Sta2
NAT1995b01	$Na_{15.2}Ca_{0.4} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	95Alb1
NAT1995d01	$Na_{15.2} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.9	M	-	H_2O	-	-	95Fin1
NAT1996a06	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	20.4	M	-	H_2O	D	823	96Bau1
NAT1996a07	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	20.6	M	-	H_2O	D	573	96Bau1
NAT1996a08	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 12H_2O$	[natrolite]	18.3	M	-	-	D/R	823	96Bau1

Table NAT.2.1 (NAT.IV.1, *F d d* 2, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT1996c01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	natrolite	17.8	M	-	H_2O	-	-	96Ghe1
NAT1999a01	$K_{0.40}Na_{15.83} \cdot Al_{16.21}Si_{23.78}O_{80} \cdot 15.36H_2O$	natrolite	17.8	M	-	H_2O	-	-	99Men1
NAT2001a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[natrolite]	18.0	M	-	H_2O	-	-	2001Lee1
NAT2001a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[natrolite]	18.1	M	-	H_2O	-	-	2001Lee1
NAT2001a03	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.6	M	-	H_2O	-	-	2001Lee1
NAT2001a04	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.7	M	-	H_2O	-	-	2001Lee1
NAT2001a05	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.0	M	-	H_2O	-	-	2001Lee1
NAT2001a06	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.3	M	-	H_2O	-	-	2001Lee1
NAT2001a07	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.8	M	-	H_2O	-	-	2001Lee1
NAT2002a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[natrolite]	18.0	M	-	H_2O	-	-	2002Lee1
NAT2002a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$	[natrolite]	18.1	M	-	H_2O	-	-	2002Lee1
NAT2002a03	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.6	M	-	H_2O	-	-	2002Lee1
NAT2002a04	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.7	M	-	H_2O	-	-	2002Lee1
NAT2002a05	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.0	M	-	H_2O	-	-	2002Lee1
NAT2002a06	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.3	M	-	H_2O	-	-	2002Lee1
NAT2002a07	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	18.8	M	-	H_2O	-	-	2002Lee1
NAT2003a01	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 16H_2O$	Na-GaSi-NAT	17.3	S	-	H_2O	-	-	2003Lee1
NAT2003a02	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 16H_2O$	Na-GaSi-NAT	17.5	S	-	H_2O	-	-	2003Lee1
NAT2003a03	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 25.76H_2O$	Na-GaSi-NAT	17.2	S	-	H_2O	-	-	2003Lee1
NAT2003a04	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.2	S	-	H_2O	-	-	2003Lee1
NAT2003a05	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.2	S	-	H_2O	-	-	2003Lee1
NAT2003a06	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.4	S	-	H_2O	-	-	2003Lee1
NAT2003a07	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.5	S	-	H_2O	-	-	2003Lee1
NAT2003a08	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.6	S	-	H_2O	-	-	2003Lee1
NAT2003a09	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	17.8	S	-	H_2O	-	-	2003Lee1
NAT2003a10	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	18.0	S	-	H_2O	-	-	2003Lee1
NAT2003a11	$Na_{16} \cdot Ga_{16}Si_{24}O_{80} \cdot 32.00H_2O$	Na-GaSi-NAT	18.2	S	-	H_2O	-	-	2003Lee1
NAT2004b01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.6	M	-	H_2O	-	-	2004Lee1
NAT2004b02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32H_2O$	[natrolite]	17.2	M	-	H_2O	-	-	2004Lee1
NAT2005d01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 14.7D_2O$	[natrolite]	18.0	M	-	D_2O	-	-	2005Ser1
NAT2005e01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16D_2O$	[natrolite]	17.8	M	-	D_2O	-	-	2005Col1
NAT2005e02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32D_2O$	[natrolite]	17.6	M	-	D_2O	-	-	2005Col1

Table NAT.2.1 (NAT.IV.1, *F d d* 2, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT2006b01	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16D_2O$	[natrolite]	17.8	M	-	D_2O	-	-	2006Dem1
NAT2006b02	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16D_2O$	[natrolite]	17.8	M	-	D_2O	-	-	2006Dem1
NAT2006b03	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32D_2O$	[natrolite]	17.6	M	-	D_2O	-	-	2006Dem1
NAT2006b04	$Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 32D_2O$	[natrolite]	17.6	M	-	D_2O	-	-	2006Dem1
NAT-XII.1.1, *F d d* 2									
NAT1972a04	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 64H_2O$	mesolite	17.6	M	-	H_2O	-	-	72Adi1
NAT1986c01	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 64H_2O$	mesolite	17.6	M	-	H_2O	-	-	86Art1
NAT1994a01	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 64H_2O$	mesolite	17.6	M	-	H_2O	-	293	94Sta1
NAT1994a02	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 59.4H_2O$	[mesolite]	17.7	M	-	H_2O	D	458	94Sta1
NAT1994b41	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 56.11H_2O$	[mesolite]	17.6	M	-	H_2O	D	383	94Sta2
NAT1994b42	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 56.14H_2O$	[mesolite]	17.6	M	-	H_2O	D	388	94Sta2
NAT1994b43	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.25H_2O$	[mesolite]	17.6	M	-	H_2O	D	392	94Sta2
NAT1994b44	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.54H_2O$	[mesolite]	17.6	M	-	H_2O	D	397	94Sta2
NAT1994b45	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.23H_2O$	[mesolite]	17.6	M	-	H_2O	D	401	94Sta2
NAT1994b46	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.17H_2O$	[mesolite]	17.6	M	-	H_2O	D	406	94Sta2
NAT1994b47	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.07H_2O$	[mesolite]	17.6	M	-	H_2O	D	410	94Sta2
NAT1994b48	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 54.94H_2O$	[mesolite]	17.6	M	-	H_2O	D	415	94Sta2
NAT1994b49	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.25H_2O$	[mesolite]	17.6	M	-	H_2O	D	420	94Sta2
NAT1994b50	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 55.10H_2O$	[mesolite]	17.6	M	-	H_2O	D	425	94Sta2
NAT1994b51	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 54.75H_2O$	[mesolite]	17.6	M	-	H_2O	D	430	94Sta2
NAT1994b52	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 54.30H_2O$	[mesolite]	17.6	M	-	H_2O	D	435	94Sta2
NAT1994b53	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 54.06H_2O$	[mesolite]	17.6	M	-	H_2O	D	440	94Sta2
NAT1994b54	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 53.53H_2O$	[mesolite]	17.6	M	-	H_2O	D	445	94Sta2
NAT1994b55	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 53.15H_2O$	[mesolite]	17.6	M	-	H_2O	D	450	94Sta2
NAT1994b56	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 52.90H_2O$	[mesolite]	17.6	M	-	H_2O	D	455	94Sta2
NAT1994b57	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 52.54H_2O$	[mesolite]	17.6	M	-	H_2O	D	460	94Sta2
NAT1994b58	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 51.95H_2O$	[mesolite]	17.6	M	-	H_2O	D	466	94Sta2
NAT1994b59	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 51.49H_2O$	[mesolite]	17.6	M	-	H_2O	D	471	94Sta2
NAT1994b60	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 50.67H_2O$	[mesolite]	17.6	M	-	H_2O	D	476	94Sta2
NAT1994b61	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 49.97H_2O$	[mesolite]	17.7	M	-	H_2O	D	482	94Sta2
NAT1994b62	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 49.23H_2O$	[mesolite]	17.7	M	-	H_2O	D	487	94Sta2
NAT1994b63	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 49.58H_2O$	[mesolite]	17.7	M	-	H_2O	D	493	94Sta2

Table NAT.2.1 (NAT.XII.1.1, *F d d* 2, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT1994b64	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 48.00H_2O$	[mesolite]	17.8	M	-	H_2O	D	498	94Sta2
NAT1994b65	$Na_{16}Ca_{16} \cdot Al_{48}Si_{72}O_{240} \cdot 47.14H_2O$	[mesolite]	17.8	M	-	H_2O	D	504	94Sta2
NAT2000c01	$Na_{15.92}Ca_{16.32} \cdot Al_{48.00}Si_{71.84}O_{240} \cdot 64H_2O$	mesolite	17.6	M	-	H_2O	-	-	2000Stu1
NAT-VIII.1.2, *F d* 1 1									
NAT1972a03	$Ca_{7.92} \cdot Al_{15.68}Si_{23.92}O_{80} \cdot 16H_2O$	scolecite	17.5	M	-	H_2O	D	573	72Adi1
NAT1979a01	$Ca_{3.92} \cdot Al_{7.72}Si_{12.28}O_{40} \cdot 12H_2O$	scolecite	17.5	M	-	H_2O	-	-	79Fäl1
NAT1984d01	$Ca_4 \cdot Al_8Si_{12}O_{40} \cdot 12H_2O$	scolecite	17.5	M	-	H_2O	-	-	84Smi1
NAT1984d02	$Ca_4 \cdot Al_8Si_{12}O_{40} \cdot 12H_2O$	scolecite	17.5	M	-	H_2O	-	-	84Smi1
NAT1985a01	$Ca_4 \cdot Al_8Si_{12}O_{40} \cdot 12H_2O$	scolecite	17.5	M	-	H_2O	-	-	85Kvi1
NAT1994b21	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	489	94Sta2
NAT1994b22	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	494	94Sta2
NAT1994b23	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	500	94Sta2
NAT1994b24	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	505	94Sta2
NAT1994b25	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	511	94Sta2
NAT1994b26	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	517	94Sta2
NAT1994b27	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	523	94Sta2
NAT1994b28	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	529	94Sta2
NAT1994b29	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	535	94Sta2
NAT1994b30	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	541	94Sta2
NAT1994b31	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	547	94Sta2
NAT1994b32	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	553	94Sta2
NAT1994b33	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	559	94Sta2
NAT1994b34	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	565	94Sta2
NAT1994b35	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	571	94Sta2
NAT1994b36	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	578	94Sta2
NAT1994b37	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	584	94Sta2
NAT1994b38	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	590	94Sta2
NAT1994b39	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	597	94Sta2
NAT1994b40	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 16.00H_2O$	[scolecite]	17.9	M	-	H_2O	D	603	94Sta2
NAT2002b01	$Ca_{3.93} \cdot Al_{7.84}Si_{12.16}O_{40} \cdot 12.21H_2O$	scolecite	17.4	M	-	H_2O	-	-	2002Com1
NAT2002b02	$Ca_{3.93} \cdot Al_{7.84}Si_{12.16}O_{40} \cdot 12.21H_2O$	[scolecite]	18.0	M	-	H_2O	-	-	2002Com1
NAT2002b03	$Ca_{3.93} \cdot Al_{7.84}Si_{12.16}O_{40} \cdot 12.21H_2O$	[scolecite]	18.4	M	-	H_2O	-	-	2002Com1

Table NAT.2.1 (NAT.VIII.1.2, *F d* 1 1, continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT2002b04	$Ca_{3.93} \cdot Al_{7.84}Si_{12.16}O_{40} \cdot 12.21H_2O$	[scolecite]	17.5	M	-	H_2O	-	-	2002Com1
NAT2005b01	$Na_8 \cdot Al_8Si_{12}O_{40} \cdot 12H_2O$	[paranatrolite]	17.0	M	-	H_2O	-	-	2005Lee2
NAT-VIII.1.3 , *F* 1 *d* 1									
NAT1972a01	$Ca_{7.92} \cdot Al_{15.68}Si_{23.92}O_{80} \cdot 23.84H_2O$	scolecite	17.5	M	-	H_2O	-	-	72Adi1
NAT1972a02	$Al_{16}Si_{24}O_{80}$		17.5	T	-	-	-	-	72Adi1
NAT1984c01	$Ca_{8.0} \cdot Al_{16.0}Si_{24.0}O_{80.0} \cdot 24H_2O$	scolecite	17.4	M	-	H_2O	-	-	84Jos1
NAT1994b01	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.54H_2O$	[scolecite]	17.5	M	-	H_2O	D	380	94Sta2
NAT1994b02	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.44H_2O$	[scolecite]	17.5	M	-	H_2O	D	384	94Sta2
NAT1994b03	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.37H_2O$	[scolecite]	17.5	M	-	H_2O	D	389	94Sta2
NAT1994b04	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.34H_2O$	[scolecite]	17.5	M	-	H_2O	D	393	94Sta2
NAT1994b05	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.52H_2O$	[scolecite]	17.5	M	-	H_2O	D	398	94Sta2
NAT1994b06	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.50H_2O$	[scolecite]	17.5	M	-	H_2O	D	402	94Sta2
NAT1994b07	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.34H_2O$	[scolecite]	17.5	M	-	H_2O	D	407	94Sta2
NAT1994b08	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 23.19H_2O$	[scolecite]	17.5	M	-	H_2O	D	412	94Sta2
NAT1994b09	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 22.82H_2O$	[scolecite]	17.5	M	-	H_2O	D	416	94Sta2
NAT1994b10	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 22.79H_2O$	[scolecite]	17.5	M	-	H_2O	D	421	94Sta2
NAT1994b11	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 22.57H_2O$	[scolecite]	17.5	M	-	H_2O	D	426	94Sta2
NAT1994b12	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 22.40H_2O$	[scolecite]	17.5	M	-	H_2O	D	431	94Sta2
NAT1994b13	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 21.84H_2O$	[scolecite]	17.5	M		H_2O	D	436	94Sta2
NAT1994b14	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 21.41H_2O$	[scolecite]	17.5	M		H_2O	D	441	94Sta2
NAT1994b15	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 21.34H_2O$	[scolecite]	17.5	M		H_2O	D	446	94Sta2
NAT1994b16	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 20.81H_2O$	[scolecite]	17.5	M		H_2O	D	451	94Sta2
NAT1994b17	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 20.44H_2O$	[scolecite]	17.6	M		H_2O	D	456	94Sta2
NAT1994b18	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 19.98H_2O$	[scolecite]	17.6	M		H_2O	D	462	94Sta2
NAT1994b19	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 19.33H_2O$	[scolecite]	17.6	M		H_2O	D	467	94Sta2
NAT1994b20	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 18.91H_2O$	[scolecite]	17.6	M		H_2O	D	472	94Sta2
NAT1997a01	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 24H_2O$	scolecite	17.5	M		H_2O	-	-	97Stu1
NAT1998a01	$Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 24H_2O$	scolecite	17.5	M		H_2O	-	-	98Kun1
NAT2004a01	$Na_{15.04}K_{1.76}Ca_{0.48} \cdot Al_{17.92}Si_{22.08}O_{80} \cdot 24.8H_2O$	paranatrolite	16.7	M		H_2O	-	-	2004Ser1
NAT2005d02	$Na_{14.8}Mg_{0.40}Ca_{0.2} \cdot Al_{16.5}Si_{23.6}O_{80} \cdot 28H_2O$	[natrolite]	16.5	M	-	D_2O	-	-	2005Ser1

Table NAT.2.1 (continued)

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T	REF
NAT-VIII.1.4, F112									
NAT1983c01	$Ba_{0.02}Na_{15.44}Sr_{0.02} \cdot Al_{15.91}Si_{24.18}O_{80}$	[natrolite]	23.3	M		H_2O	D	623	83Alb1
NAT1985b01	$Rb_{16} \cdot Ga_{16}Ge_{24}O_{80}$		18.2	S		-	-	-	85Kla1
NAT1987a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T		-	-	-	87Dem1
NAT1987a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T		-	-	-	87Dem1
NAT1987a03	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T		-	-	-	87Dem1
NAT1987a04	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T		-	-	-	87Dem1
NAT1987a05	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T		-	-	-	87Dem1
NAT1987a06	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T	-	-	-	-	87Dem1
NAT1987a07	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T	-	-	-	-	87Dem1
NAT1987a08	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T	-	-	-	-	87Dem1
NAT1987a09	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T	-	-	-	-	87Dem1
NAT1987a10	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$		23.3	T	-	-	-	-	87Dem1
NAT1991a06	$(NH_4)_9 \cdot Al_{9.0}Si_{11.0}O_{40} \cdot 8H_2O$	[NH_4-gonnardite]	18.0	M	NH_4	H_2O	-	-	91Art1
NAT1995a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	22.4	M	-	-	D	548	95Jos1
NAT1996a01	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	22.5	M	-	-	D	598	96Bau1
NAT1996a02	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	22.5	M	-	-	D	573	96Bau1
NAT1996a03	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	21.4	M	-	-	D	723	96Bau1
NAT1996a04	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	21.0	M	-	-	D	773	96Bau1
NAT1996a05	$Na_{16} \cdot Al_{16}Si_{24}O_{80}$	[natrolite]	22.3	M	-	-	D	573	96Bau1
NAT-XVI.1.4 *C*112$_1$									
NAT1992a01	$(NH_4)_{16} \cdot Al_{16}Si_{24}O_{80}$	[NH_4-natrolite]	18.6	M	NH_4	-	-	-	92Stu1
NAT1993a01	$(NH_4)_{16} \cdot Al_{16}Si_{24}O_{80}$	[NH_4-natrolite]	18.6	M	NH_4	-	-	-	93Stu1
NAT1996b01	$(H_3O)_{16} \cdot Al_{16}Si_{24}O_{80}$	[H_3O-natrolite]	18.5	M	H_3O	-	C	523	96Stu1

Table NAT.2.2 Structural parameters of NAT-type compounds.

code	*a* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT-II, *I* $\bar{4}$ 2 *d*								
NAT1986a01	13.141(8)	6.638(2)	1146	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	86Mik1
NAT1986b01	13.21(1)	6.622(4)	1156	½, 0, ¼	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	86Maz1
NAT1991a01	13.1252(3)	6.6219(4)	1141	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	91Art1
NAT1991a02	13.1944(6)	6.6116(7)	1151	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	91Art1
NAT1991a03	13.2580(6)	6.6054(6)	1161	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	91Art1
NAT1991a04	13.2163(3)	6.6233(4)	1157	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	91Art1
NAT1991a05	13.7276(3)	6.5557(3)	1235	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	91Art1
NAT1991b01	13.196(5)	6.663(2)	1160	0, 0, ½	**a**, **b**, **c**	*x*, *y*, *z*-½	293	91Mal1
NAT1995c01	13.070(9)	6.580(6)	1124	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	95Ras1
NAT1999b01	13.2670(4)	6.6023(6)	1162	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	99Art1
NAT2000a01	13.639(2)	6.545(1)	1218	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	293	2000Lee1
NAT2000b01	13.314(2)	6.818(1)	1209	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	298	2000Tri1
NAT2000d01	13.197(7)	6.630(9)	1155	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	2000Eva1
NAT2002c01	13.751(2)	6.605(1)	1249	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	2002Lee2
NAT2002c02	13.616(2)	6.550(1)	1214	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	113	2002Lee2
NAT2005a01	13.1988(1)	6.6288(1)	1155	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	2005Lee1
NAT2005a02	13.0666(1)	6.6632(1)	1138	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	373	2005Lee1
NAT2005a03	12.9815(1)	6.6808(1)	1126	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	473	2005Lee1
NAT2005a04	12.920(1)	6.6950(9)	1118	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	573	2005Lee1
NAT2005a05	13.1503(2)	6.2469(1)	1080	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	573	2005Lee1
NAT2006a01	13.1988(1)	6.6288(1)	1155	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	2006Lee1
NAT2006a02	12.959(1)	6.5446(7)	1099	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	- [1)]	2006Lee1
NAT2006a03	12.761(1)	6.5127(6)	1061	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	- [2)]	2006Lee1
NAT2006a04	12.910(2)	6.540(1)	1090	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	- [3)]	2006Lee1

[1)] at 4.2(1) GPa
[2)] at 6.9(1) GPa
[3)] at 5.4(1) GPa on release

Table NAT.2.2 (continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT-IV.1, *F d d* 2									
NAT1933a01	18.3(1)	18.6(1)	6.57(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	33Tay1
NAT1960a01	18.30(1)	18.63(1)	6.60(2)	2250	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	60Mei1
NAT1963a01	18.30(1)	18.63(1)	6.60(2)	2250	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	63Gab1
NAT1964a01	18.30	18.63	6.60	2250	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	64Tor1
NAT1973a01	18.43	18.71	6.52	2248	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	298	73Pea1
NAT1973a02	18.43	18.71	6.52	2248	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	361	73Pea1
NAT1973a03	18.43	18.71	6.52	2248	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	419	73Pea1
NAT1973a04	18.43	18.71	6.52	2248	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	471	73Pea1
NAT1981a01	18.35(1)	18.59(1)	6.608(4)	2254	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	81Alb1
NAT1983a01	18.319(4)	18.595(4)	6.597(1)	2247	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	83Hes1
NAT1983b01	18.326(5)	18.652(5)	6.601(3)	2256	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	83Pec1
NAT1984a01	18.285(2)	18.630(2)	6.585(1)	2243	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	84Kir1
NAT1984a02	18.296(3)	18.647(3)	6.585(1)	2247	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	84Kir1
NAT1984a03	18.296(3)	18.647(3)	6.585(1)	2247	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	84Kir1
NAT1984a04	18.296(3)	18.647(3)	6.585(1)	2247	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	84Kir1
NAT1984b01	18.272(6)	18.613(6)	6.593(2)	2242	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	20	84Art1
NAT1987b01	19.3173(2)	19.7672(2)	6.48206(6)	2467	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	87Yam1
NAT1988a01	17.678(5)	18.509(5)	6.488(5)	2123	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	88Sie1
NAT1988c01	18.423(4)	18.826(3)	6.652(1)	2307	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	296	88Xie1
NAT1989b01	17.678(5)	18.509(5)	6.488(5)	2123	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	89Sie1
NAT1990a01	17.678(5)	18.509(5)	6.488(5)	2123	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Bau1
NAT1990a02	18.307(2)	18.623(2)	6.5872(4)	2246	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Bau1
NAT1990a03	19.27(4)	19.66(4)	6.469(5)	2451	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Bau1
NAT1990b01	18.305(3)	18.632(3)	6.589(2)	2247	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Kro1
NAT1990b02	18.367(2)	18.583(1)	6.599(3)	2252	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Kro1
NAT1990b03	18.372(2)	18.576(2)	6.606(3)	2254	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Kro1
NAT1990b04	17.704(4)	18.540(5)	6.495(2)	2132	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	90Kro1
NAT1993b01	18.2929(7)	18.6407(9)	6.5871(6)	2246	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	93Stu2
NAT1994a03	18.11287(8)	18.63331(8)	6.56618(3)	2216	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	94Sta1
NAT1994a04	18.2807(4)	18.7242(4)	6.5484(2)	2241	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	94Sta1
NAT1994a05	18.0812(2)	18.5758(2)	6.56504(6)	2205	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	94Sta1

Table NAT.2.2 (NAT-IV.1, *F d d* 2, continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT1994a06	18.6180(9)	19.0312(9)	6.5421(3)	2318	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	94Sta1
NAT1994b66	18.2980(6)	18.7219(7)	6.5571(2)	2246	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	510	94Sta2
NAT1994b67	18.2808(8)	18.7155(8)	6.5607(3)	2245	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	515	94Sta2
NAT1994b68	18.2122(9)	18.6876(9)	6.5616(3)	2233	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	521	94Sta2
NAT1994b69	18.1892(6)	18.6719(6)	6.5623(2)	2229	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	527	94Sta2
NAT1994b70	18.1785(6)	18.6595(6)	6.5626(2)	2226	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	533	94Sta2
NAT1994b71	18.1671(5)	18.6452(5)	6.5626(2)	2223	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	539	94Sta2
NAT1994b72	18.1559(5)	18.6329(5)	6.5621(2)	2220	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	545	94Sta2
NAT1994b73	18.1419(5)	18.6171(5)	6.5616(2)	2216	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	551	94Sta2
NAT1994b74	18.1311(6)	18.6064(6)	6.5610(2)	2213	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	557	94Sta2
NAT1994b75	18.1238(6)	18.5979(6)	6.5606(2)	2211	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	563	94Sta2
NAT1994b76	18.1154(5)	18.5883(6)	6.5599(2)	2209	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	570	94Sta2
NAT1994b77	18.1091(5)	18.5821(6)	6.5594(2)	2207	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	576	94Sta2
NAT1994b78	18.1039(6)	18.5763(6)	6.5589(2)	2206	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	582	94Sta2
NAT1995b01	18.347(7)	18.561(4)	6.587(4)	2243	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	95Alb1
NAT1995d01	18.2984(7)	18.6502(8)	6.5589(3)	2238	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	95Fin1
NAT1996a06	17.32(1)	17.64(2)	6.416(2)	1960	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	823	96Bau1
NAT1996a07	17.33(2)	17.55(2)	6.385(3)	1942	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	573	96Bau1
NAT1996a08	18.22(2)	18.33(2)	6.536(7)	2184	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	96Bau1
NAT1996c01	18.288(2)	18.631(2)	6.583(1)	2243	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	298	96Ghe1
NAT1999a01	18.334(3)	18.606(3)	6.602(1)	2252	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	99Men1
NAT2001a01	18.226(2)	18.583(2)	6.579(1)	2228	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [1]	2001Lee1
NAT2001a02	18.180(4)	18.531(4)	6.566(2)	2212	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s . [2]	2001Lee1
NAT2001a03	18.390(6)	18.829(6)	6.547(2)	2267	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [3]	2001Lee1
NAT2001a04	18.378(3)	18.818(3)	6.545(1)	2264	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [4]	2001Lee1
NAT2001a05	18.233(3)	18.679(3)	6.530(1)	2224	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [5]	2001Lee1
NAT2001a06	18.097(2)	18.518(2)	6.512(1)	2182	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [6]	2001Lee1
NAT2001a07	17.924(2)	18.325(2)	6.487(1)	2131	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [7]	2001Lee1
NAT2002a01	18.226(2)	18.583(2)	6.579(1)	2228	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [1]	2002Lee1
NAT2002a02	18.180(4)	18.531(4)	6.566(2)	2212	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [2]	2002Lee1
NAT2002a03	18.390(6)	18.829(6)	6.547(2)	2267	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [3]	2002Lee1

[1] at 0.40 GPa [2] at 0.84 GPa [3] at 1.51 GPa [4] at 1.72 GPa [5] at 2.42 GPa [6] at 3.58 GPa [7] at 5.01 GPa

Table NAT.2.2 (NAT-IV.1, *F d d* 2, continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT2002a04	18.378(3)	18.818(3)	6.545(1)	2264	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [1)]	2002Lee1
NAT2002a05	18.233(3)	18.679(3)	6.530(1)	2224	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [2)]	2002Lee1
NAT2002a06	18.097(2)	18.518(2)	6.512(1)	2182	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [3)]	2002Lee1
NAT2002a07	17.924(2)	18.325(2)	6.487(1)	2131	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [4)]	2002Lee1
NAT2003a01	18.400(1)	18.842(1)	6.6539(4)	2307	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	2003Lee1
NAT2003a02	18.357(1)	18.802(1)	6.6386(4)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [5)]	2003Lee1
NAT2003a03	18.482(3)	18.991(3)	6.6254(7)	2325	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [6)]	2003Lee1
NAT2003a04	18.476(1)	18.998(1)	6.6334(4)	2328	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [7)]	2003Lee1
NAT2003a05	18.454(1)	18.976(1)	6.6306(4)	2322	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [8)]	2003Lee1
NAT2003a06	18.398(1)	18.911(1)	6.6258(4)	2305	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [9)]	2003Lee1
NAT2003a07	18.342(1)	18.853(1)	6.6162(4)	2288	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [10)]	2003Lee1
NAT2003a08	18.276(1)	18.783(1)	6.6065(4)	2268	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [11)]	2003Lee1
NAT2003a09	18.197(1)	18.695(1)	6.5958(4)	2244	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [12)]	2003Lee1
NAT2003a10	18.111(1)	18.597(1)	6.5817(4)	2217	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [13)]	2003Lee1
NAT2003a11	18.041(1)	18.508(1)	6.5711(4)	2194	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [14)]	2003Lee1
NAT2004b01	18.4277(7)	18.8567(7)	6.5528(3)	2277	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT [15)]	2004Lee1
NAT2004b02	18.6981(7)	19.0339(6)	6.5193(2)	2320	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	473 [15)]	2004Lee1
NAT2005d01	18.2126(9)	18.5695(9)	6.5741(4)	2223	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [16)]	2005Ser1
NAT2005e01	18.2933(11)	18.6282(12)	6.5839(4)	2244	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	2005Col1
NAT2005e02	18.394(4)	18.8296(26)	6.5463(10)	2267	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [17)]	2005Col1
NAT2006b01	18.2933(11)	18.6282(12)	6.5839(4)	2244	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	300	2006Dem1
NAT2006b02	18.2933(11)	18.6282(12)	6.5839(4)	2244	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	50	2006Dem1
NAT2006b03	18.394(4)	18.8296(26)	6.5463(10)	2267	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	300 [4)]	2006Dem1
NAT2006b04	18.394(4)	18.8296(26)	6.5463(10)	2267	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	50 [4)]	2006Dem1
NAT-XII.1.1, *F d d* 2									
NAT1972a04	18.410(3)	56.674(7)	6.547(2)	6831	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	72Adi1
NAT1986c01	18.4049(8)	56.655(6)	6.5443(4)	6824	¼, ¼, 0	**a**, **b**, **c**	*x*+¼, *y*+¼, *z*	294	86Art1
NAT1994a01	18.4071(4)	56.668(1)	6.5464(2)	6828	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	293	94Sta1
NAT1994a02	18.3586(8)	56.537(2)	6.5373(3)	6785	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	293	94Sta1
NAT1994b41	18.4075(6)	56.651(2)	6.5455(2)	6826	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	383	94Sta2

[1)] at 1.72 GPa [2)] at 2.42 GPa [3)] at 3.58 GPa [4)] at 5.01 GPa [5)] at 0.35 GPa [6)] at 0.61 GPa [7)] at 0.90 GPa [8)] at 1.18 GPa [9)] at 1.55 GPa
[10)] at 1.91 GPa [11)] at 2.43 GPa [12)] at 2.79 GPa [13)] at 3.78 GPa [14)] at 4.46 GPa [15)] at 1.7 GPa [16)] at 0.9 GPa [17)] at 1.87 GPa

Table NAT.2.2 (NAT-IV.1, *F d d* 2, continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT1994b42	18.4081(5)	56.653(2)	6.5457(2)	6826	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	388	94Sta2
NAT1994b43	18.4081(6)	56.655(2)	6.5459(2)	6827	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	392	94Sta2
NAT1994b44	18.4084(5)	56.654(2)	6.5462(2)	6827	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	397	94Sta2
NAT1994b45	18.4092(5)	56.656(2)	6.5466(2)	6828	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	401	94Sta2
NAT1994b46	18.4096(5)	56.656(2)	6.5471(2)	6829	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	406	94Sta2
NAT1994b47	18.4098(5)	56.656(2)	6.5473(2)	6829	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	410	94Sta2
NAT1994b48	18.4098(5)	56.656(2)	6.5477(2)	6829	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	415	94Sta2
NAT1994b49	18.4096(5)	56.657(2)	6.5481(2)	6830	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	420	94Sta2
NAT1994b50	18.4085(6)	56.654(2)	6.5484(2)	6829	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	425	94Sta2
NAT1994b51	18.4074(6)	56.651(2)	6.5488(2)	6829	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	430	94Sta2
NAT1994b52	18.4054(5)	56.648(2)	6.5493(2)	6828	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	435	94Sta2
NAT1994b53	18.4032(6)	56.641(2)	6.5498(2)	6827	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	440	94Sta2
NAT1994b54	18.3998(6)	56.634(2)	6.5502(2)	6826	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	445	94Sta2
NAT1994b55	18.3966(5)	56.624(2)	6.5510(2)	6824	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	450	94Sta2
NAT1994b56	18.3914(6)	56.613(2)	6.5514(2)	6821	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	455	94Sta2
NAT1994b57	18.3850(6)	56.595(2)	6.5522(2)	6818	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	460	94Sta2
NAT1994b58	18.3767(6)	56.574(2)	6.5528(2)	6813	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	466	94Sta2
NAT1994b59	18.3703(6)	56.558(2)	6.5536(2)	6809	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	471	94Sta2
NAT1994b60	18.3603(6)	56.531(2)	6.5546(2)	6803	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	476	94Sta2
NAT1994b61	18.3483(6)	56.499(2)	6.5553(2)	6796	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	482	94Sta2
NAT1994b62	18.3350(6)	56.460(2)	6.5561(2)	6787	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	487	94Sta2
NAT1994b63	18.3176(8)	56.396(2)	6.5575(3)	6774	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	493	94Sta2
NAT1994b64	18.3049(8)	56.243(2)	6.5569(3)	6750	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	498	94Sta2
NAT1994b65	18.3042(7)	56.189(2)	6.5565(2)	6743	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	504	94Sta2
NAT2000c01[1])	18.412(2)	56.670(5)	6.548(1)	6832	¼, ¼, 0	**a**, **b**, **c**	*x*-¼, *y*-¼, *z*	RT	2000Stu1

[1]) Lattice constants from personal communication by A. Kirfel.

Table NAT.2.2 (continued)

NAT-VIII.1.2, *Fd*1 1

code	*a* [Å]	*b* [Å]	*c* [Å]	α [°]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT1972a03	18.604(3)	18.871(4)	6.529(2)	89.84(5)	2292	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	298	72Adi1
NAT1979a01	18.956(2)	18.482(2)	6.5174(4)	89.366(9)	2283	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*x*, *y*, *z*	n.s.	79Fäl1
NAT1984d01	18.96(1)	18.50(3)	6.521(4)	90.5(2)	2287	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*x*, *y*, *z*	n.s.	84Smi1
NAT1984d02	18.968(1)	18.4971(9)	6.5222(4)	90.618(5)	2288	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*x*, *y*, *z*	n.s.	84Smi1
NAT1985a01	18.948(3)	18.461(2)	6.516(2)	89.48(2)	2279	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*x*, *y*, *z*	20	85Kvi1
NAT1994b21	18.1465(7)	18.8604(7)	6.5396(3)	88.986(2)	2238	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	489	94Sta2
NAT1994b22	18.1391(6)	18.8598(6)	6.5396(2)	88.966(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	494	94Sta2
NAT1994b23	18.1373(6)	18.8601(6)	6.5400(2)	88.957(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	500	94Sta2
NAT1994b24	18.1353(6)	18.8591(6)	6.5402(2)	88.948(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	505	94Sta2
NAT1994b25	18.1350(6)	18.8589(6)	6.5404(2)	88.941(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	511	94Sta2
NAT1994b26	18.1348(6)	18.8577(6)	6.5406(2)	88.931(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	517	94Sta2
NAT1994b27	18.1353(6)	18.8574(6)	6.5408(2)	88.925(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	523	94Sta2
NAT1994b28	18.1353(6)	18.8572(6)	6.5413(2)	88.917(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	529	94Sta2
NAT1994b29	18.1367(6)	18.8575(6)	6.5417(2)	88.908(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	535	94Sta2
NAT1994b30	18.1368(6)	18.8573(6)	6.5420(2)	88.902(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	541	94Sta2
NAT1994b31	18.1371(6)	18.8554(6)	6.5424(2)	88.894(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	547	94Sta2
NAT1994b32	18.1374(6)	18.8556(6)	6.5428(2)	88.886(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	553	94Sta2
NAT1994b33	18.1369(6)	18.8543(6)	6.5428(2)	88.879(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	559	94Sta2
NAT1994b34	18.1364(6)	18.8533(6)	6.5426(2)	88.880(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	565	94Sta2
NAT1994b35	18.1368(6)	18.8543(6)	6.5429(2)	88.882(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	571	94Sta2
NAT1994b36	18.1377(6)	18.8526(6)	6.5432(2)	88.868(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	578	94Sta2
NAT1994b37	18.1369(6)	18.8495(6)	6.5442(2)	88.851(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	584	94Sta2
NAT1994b38	18.1361(6)	18.8478(6)	6.5446(2)	88.843(2)	2237	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	590	94Sta2
NAT1994b39	18.1350(6)	18.8451(6)	6.5448(2)	88.838(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	597	94Sta2
NAT1994b40	18.1332(6)	18.8443(6)	6.5444(2)	88.840(2)	2236	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	603	94Sta2
NAT2002b01	19.030(3)	18.481(7)	6.533(2)	90.54(3)	2298	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*y*-1/8, 1/2*z*-1/4, *x*-1/2*z*+1/4	n.s.	2002Com1
NAT2002b02	18.804(5)	18.30(1)	6.471(4)	90.35(7)	2226	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*y*-1/8, 1/2*z*-1/4, *x*-1/2*z*+1/4	n.s. [1]	2002Com1
NAT2002b03	18.631(6)	18.16(1)	6.430(4)	90.11(7)	2175	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*y*-1/8, 1/2*z*-1/4, *x*-1/2*z*+1/4	n.s. [2]	2002Com1

[1] at 1.77 GPa [2] at 3.38 GPa

Table NAT.2.2 (NAT-VIII.1.2, *F d* 1 1, continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	α [°]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT2002b04	18.842(4)	18.550(7)	6.542(2)	90.52(4)	2286	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*y*-1/8, 1/2*z*-1/4, *x*-1/2*z*+1/4	n.s.	2002Com1
NAT2005b01	19.293(1)	18.881(2)	6.4800(4)	88.46(1)	2360	0, 1/8, 1/2	**b**, **a**+2**c**, **a**	*y*-1/8, 1/2*z*-1/4, *x*-1/2*z*+1/4	n.s. [1)]	2005Lee2

NAT-VIII.1.3, *F* 1 *d* 1

code	*a* [Å]	*b* [Å]	*c* [Å]	β [°]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT1972a01	18.503(3)	18.966(4)	6.531(2)	90.62(5)	2292	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	72Adi1
NAT1972a02	18.503(3)	18.966(4)	6.531(2)	90.62(5)	2292	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	72Adi1
NAT1984c01	18.508(5)	18.981(5)	6.527(2)	90.64(1)	2293	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	84Jos1
NAT1994b01	18.5106(5)	18.9641(5)	6.5225(2)	90.700(2)	2289	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	380	94Sta2
NAT1994b02	18.5109(5)	18.9639(6)	6.5227(2)	90.708(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	384	94Sta2
NAT1994b03	18.5119(5)	18.9637(5)	6.5229(2)	90.715(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	389	94Sta2
NAT1994b04	18.5121(5)	18.9632(5)	6.5230(2)	90.723(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	393	94Sta2
NAT1994b05	18.5136(5)	18.9633(5)	6.5237(2)	90.734(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	398	94Sta2
NAT1994b06	18.5148(6)	18.9634(6)	6.5243(2)	90.743(2)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	402	94Sta2
NAT1994b07	18.5152(5)	18.9622(5)	6.5247(2)	90.755(2)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	407	94Sta2
NAT1994b08	18.5150(6)	18.9610(6)	6.5254(2)	90.770(2)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	412	94Sta2
NAT1994b09	18.5153(5)	18.9597(6)	6.5262(2)	90.784(2)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	416	94Sta2
NAT1994b10	18.5137(6)	18.9562(6)	6.5269(2)	90.799(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	421	94Sta2
NAT1994b11	18.5114(6)	18.9517(6)	6.5273(2)	90.820(2)	2290	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	426	94Sta2
NAT1994b12	18.5090(6)	18.9464(6)	6.5287(2)	90.843(2)	2289	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	431	94Sta2
NAT1994b13	18.5040(6)	18.9390(6)	6.5295(2)	90.872(2)	2288	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	436	94Sta2
NAT1994b14	18.4971(6)	18.9293(6)	6.5303(2)	90.901(2)	2286	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	441	94Sta2
NAT1994b15	18.4910(6)	18.9193(6)	6.5315(2)	90.932(2)	2285	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	446	94Sta2
NAT1994b16	18.4824(6)	18.9047(6)	6.5328(2)	90.971(2)	2282	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	451	94Sta2
NAT1994b17	18.4702(6)	18.8872(6)	6.5338(2)	91.009(2)	2279	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	456	94Sta2
NAT1994b18	18.4540(6)	18.8625(6)	6.5356(2)	91.053(2)	2275	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	462	94Sta2
NAT1994b19	18.4355(6)	18.8388(6)	6.5368(2)	91.088(2)	2270	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	467	94Sta2
NAT1994b20	18.4227(6)	18.8200(6)	6.5379(2)	91.113(2)	2266	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	472	94Sta2
NAT1997a01	18.502(1)	18.974(2)	6.525(1)	90.615(7)	2291	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s.	97Stu1
NAT1998a01	18.489(2)	18.959(2)	6.519(1)	90.61(1)	2285	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	98Kun1

[1)] at 0.99 GPa

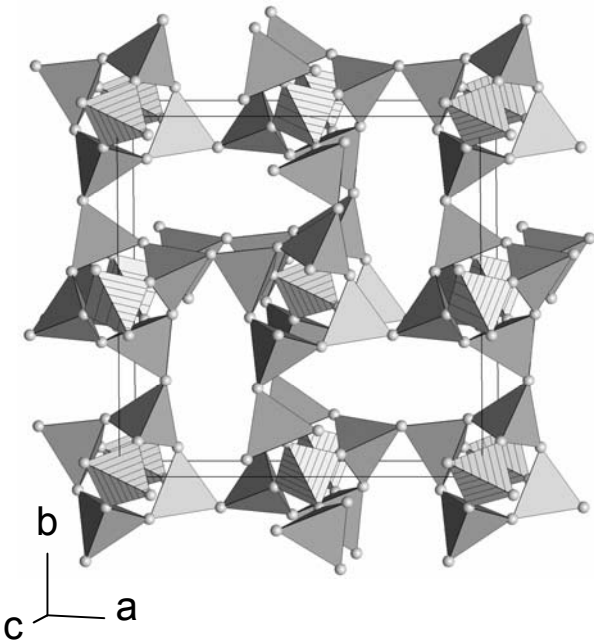
Table NAT.2.2 (NAT-VIII.1.3, *F* 1 *d* 1, continued)

code	*a* [Å]	*b* [Å]	*c* [Å]	β [°]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT2004a01	18.971(4)	19.204(3)	6.595(1)	91.60(2)	2402	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	2004Ser1
NAT2005d02	18.8971(6)	19.3142(6)	6.4833(2)	91.584(3)	2365	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	n.s. [1)]	2005Ser1
NAT-VIII.1.4, *F* 1 1 2										
code	*a* [Å]	*b* [Å]	*c* [Å]	γ [°]	*V* [Å^3]	shift	matrix	coord. trans.	*T* [K]	reference
NAT1983c01	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	83Alb1
NAT1985b01	18.055(2)	18.055(2)	6.727(1)	90	2193	½, 0, ¼	**a**+**b**, -**a**+**b**, **c**	½(*x*+*y*)-¼, ½(-*x*+*y*)+¼, *z*-¼	-	85Kla1
NAT1987a01	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a02	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a03	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a04	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a05	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a06	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a07	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a08	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a09	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1987a10	16.01	16.73	6.40	90	1714	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	-	87Dem1
NAT1991a06	18.153(1)	18.480(1)	6.6224(4)	91.124(7)	2221	¼, ¼, 0.0228	**a**+**b**, -**a**+**b**, **c**	½(*x*+*y*)-¼, ½(-*x*+*y*), *z*-0.0228	n.s.	91Art1
NAT1995a01	16.28(2)	17.045(9)	6.434(4)	90.08(6)	1785	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	548	95Jos1
NAT1996a01	16.223(7)	17.03(2)	6.438(3)	90.01(6)	1779	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	598	96Bau1
NAT1996a02	16.24(1)	17.02(1)	6.429(2)	90.02(7)	1777	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	573	96Bau1
NAT1996a03	16.58(2)	17.43(1)	6.461(1)	90.03(8)	1866	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	723	96Bau1
NAT1996a04	16.74(2)	17.62(1)	6.465(1)	90.03(7)	1907	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	773	96Bau1
NAT1996a05	16.29(2)	17.08(1)	6.449(2)	90.04(9)	1795	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	573	96Bau1
NAT-XVI.1.4, *C* 1 1 2_1										
NAT1992a01	17.899(2)	18.390(2)	6.529(1)	90.00(1)	2149	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	92Stu1
NAT1993a01	17.899(2)	18.390(2)	6.529(1)	90.00(1)	2149	0, 0, 0	**a**, **b**, **c**	*x*, *y*, *z*	RT	93Stu1
NAT1996b01	18.474(4)	17.912(6)	6.542(2)	90.00(1)	2165	0, 0, 0	**b**, -**a**, **c**	*y*, -*x*, *z*	RT	96Stu1

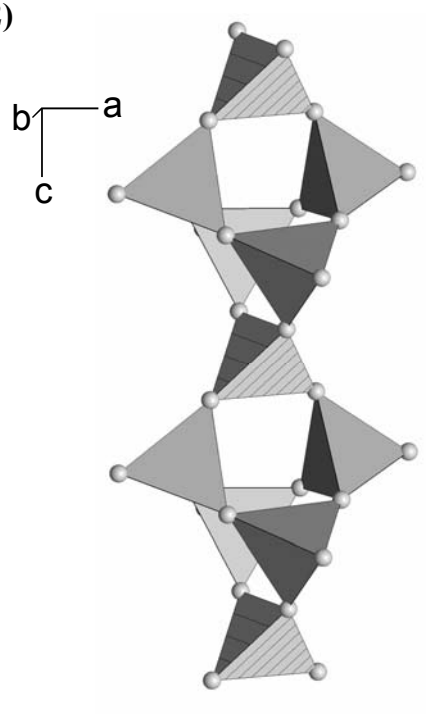
[1)] at 1.0 GPa

NAT.3 Framework structures

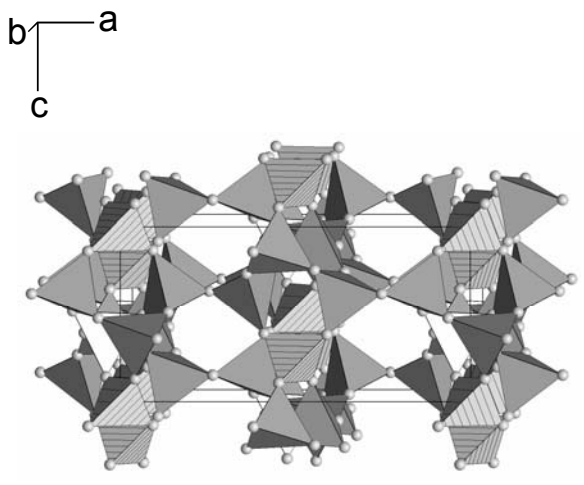
NAT.3.1 NAT-II compounds ($I\bar{4}2d$, IT #122)



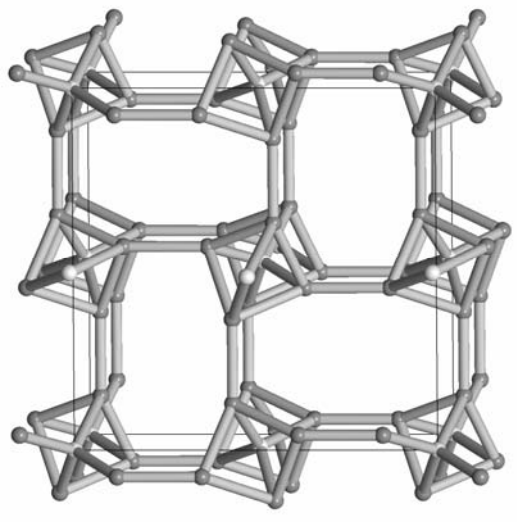
a Polyhedral representation. $(Al,Si)O_4$ tetrahedra are hatched. View parallel **c** rotated by 5° about **a** and **b**.



b The natrolite chain (**fib** unit). View parallel **b** rotated by 10° about **a** and 2° about **c**.



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



d Ball and stick model corresponding to a).

Fig. NAT.3.1.1 Projections of the NAT-II crystal structure of tetranatrolite $Na_8 \cdot Al_8Si_{12}O_{40} \cdot 8H_2O$ (NAT1995c01, 95Ras1).

Table NAT.3.1.1 Atomic coordinates and site definitions for tetranatrolite $Na_8 \cdot Al_8Si_{12}O_{40} \cdot 8H_2O$ (NAT1995c01, 95Ras1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
(Si,Al)1	-0.0576(2)	0.8662(2)	0.6209(6)	0.7(1)	1	16(e)	8 / 8
Si2	0	0	0	0.7(1)	$\bar{4}$ . .	4(a)	4
O1	-0.0448(7)	0.9090(6)	0.864(2)	1.6(2)	1	16(e)	16
O2	0.1381(8)	0.0589(7)	0.487(2)	1.9(2)	1	16(e)	16
O3	0.8878(9)	3/4	5/8	1.2(2)	. 2 .	8(d)	8
Na1	0.6895(6)	1/4	1/8	2.1(1)	. 2 .	8(d)	8
OW1	0.132(1)	¼	1/8	2.5(3)	. 2 .	8(d)	8
H1	0.07(1)	0.21(1)	0.03(3)	3	1	16(e)	16

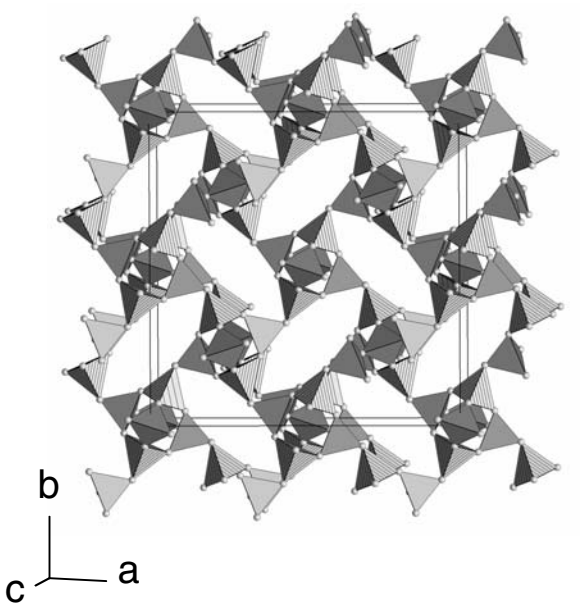
Table NAT.3.1.2 Selected interatomic distances and angles for tetranatrolite $Na_8 \cdot Al_8Si_{12}O_{40} \cdot 8H_2O$ (NAT1995c01, 95Ras1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
(Si,Al)1 - O3	1.678(6)	129.7(7)	Si2 - O1	1.599(10)	143.7(7)
(Si,Al)1 - O2	1.681(10)	136.6(7)	Si2 - O1	1.599(10)	143.7(7)
(Si,Al)1 - O2	1.686(11)	136.6(7)	Si2 - O1	1.599(10)	143.7(7)
(Si,Al)1 - O1	1.703(13)	143.7(7)	Si2 - O1	1.599(10)	143.7(7)
mean	1.687	136.7	mean	1.599	143.7

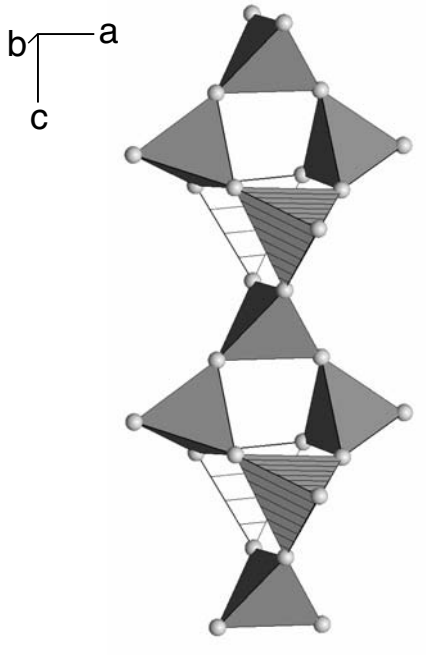
NAT.3.2 NAT-IV compounds (*F d d* 2, IT #43)

Table NAT.3.2.1 Atomic coordinates and site definitions for natrolite $Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$ (NAT1993b01, 93Stu2).

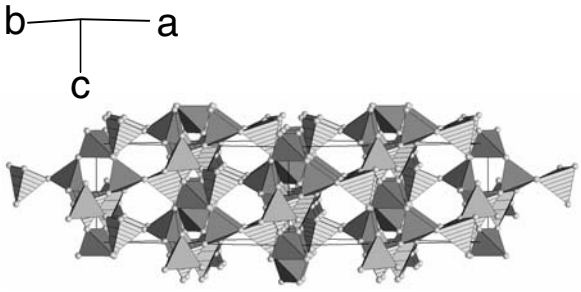
atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al 11	0.46261(1)	0.40626(1)	0.61525(2)	0.48	1	16(b)	16
Si12	0.34677(1)	0.78865(1)	0.12273(2)	0.46	1	16(b)	16
Si2	0	0	0	0.53	. . 2	8(a)	8
O11	0.47731(2)	0.43147(1)	0.86619(5)	1.14	1	16(b)	16
O12	0.31965(1)	0.77267(2)	0.89022(4)	1.17	1	16(b)	16
O21	0.09850(1)	0.03512(1)	0.50019(5)	1.04	1	16(b)	16
O22	0.70637(1)	0.15267(2)	0.22579(4)	1.03	1	16(b)	16
O3	0.42990(1)	0.31817(1)	0.60974(4)	0.68	1	16(b)	16
Na1	0.22074(1)	0.03077(1)	0.61761(4)	1.32	1	16(b)	16
OW1	0.05648(2)	0.18951(2)	0.11087(7)	1.75	1	16(b)	16
H1	0.0520(7)	0.1440(6)	0.057(2)	4.34	1	16(b)	16
H2	0.1010(6)	0.1883(6)	0.161(2)	4.34	1	16(b)	16



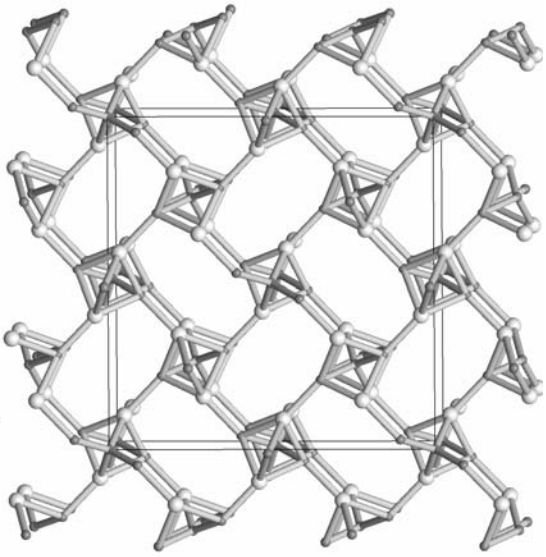
a Polyhedral representation. AlO_4 tetrahedra are hatched. View parallel **c** rotated by 4° about **a** and **b**.



b The natrolite chain (**fib** unit). View parallel **b** rotated by 5° about **a** and 1° about **c**.



c Polyhedral representation. View parallel [110] rotated by 1° about [1 $\bar{1}$ 0] and [001]. Scale is 84 % of a).



d Ball and stick model corresponding to a).

Fig. NAT.3.2.1 Projections of the NAT-IV crystal structure of natrolite $Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$ (NAT1993b01, 93Stu2).

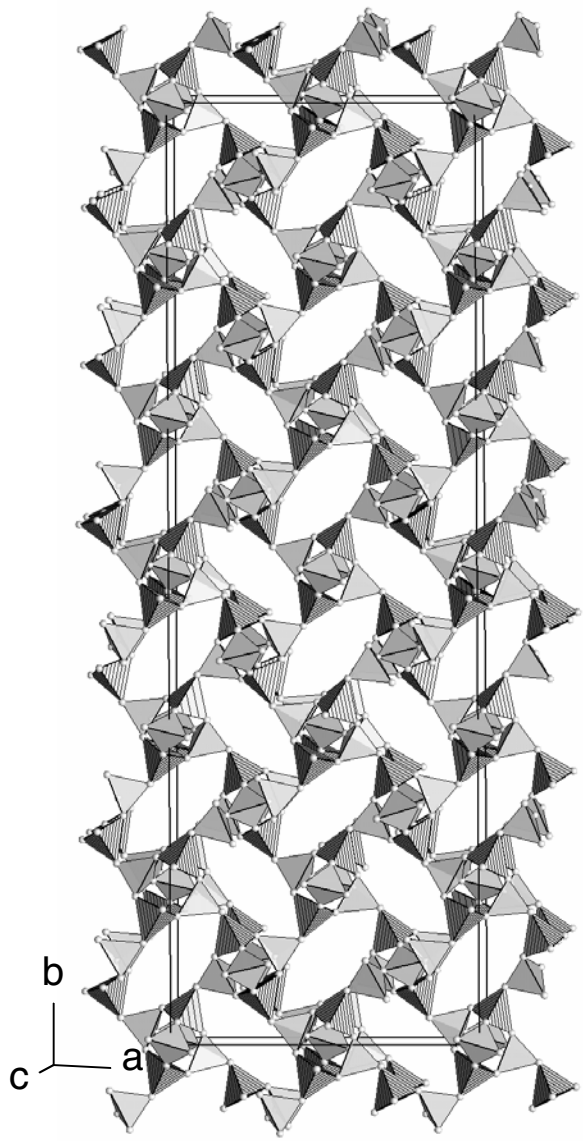
Table NAT.3.2.2 Selected interatomic distances and angles for natrolite $Na_{16} \cdot Al_{16}Si_{24}O_{80} \cdot 16H_2O$ (NAT1993b01, 93Stu2).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 1 - O21	1.7373(3)	138.71(1)	Si12 - O21	1.6115(3)	138.71(1)
Al 1 - O11	1.7394(4)	140.91(2)	Si12 - O22	1.6132(3)	135.02(1)
Al 1 - O22	1.7449(3)	135.02(1)	Si12 - O3	1.6196(2)	129.76(1)
Al 1 - O3	1.7479(2)	129.76(1)	Si12 - O12	1.6372(3)	144.53(2)
mean	1.7424	136.10	mean	1.6204	137.01
Si2 - O11	1.6066(3)	140.91(2)			
Si2 - O11	1.6066(3)	140.91(2)			
Si2 - O12	1.6294(3)	144.53(2)			
Si2 - O12	1.6294(3)	144.53(2)			
mean	1.6180	142.72			

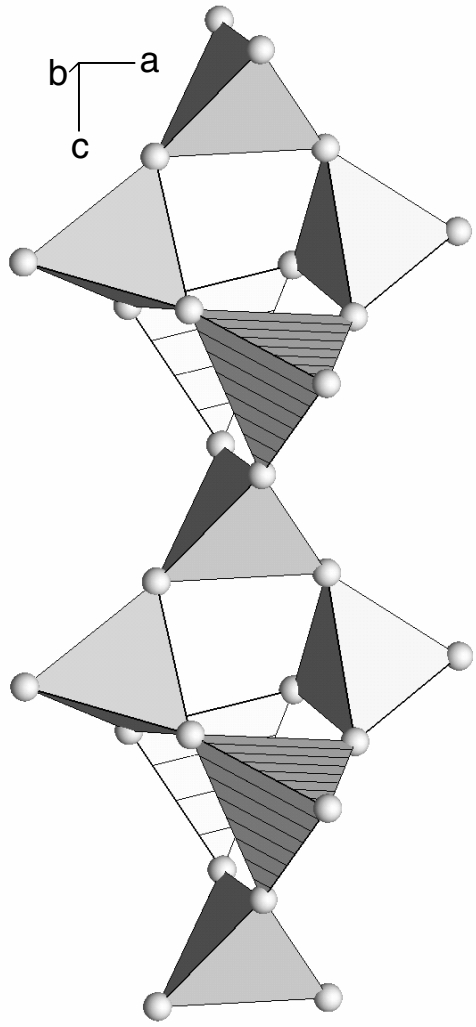
NAT.3.3 NAT-XII.1 compounds (*F d d* 2 , IT #43)

Table NAT.3.3.2 Selected interatomic distances and angles for mesolite, $Na_{15.92}Ca_{16.32} \cdot Al_{48.00}Si_{71.84}O_{240} \cdot 64H_2O$ (NAT2000c01, 2000Stu1).

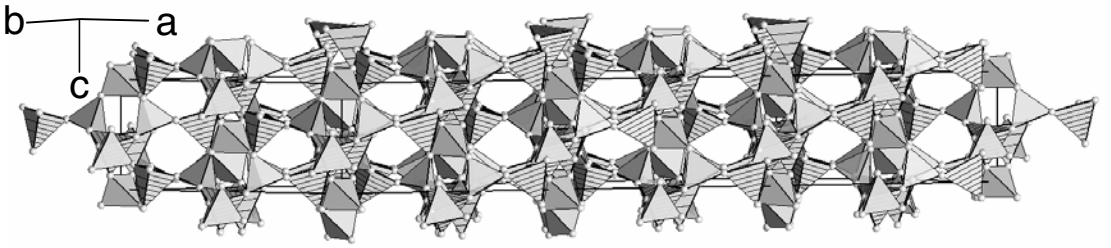
	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11a - O22b	1.731(1)	136.4(1)	Al 11b - O21a	1.727(1)	143.2(1)
Al 11a - O21b	1.737(1)	129.5(1)	Al 11b - O32	1.733(1)	134.5(1)
Al 11a - O11a	1.739(1)	148.0(1)	Al 11b - O11b	1.736(1)	139.4(1)
Al 11a - O31	1.741(1)	136.7(1)	Al 11b - O22c	1.763(1)	126.7(1)
mean	1.737	137.8	mean	1.740	136.0
Al 11c - O22a	1.744(1)	135.1(1)	Si12a - O21a	1.606(1)	143.2(1)
Al 11c - O33	1.748(1)	131.5(1)	Si12a - O33	1.611(1)	131.5(1)
Al 11c - O11c	1.749(1)	133.2(1)	Si12a - O22c	1.630(1)	126.7(1)
Al 11c - O21c	1.756(1)	135.2(1)	Si12a - O12a	1.633(1)	144.1(1)
mean	1.749	133.8	mean	1.620	136.4
Si12b - O22b	1.599(1)	136.4(1)	Si12c - O21b	1.611(1)	129.5(1)
Si12b - O31	1.614(1)	136.7(1)	Si12c - O22a	1.617(1)	135.1(1)
Si12b - O21c	1.634(1)	135.2(1)	Si12c - O32	1.620(1)	134.5(1)
Si12b - O12b	1.643(1)	133.4(1)	Si12c - O12c	1.629(1)	153.6(1)
mean	1.622	135.4	mean	1.619	138.2
Si21 - O11b	1.605(1)	139.4(1)	Si22 - O11a	1.596(1)	148.0(1)
Si21 - O11b	1.605(1)	139.4(1)	Si22 - O11c	1.612(1)	133.2(1)
Si21 - O12a	1.633(1)	144.1(1)	Si22 - O12c	1.618(1)	153.6(1)
Si21 - O12a	1.633(1)	144.1(1)	Si22 - O12b	1.644(1)	133.4(1)
mean	1.619	141.8	mean	1.618	142.1



a Polyhedral representation. AlO_4 tetrahedra are hatched. View parallel **c** rotated by 4° about **a** and **b**.



b The natrolite chain (**fib** unit). View parallel **b** rotated by 5° about **a** and 1° about **c**.



c Polyhedral representation. View approximately parallel [310].

Fig. NAT.3.3.1 Projections of the NAT-XII.1 crystal structure of mesolite, $Na_{15.92}Ca_{16.32} \cdot Al_{48.00}Si_{71.84}O_{240} \cdot 64H_2O$ (NAT2000c01, 2000Stu1).

Table NAT.3.3.1 Atomic coordinates and site definitions for mesolite, $Na_{15.92}Ca_{16.32} \cdot Al_{48.00}Si_{71.84}O_{240} \cdot 64H_2O$ (NAT2000c01, 2000Stu1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al11a	0.45151(2)	0.13765(1)	0.6430(1)	0.52	1	16(b)	16
Al11b	0.46308(2)	0.46976(1)	0.6131(1)	0.50	1	16(b)	16
Al11c	0.46373(2)	0.80211(1)	0.6430(1)	0.52	1	16(b)	16
Si12a	0.34500(2)	0.26431(1)	0.1222(1)	0.49	1	16(b)	16
Si12b	0.33791(2)	0.59687(1)	0.1522(1)	0.52	1	16(b)	16
Si12c	0.34815(2)	0.93021(1)	0.1506(1)	0.50	1	16(b)	16
Si21	0	0	0	0.55	. . 2	8(a)	8
Si22	-0.00431(2)	0.33181(1)	0.0275(1)	0.53	1	16(b)	16
O11a	0.48495(6)	0.14682(2)	0.8783(2)	1.16	1	16(b)	16
O11b	0.48192(6)	0.47711(2)	0.8649(2)	1.02	1	16(b)	16
O11c	0.47710(5)	0.80807(2)	0.9023(2)	0.95	1	16(b)	16
O12a	0.31979(5)	0.25698(2)	0.8916(2)	1.04	1	16(b)	16
O12b	0.32621(5)	0.58890(2)	0.9132(2)	0.94	1	16(b)	16
O12c	0.31269(5)	0.92206(2)	0.9339(2)	1.05	1	16(b)	16
O21a	0.09344(5)	0.00870(2)	0.5153(2)	0.97	1	16(b)	16
O21b	0.11068(5)	0.34186(2)	0.5516(2)	0.97	1	16(b)	16
O21c	0.09621(5)	0.67664(2)	0.5447(2)	0.90	1	16(b)	16
O22a	0.70582(5)	0.05064(2)	0.2530(2)	1.01	1	16(b)	16
O22b	0.72813(5)	0.38646(2)	0.2179(2)	0.99	1	16(b)	16
O22c	0.70948(5)	0.71538(2)	0.2093(2)	0.87	1	16(b)	16
O31	0.41645(5)	0.10931(2)	0.6711(2)	0.79	1	16(b)	16
O32	0.42641(5)	0.44166(2)	0.5965(2)	0.70	1	16(b)	16
O33	0.42741(5)	0.77381(2)	0.6136(2)	0.71	1	16(b)	16
Na1	0.71747(3)	0.51095(1)	0.6316(2)	1.51	1	16(b)	16
Ca1	-0.02197(1)	0.57739(1)	0.8815(1)	0.92	1	16(b)	16
OW60	0.5315(1)	0.56608(3)	0.0760(3)	2.79	1	16(b)	16
OW61	-0.04922(8)	0.59820(3)	0.1835(3)	2.46	1	16(b)	16
OW62	0.80341(7)	0.51845(2)	0.3771(3)	1.67	1	16(b)	16
OW7	0.56792(6)	0.60685(2)	0.3648(3)	2.06	1	16(b)	16
H61	0.523(1)	0.5544(3)	0.009(5)	3.16	1	16(b)	16
H62	0.573(1)	0.5699(7)	0.038(8)	14.21	1	16(b)	16
H63	0.910(1)	0.5935(6)	0.234(6)	11.05	1	16(b)	16
H64	-0.033(1)	0.6068(5)	0.269(4)	4.74	1	16(b)	16
H65	0.796(1)	0.5321(3)	0.316(5)	3.95	1	16(b)	16
H66	0.845(1)	0.5197(4)	0.430(5)	3.95	1	16(b)	16
H71	0.612(1)	0.6040(6)	0.315(8)	11.05	1	16(b)	16
H72	0.555(2)	0.6213(4)	0.330(9)	12.63	1	16(b)	16

NAT.3.4 NAT-VIII.2 compounds (*F d* 1 1, IT #9)

Crystal structure projections are essentially identical with Fig. NAT.3.2.1.

Table NAT.3.4.1 Atomic coordinates and site definitions for scolecite, $Ca_{7.92} \cdot Al_{15.68}Si_{23.92}O_{80} \cdot 16H_2O$ (NAT1972a03, 72Adi1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al11a	0.4563(3)	0.4192(4)	0.615(1)	0.93(9)	1	8(a)	8
Al11b	0.5379(3)	0.5986(4)	0.615(1)	0.93(9)	1	8(a)	8
Si12a	0.3403(3)	0.8007(4)	0.119(1)	0.91(8)	1	8(a)	8
Si12b	0.6563(2)	0.2153(3)	0.129(1)	0.81(8)	1	8(a)	8
Si2	0	0	0	1.03(8)	1	8(a)	8
O11a	0.4810(7)	0.4302(7)	0.874(2)	1.4(2)	1	8(a)	8
O11b	0.5146(7)	0.5665(7)	0.860(2)	1.7(2)	1	8(a)	8
O12a	0.3165(7)	0.7654(7)	0.905(2)	1.3(2)	1	8(a)	8
O12b	0.6759(6)	0.2339(7)	0.886(2)	1.3(2)	1	8(a)	8
O21a	0.1007(6)	0.0381(7)	0.518(2)	1.0(2)	1	8(a)	8
O21b	0.9017(7)	-0.0088(8)	0.541(3)	1.9(2)	1	8(a)	8
O22a	0.7168(7)	0.1600(7)	0.214(2)	1.5(2)	1	8(a)	8
O22b	0.2827(7)	0.8582(8)	0.197(2)	1.6(2)	1	8(a)	8
O31	0.4195(6)	0.3352(7)	0.582(2)	1.1(2)	1	8(a)	8
O32	0.5779(7)	0.6830(7)	0.642(2)	1.3(2)	1	8(a)	8
Ca1	0.2319(2)	0.0288(3)	0.610(1)	1.25(7)	1	8(a)	8
OW1	0.9522(9)	0.8090(9)	0.080(3)	2.8(3)	1	8(a)	8
OW2	0.045(1)	0.222(1)	0.179(3)	1.6(3)	1	8(a)	8

Table NAT.3.4.2 Selected interatomic distances and angles for scolecite, $Ca_{7.92} \cdot Al_{15.68}Si_{23.92}O_{80} \cdot 16H_2O$ (NAT1972a03, 72Adi1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11a - O31	1.74(2)	134(1)	Al 11b - O22b	1.72(2)	130(1)
Al 11a - O22a	1.74(2)	134(1)	Al 11b - O21a	1.75(1)	133(1)
Al 11a - O11a	1.77(2)	131(1)	Al 11b - O11b	1.77(2)	147(1)
Al 11a - O21b	1.77(2)	133(1)	Al 11b - O32	1.77(2)	137(1)
mean	1.76	133	mean	1.75	138
Si12a - O21b	1.59(2)	133(1)	Si12b - O32	1.58(1)	137(1)
Si12a - O22b	1.61(2)	130(1)	Si12b - O22a	1.63(1)	134(1)
Si12a - O12a	1.61(2)	146(1)	Si12b - O21a	1.65(2)	133(1)
Si12a - O31	1.63(1)	134(1)	Si12b - O12b	1.66(2)	137(1)
mean	1.61	136	mean	1.63	135
Si2 - O11b	1.57(1)	147(1)			
Si2 - O11a	1.59(1)	131(1)			
Si2 - O12a	1.62(1)	146(1)			
Si2 - O12b	1.67(1)	137(1)			
mean	1.61	140			

NAT.3.5 NAT-VIII.3 compounds (*F* 1 *d* 1, IT #9)

Crystal structure projections are essentially identical with Fig. NAT.3.2.1.

Table NAT.3.5.1 Atomic coordinates and site definitions for scolecite, $Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 24H_2O$ (NAT1997a01, 97Stu1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al11a	0.45014(1)	0.41292(1)	0.61564(4)	0.49	1	8(a)	8
Al11b	0.53302(1)	0.59168(1)	0.61120(3)	0.46	1	8(a)	8
Si12a	0.33444(1)	0.79244(1)	0.12550(3)	0.45	1	8(a)	8
Si12b	0.64989(1)	0.20685(1)	0.12019(3)	0.46	1	8(a)	8
Si2	0	0.00440(1)	0	0.48	1	8(a)	8
O11a	0.48314(3)	0.43812(2)	0.85594(8)	1.01	1	8(a)	8
O11b	0.51589(3)	0.57450(2)	0.86835(7)	0.92	1	8(a)	8
O12a	0.32178(2)	0.76486(3)	0.88908(7)	0.88	1	8(a)	8
O12b	0.68275(2)	0.23369(3)	0.90256(7)	0.96	1	8(a)	8
O21a	0.09211(2)	0.02626(2)	0.52419(7)	0.85	1	8(a)	8
O21b	0.89248(2)	-0.02049(2)	0.53072(7)	0.97	1	8(a)	8
O22a	0.70456(2)	0.14622(2)	0.20885(8)	0.90	1	8(a)	8
O22b	0.26956(2)	0.84358(2)	0.18755(8)	0.95	1	8(a)	8
O31	0.41280(2)	0.32898(2)	0.64013(7)	0.72	1	8(a)	8
O32	0.57062(2)	0.67464(2)	0.57552(7)	0.68	1	8(a)	8
Ca1	0.47393(1)	0.73179(1)	0.36470(3)	0.87	1	8(a)	8
OW11	0.53024(8)	0.70120(5)	0.0625(2)	2.59	1	8(a)	8
OW12	0.44574(5)	0.79528(6)	0.6629(2)	2.30	1	8(a)	8
OW3	0.56282(4)	0.82040(3)	0.3583(2)	1.92	1	8(a)	8
H11	0.514(3)	0.667(2)	0.006(7)	6.63	1	8(a)	8
H12	0.567(2)	0.727(2)	0.020(6)	4.11	1	8(a)	8
H13	0.421(2)	0.772(2)	0.714(6)	5.05	1	8(a)	8
H14	0.484(3)	0.800(3)	0.728(9)	7.82	1	8(a)	8
H31	0.606(2)	0.819(2)	0.332(5)	3.95	1	8(a)	8
H32	0.550(2)	0.861(2)	0.378(5)	3.63	1	8(a)	8

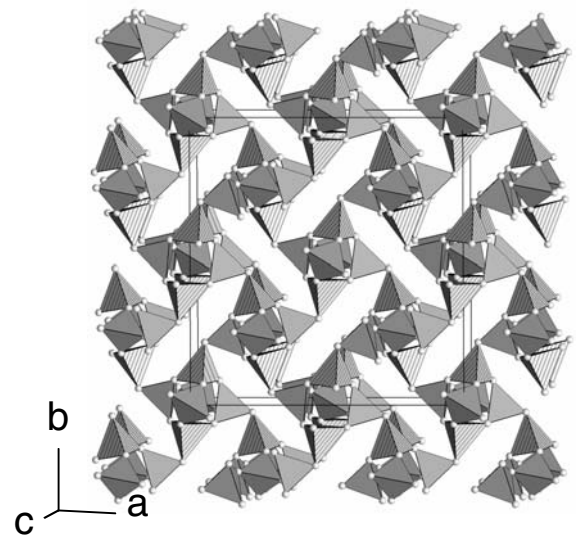
Table NAT.3.5.2 Selected interatomic distances and angles for scolecite, $Ca_8 \cdot Al_{16}Si_{24}O_{80} \cdot 24H_2O$ (NAT1997a01, 97Stu1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11a - O21b	1.740(1)	134.22(3)	Al 11b - O32	1.738(1)	133.14(3)
Al 11a - O11a	1.743(1)	143.97(3)	Al 11b - O11b	1.742(1)	134.74(3)
Al 11a - O31	1.744(1)	138.21(3)	Al 11b - O21a	1.753(1)	135.11(3)
Al 11a - O22b	1.746(1)	133.27(3)	Al 11b - O22a	1.766(1)	127.59(3)
mean	1.743	137.42	mean	1.749	132.65
Si12a - O22b	1.599(1)	133.27(3)	Si12b - O21b	1.605(1)	134.22(3)
Si12a - O31	1.609(1)	138.21(3)	Si12b - O32	1.613(1)	133.14(3)
Si12a - O21a	1.630(1)	135.11(3)	Si12b - O12b	1.632(1)	151.06(3)
Si12a - O12a	1.643(1)	134.12(3)	Si12b - O22a	1.634(1)	127.59(3)
mean	1.620	135.18	mean	1.621	136.50

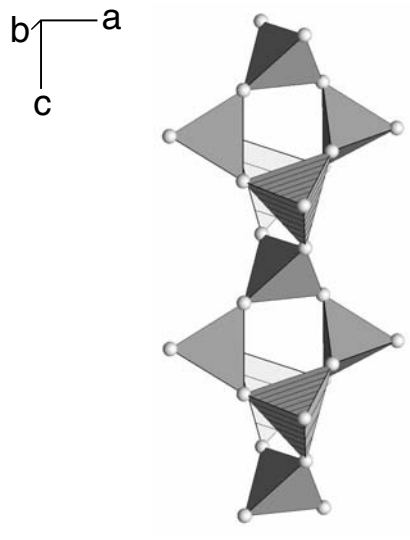
Table NAT.3.5.2 (continued)

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si2 - O11a	1.599(1)	143.97(3)	Si2 - O12b	1.618(1)	151.06(3)
Si2 - O11b	1.612(1)	134.74(3)	Si2 - O12a	1.642(1)	134.12(3)
			mean	1.618	140.97

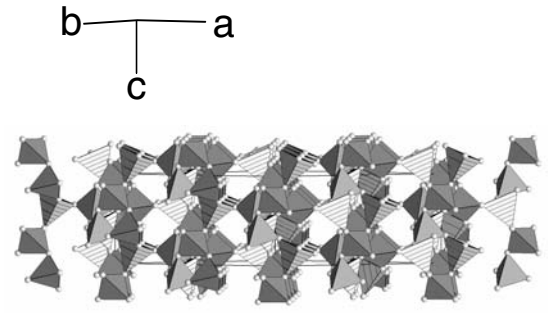
NAT.3.6 NAT.VIII.4 compounds (*F* 1 1 2, IT #5)



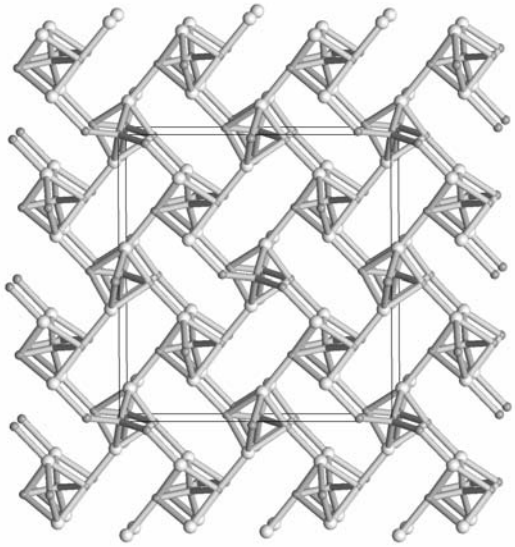
a Polyhedral representation. AlO_4 tetrahedra are hatched. View parallel **c** rotated by 4° about **a** and **b**.



b The natrolite chain (**fib** unit). View parallel **b** rotated by 10° about **a** and 1° about **c**.



c Polyhedral representation. View parallel [110] rotated by 1° about [1 $\bar{1}$ 0] and [001]. Scale is 80 % of a).



d Ball and stick model corresponding to a).

Fig. NAT.3.6.1 Projections of the NAT-VIII.4 crystal structure of metanatrolite, $Na_{16} \cdot Al_{16}Si_{24}O_{80}$ (NAT1996a01, 96Bau1).

Table NAT.3.6.1 Atomic coordinates and site definitions for metanatrolite, $Na_{16} \cdot Al_{16}Si_{24}O_{80}$ (NAT1996a01, 96Bau1).

atom	*x*	*y*	*z*	*B* [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al11a	0.0264(2)	0.1055(1)	0.6050(5)	2.27(6)	1	8(c)	8
Al11b	0.7676(1)	0.1424(1)	0.3613(5)	2.39(7)	1	8(c)	8
Si12a	0.3629(1)	0.2650(1)	0.6151(4)	2.31(6)	1	8(c)	8
Si12b	0.1104(1)	-0.0214(1)	0.3617(4)	2.20(6)	1	8(c)	8
Si21	0	0	-0.01031(6)	2.50(9)	2	4(a)	4
Si22	¼	¼	0.2408(6)	2.40(9)	2	4(b)	4
O11a	0.4587(3)	0.4299(3)	0.860(1)	3.9(1)	1	8(c)	8
O11b	0.7641(3)	0.8289(3)	0.1100(9)	3.32(9)	1	8(c)	8
O12a	0.3312(3)	0.7350(3)	0.887(1)	3.6(1)	1	8(c)	8
O12b	0.5721(4)	0.4586(3)	0.132(1)	3.6(1)	1	8(c)	8
O21a	0.0905(4)	0.0699(3)	0.405(1)	3.8(1)	1	8(c)	8
O21b	0.6465(4)	0.8033(4)	0.783(1)	3.9(1)	1	8(c)	8
O22a	0.3084(4)	0.8407(4)	0.180(1)	4.3(1)	1	8(c)	8
O22b	0.5724(4)	0.4243(3)	0.544(1)	3.8(1)	1	8(c)	8
O31	0.4588(4)	0.2916(3)	0.595(1)	3.4(1)	1	8(c)	8
O32	0.7083(4)	0.9584(3)	0.848(1)	3.1(1)	1	8(c)	8
Na1	0.0620(4)	0.1828(4)	0.132(1)	7.4(2)	1	8(c)	7.5(1)
Na2	0.3110(9)	0.063(1)	0.329(2)	5.2(3)	1	8(c)	3.76
Na21	0.287(1)	0.0728(8)	0.399(2)	5.6(4)	1	8(c)	3.76

Table NAT.3.6.2 Selected interatomic distances and angles for metanatrolite, $Na_{16} \cdot Al_{16}Si_{24}O_{80}$ (NAT1996a01, 96Bau1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11a - O22b	1.727(7)	133.4(4)	Al 11b - O22a	1.724(7)	134.3(5)
Al 11a - O21a	1.762(7)	125.2(4)	Al 11b - O21b	1.746(7)	131.1(4)
Al 11a - O11a	1.763(7)	133.0(4)	Al 11b - O11b	1.751(6)	132.3(3)
Al 11a - O31	1.770(6)	113.7(4)	Al 11b - O32	1.762(6)	114.8(4)
mean	1.755	126.3	mean	1.746	128.1
Si12a - O21b	1.595(7)	131.1(4)	Si12b - O21a	1.613(6)	125.2(4)
Si12a - O22a	1.617(7)	134.3(5)	Si12b - O22b	1.616(6)	133.4(4)
Si12a - O31	1.626(7)	113.7(4)	Si12b - O32	1.627(7)	114.8(4)
Si12a - O12a	1.640(7)	135.8(4)	Si12b - O12b	1.642(8)	133.0(4)
mean	1.620	128.7	mean	1.624	126.6
Si21 - O11a	1.605(5)	133.0(4)	Si22 - O11b	1.602(6)	132.3(3)
Si21 - O11a	1.605(5)	133.0(4)	Si22 - O11b	1.602(6)	132.3(3)
Si21 - O12b	1.644(7)	132.3(4)	Si22 - O12a	1.637(6)	135.8(4)
Si21 - O12b	1.644(7)	132.3(4)	Si22 - O12a	1.637(6)	135.8(4)
mean	1.625	132.7	mean	1.620	134.1

NAT.3.7 NAT-XVI.4 compounds (*C* 1 1 2_1, IT #5)

Crystal structure projections are essentially identical with Fig. NAT.3.2.1.

Table NAT.3.7.1 Atomic coordinates and site definitions for NH_4-natrolite, $(NH_4)_{16} \cdot Al_{16}Si_{24}O_{80}$ (NAT1992a01, 92Stu1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
Al11A	0.03541(6)	0.09234(5)	0.6170(2)	0.68	1	4(c)	4
Al11B	0.03511(6)	0.59761(5)	0.1169(2)	0.67	1	4(c)	4
Al11C	0.78664(6)	0.15342(6)	0.3645(2)	0.68	1	4(c)	4
Al11D	0.78416(6)	0.65594(6)	0.8653(2)	0.68	1	4(c)	4
Si12A	0.34558(4)	0.28565(5)	0.6255(2)	0.67	1	4(c)	4
Si12B	0.35124(4)	0.78483(5)	0.1245(2)	0.64	1	4(c)	4
Si12C	0.09972(5)	-0.03602(5)	0.3742(2)	0.73	1	4(c)	4
Si12D	0.09742(5)	0.46684(5)	0.8731(1)	0.67	1	4(c)	4
Si21	-0.00034(7)	-0.00714(3)	0.0007(2)	0.80	1	4(c)	4
Si22	0.24290(3)	0.24993(7)	0.2496(2)	0.91	1	4(c)	4
O11A	0.4839(1)	0.4191(1)	0.8726(4)	1.26	1	4(c)	4
O11B	0.4884(1)	0.9371(1)	0.3579(4)	1.38	1	4(c)	4
O11C	0.7313(1)	0.8228(1)	0.1196(4)	1.61	1	4(c)	4
O11D	0.7409(1)	0.3211(1)	0.6146(4)	1.64	1	4(c)	4
O12A	0.3326(1)	0.7666(1)	0.8803(3)	1.29	1	4(c)	4
O12B	0.3132(1)	0.2613(2)	0.3998(4)	1.59	1	4(c)	4
O12C	0.5748(2)	0.4829(1)	0.1414(4)	1.69	1	4(c)	4
O12D	0.5736(1)	0.9936(1)	0.6476(4)	1.49	1	4(c)	4
O21A	0.1022(1)	0.0382(1)	0.5054(5)	1.67	1	4(c)	4
O21B	0.0985(1)	0.5345(1)	0.0275(5)	1.53	1	4(c)	4
O21C	0.6496(1)	0.7872(1)	0.7583(5)	1.65	1	4(c)	4
O21D	0.6495(1)	0.2821(1)	0.2805(4)	1.24	1	4(c)	4
O22A	0.2928(1)	0.8439(1)	0.2049(4)	1.42	1	4(c)	4
O22B	0.2955(1)	0.3487(1)	0.7227(4)	1.54	1	4(c)	4
O22C	0.5439(1)	0.4052(2)	0.4688(4)	1.61	1	4(c)	4
O22D	0.5396(1)	0.9052(1)	-0.0520(4)	1.04	1	4(c)	4
O31a	0.4297(1)	0.3147(1)	0.5870(4)	0.99	1	4(c)	4
O31b	0.4348(1)	0.8180(1)	0.1280(4)	0.89	1	4(c)	4
O32a	0.6816(1)	0.9365(1)	0.8569(5)	1.12	1	4(c)	4
O32b	0.6843(1)	0.4335(1)	0.3604(5)	1.09	1	4(c)	4
N1	0.4474(1)	0.2852(1)	0.0900(3)	1.64	1	4(c)	4
H11	0.425(1)	0.287(1)	0.224(3)	1.64	1	4(c)	4
H12	0.454(1)	0.3353(9)	0.054(4)	1.64	1	4(c)	4
H13	0.495(1)	0.264(1)	0.091(3)	1.64	1	4(c)	4
H14	0.415(1)	0.261(1)	0.001(3)	1.64	1	4(c)	4
N2	0.4741(1)	0.8104(1)	0.6512(4)	1.69	1	4(c)	4
H21	0.509(1)	0.837(1)	0.740(3)	1.69	1	4(c)	4
H22	0.454(1)	0.840(1)	0.547(3)	1.69	1	4(c)	4
H23	0.429(1)	0.789(1)	0.719(3)	1.69	1	4(c)	4
H24	0.495(1)	0.771(1)	0.583(3)	1.69	1	4(c)	4
N3	0.7208(2)	0.4438(2)	0.8947(5)	2.94	1	4(c)	4
H31	0.731(1)	0.410(1)	0.786(3)	2.94	1	4(c)	4
H32	0.725(1)	0.422(1)	0.027(3)	2.94	1	4(c)	4

Table NAT.3.7.1 (continued)

atom	*x*	*y*	*z*	B_{eq} [Å^2]	Site symmetry	Wyckoff position	no. of atoms in unit cell
H33	0.752(1)	0.486(1)	0.886(4)	2.94	1	4(c)	4
H34	0.671(1)	0.461(1)	0.863(4)	2.94	1	4(c)	4
N4	0.2940(2)	0.5437(2)	0.8640(7)	n.p.d.	1	4(c)	4
H41	0.277(2)	0.576(1)	0.762(4)	n.p.d.	1	4(c)	4
H42	0.334(1)	0.516(1)	0.817(5)	n.p.d.	1	4(c)	4
H43	0.309(2)	0.571(1)	0.978(3)	n.p.d.	1	4(c)	4
H44	0.252(1)	0.514(2)	0.909(4)	n.p.d.	1	4(c)	4

Table NAT.3.7.2 Selected interatomic distances and angles for NH_4-natrolite, $(NH_4)_{16} \cdot Al_{16}Si_{24}O_{80}$ (NAT1992a01, 92Stu1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 11A - O11B	1.717(3)	144.9(2)	Al 11B - O22C	1.714(2)	139.0(2)
Al 11A - O21A	1.718(2)	134.2(1)	Al 11B - O21B	1.725(2)	136.7(1)
Al 11A - O31b	1.734(2)	130.0(1)	Al 11B - O11A	1.731(3)	133.0(1)
Al 11A - O22D	1.738(2)	132.1(1)	Al 11B - O31a	1.742(2)	128.7(1)
mean	1.727	135.3	mean	1.728	134.4
Al 11C - O21C	1.725(2)	139.1(1)	Al 11D - O22A	1.730(2)	136.2(1)
Al 11C - O22B	1.738(2)	132.1(1)	Al 11D - O21D	1.736(2)	132.2(1)
Al 11C - O32a	1.749(2)	129.0(1)	Al 11D - O32b	1.739(2)	129.1(1)
Al 11C - O11C	1.752(3)	137.5(1)	Al 11D - O11D	1.740(3)	139.4(1)
mean	1.741	134.4	mean	1.737	134.2
Si12A - O22B	1.597(2)	132.1(1)	Si12B - O21C	1.587(3)	139.1(1)
Si12A - O21D	1.608(2)	132.2(1)	Si12B - O22A	1.597(2)	136.2(1)
Si12A - O31a	1.617(2)	128.7(1)	Si12B - O31b	1.615(2)	130.0(1)
Si12A - O12B	1.646(3)	148.9(2)	Si12B - O12A	1.663(2)	135.0(1)
Mean	1.617	135.5	Mean	1.616	135.1
Si12C - O22C	1.596(3)	139.0(2)	Si12D - O21B	1.601(3)	136.7(1)
Si12C - O21A	1.612(3)	134.2(1)	Si12D - O12D	1.610(3)	142.3(2)
Si12C - O32b	1.617(2)	129.1(1)	Si12D - O32a	1.610(2)	129.0(1)
Si12C - O12C	1.622(3)	140.8(2)	Si12D - O22D	1.611(2)	132.1(1)
mean	1.612	135.8	mean	1.608	135.0
Si21 - O11B	1.604(2)	144.9(2)	Si22 - O11C	1.600(2)	137.5(1)
Si21 - O11A	1.618(2)	133.0(1)	Si22 - O11D	1.602(2)	139.4(1)
Si21 - O12C	1.639(4)	140.8(2)	Si22 - O12B	1.609(2)	148.9(2)
Si21 - O12D	1.644(2)	142.3(2)	Si22 - O12A	1.627(2)	135.0(1)
mean	1.626	140.3	mean	1.609	140.2

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

NAT.5 Flexibility and apertures

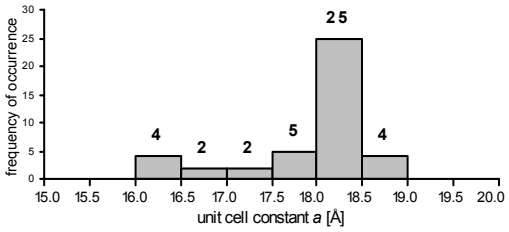


Fig. NAT.5.1 Histogram of 42 unit cell constants *a* of aluminosilicates of NAT-type determined by single crystal methods in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples. The extreme values of *a* are 16.223 Å and 18.971 Å, the mean value is 17.974 Å.

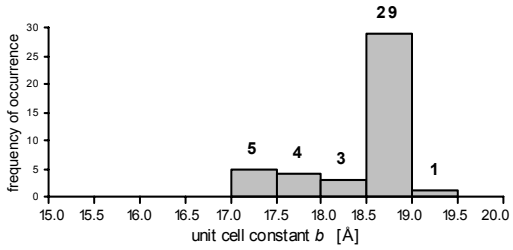


Fig. NAT.5.2 Histogram of 42 unit cell constants *b* of aluminosilicates of NAT-type determined by single crystal methods in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples. The extreme values of *b* are 17.018 Å and 19.204 Å, the mean value is 18.382 Å.

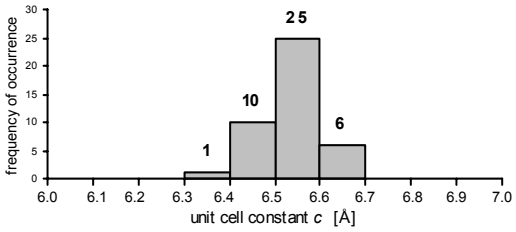


Fig. NAT.5.3 Histogram of 42 unit cell constants *c* of aluminosilicates of NAT-type determined by single crystal methods in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples. The extreme values of **c** are 6.385 Å and 6.608 Å, the mean value is 6.537 Å. Observe: the scale on the abscissa in this diagram is different from Figures NAT.5.1 and NAT.5.2.

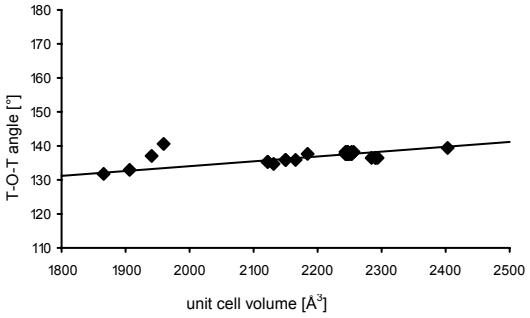


Fig. NAT.5.4 Mean T-O-T angles from 42 single crystal structure determinations of aluminosilicates of NAT-type performed in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples, are plotted against the unit cell volume, V. The extreme values of V are 1777 Å^3 and 2402 Å^3, the mean is 2163 Å^3. The extreme values of T-O-T(mean) are 129.1° and 140.6°, mean 136.4°. The line is a least-squares fit to all points.

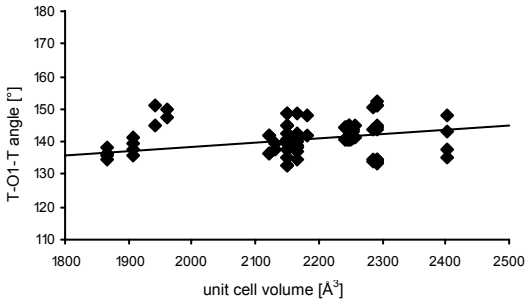


Fig. NAT.5.5 Individual angles T-O1-T from 42 single crystal structure determinations of aluminosilicates of NAT-type performed in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples, are plotted against the unit cell volume, V. The plot shows 124 pairs of experimental values. The extreme values of V are 1777 Å^3 and 2402 Å^3, the mean is 2163 Å^3. The extreme values of T-O1-T are 132.7° and 152.4°, the mean is 140.5°. The line is a least-squares fit to all points.

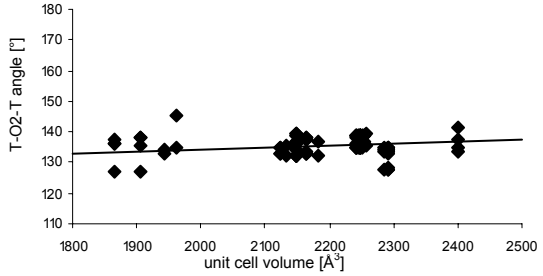


Fig. NAT.5.6 Indidvidual angles T-O2-T from 42 single crystal structure determinations of aluminosilicates of NAT-type performed in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples, are plotted against the unit cell volume, V. The plot shows 124 pairs of experimental values. The extreme values of V are 1777 Å^3 and 2402 Å^3, the mean is 2163 Å^3. The extreme values of T-O2-T are 125.2° and 145.3°, the mean is 135.0°. The line is a least-squares fit to all points.

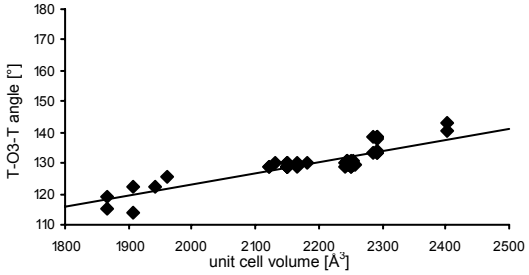


Fig. NAT.5.7 Individual angles T-O3-T from 42 single crystal structure determinations of aluminosilicates of NAT-type performed in space groups *Fdd*2, *F*1*d*1, *F*112 and $C112_1$, but excluding mesolite samples, are plotted against the unit cell volume, V. The plot shows 62 pairs of experimental values. The extreme values of V are 1777 Å^3 and 2402 Å^3, the mean is 2163 Å^3. The extreme values of T-O3-T are 113.9° and 142.8°, the mean is 128.0°. The line is a least-squares fit to all points.

When Pauling described the crystal structure of the NAT-type framework [30Pau1] he pointed out that the **fib** chains could rotate about their axes and cause the structure to collapse: the 8-ring pores between the fibers would become smaller and consequently the *a* and *b* unit cell constants would shrink. One can see that clearly when observing the spread of the unit cell constants *a* and *b* in a number of NAT-type frameworks filled with various cations and either in the hydrated or the dehydrated state (Figs. NAT.5.1 and NAT.5.2). The ratio between the largest and the smallest *a* and *b* cell constants are 1.17 and 1.12, while for the **c** constants it is 1.04. The latter value is similar to ratios encountered for the noncollapsible [92Bau1] frameworks of the FAU- or LTA-types. In a collapsible framework the mean T-O-T angle decreases as the volume of the unit cell becomes smaller (Fig. NAT.5.4). The same is true of

the individual angles T-O1-T, T-O2-T and T-O3-T (Figs. NAT.5.5, NAT.5.6 and NAT.5.7). All these angles corotate [92Bau1] as the framework collapses. The slope is steepest for T-O3-T *vs.* volume, because the oxygen atoms O3 connect the **fib** chains and serve as hinges between them as they rotate. The T-O3-T angle of 113.9° in NAT1996a04 is the narrowest such angle observed in any aluminosilicate or silicate. Such small angles are one of the limiting factors halting the further collapse of a tetrahedral aluminosilicate framework [92Bau2, 95Bau1]. The mean angle of 136° in NAT-type compounds is clearly smaller than the maximum of the distribution of T-O-T angles in aluminosilicate zeolites (about 143° [95Bau1]).

The 8-ring openings in the framework of natrolite have free diameters ranging from about 2.5 Å to 4 Å. Inasmuch as the framework can easily expand and collapse the actual values can vary considerably.

NAT.6 Other information

NAT-type compounds are mentioned in a few patents and patent applications. However, it does not appear that many useful applications of NAT-type compounds are known.

The chemistry of gonnardite, mesolite, natrolite, paranatrolite, scolecite and tetranatrolite was explored by [82Alb1] and [92Ros1].

Crystal structures which share some of their features with the topology of the NAT-type have been determined recently: $K_{2.6}Li_{5.4} \cdot Li_4Si_{16}O_{38} \cdot 4.3H_2O$ [2006Par1] and $Ge_3O_5(OH)_4[C_2N_2\ H_{10}]$ [2006Sne1].

NAT.7 Ignored work

The following papers have not been incorporated into this compilation:

1. [89Pec1], it is not possible to recover from the information on tetranatrolite given in this paper a meaningful description of its crystal structure;
2. [81Pec1], atomic coordinates and the esd's of the H-atoms are inconsistent with the experimental data.
3. [84Pec1], the text of the part of this paper referring to the neutron diffraction study is essentially identical to the text of [83Pec1].
4. [82Pec1], the values of most coordinates in this refinement of mesolite are essentially identical with the corresponding values in [72Adi1].
5. [82Pec2], for the crystal structure of scolecite the space group is given as Cc, however, the cell constants and the coordinates do not fit this description. They correspond to the F1d1 setting as used in [72Adi1]. The positional coordinates in [82Pec1] are essentially identical to those in [72Adi1].
6. [88Pec1], the atomic coordinates, the thermal parameters and the estimated standard deviations of both reported in [88Pec1] for paranatrolite bear a strong resemblance to the data previously reported for the neutron diffraction crystal structure refinement of scolecite [84Jos1]. The anisotropic thermal parameters of paranatrolite correspond in minute detail to the data given in [84Jos1]. Compare also the discussion of [88Pec1] in [91Bau1].

Because of the similarities between the numerical values of [84Jos1] and [88Pec1] (and of the resemblance between [72Adi1] and [82Pec1, 82Pec2] as well), which all are extremely unlikely to have happened by coincidence, we have listed here the earlier work only.

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Gone to press May 1, 2006