called 'Mo,Al', aluminium and molybdenum ions are distributed at random. It is worth pointing out that the 'Mo' octahedra which share their corners with six different P_2O_7 groups are almost regular (Table 2) with Mo—O distances ranging from 1·986 to 2·016 Å. The 'Mo,Al' octahedra exhibit much smaller distances in agreement with the size of aluminium. Moreover they are more distorted owing to the fact that each 'Mo,Al' octahedron shares the four corners of its basal plane with two P_2O_7 groups (Fig. 2), the two other opposite apices being linked to two different diphosphate groups. The molybdenum valency in the different sites is not clearly established. The calculation of the sum of the electrostatic bond strengths according to the theory developed by Zachariasen (1978) leads to the valent state of 4·18 for the octahedra only occupied by molybdenum. This suggests that the 'Mo' octahedra are occupied by tetravalent molybdenum in agreement with the Mo—O distances (Table 2), whereas trivalent molybdenum and aluminium are statistically distributed over the same octahedral site. Nevertheless the latter distribution is rather unexpected owing to the large size of Mo^{III} compared to aluminium.

A second characteristic of this structure deals with the behaviour of K^+ cations which is different from that of Na^+. This cation is indeed surrounded by eight O atoms with K—O distances ranging from 2·52 to 3·22 Å (Table 2) against six for Na^+ (2·33 to 3·20 Å). This can be explained by the fact that the K^+ cations are located at a centre of symmetry, *i.e.* on the axis of the tunnels, while the Na^+ cations are off-centre. Consequently, the vibration of K^+ is preferentially oriented along the axis of the tunnel. Its thermal factor, B_{eq}, smaller than that of Na^+, is consistent with its larger size.

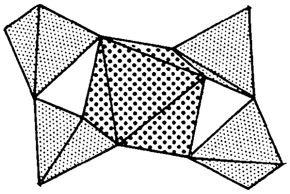

Fig. 2. The $(Mo,Al)P_4O_{16}$ unit.

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Thomsonite, a Neutron Diffraction Study at 13 K

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Abstract. The crystal structure of the natural thomsonite, $Na_{1\cdot00}Ca_{1\cdot88}Sr_{0\cdot12}Al_5Si_5O_{20}.6H_2O$, at 13 K [$M_r$ = 812·3, orthorhombic, *Pncn*, $a = 13{\cdot}1043\ (14)$, $b = 13{\cdot}0569\ (18)$, $c = 13{\cdot}2463\ (30)$ Å, $V = 2266\ (1)$ Å^3, $Z = 4$, $D_x = 2{\cdot}381$ g cm^{-3}, $\mu = 0{\cdot}886$ cm^{-1}] has been refined from neutron diffraction data [$\lambda = 1{\cdot}1588\ (1)$ Å]. 4513 (3004 unique) reflections resulted in $R(F^2) = 0{\cdot}0369$. The structure is generally very close to the room-temperature structure [Pluth, Smith & Kvick, (1985). *Zeolites*, **5**, 74–80] and shows no sign of

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cation ordering. Among the significant differences are decreased *T*—O—*T* angles, a higher degree of asymmetry of the Ca coordination and a strengthening of the shortest hydrogen bonds at 13 K.

Introduction. Previous structure determinations of thomsonite at room temperature [Alberti, Vezzalini & Tazzoli (1981), Pechar (1982) (X-rays) and Pluth, Smith & Kvick (1985) (neutrons), PSK hereafter] have demonstrated disorder, temporal or spatial, in the cation sites: the Ca site consists of two positions only 0·565 (3) Å apart, precluding simultaneous occupancy; the so-called NaCa site has a random distribution of Na and Ca. It was suggested that at lower temperature there might be an ordering of these sites analogous to the situation in anorthite and Na,Ca feldspar (reviewed by Smith & Brown, 1988). The present structure determination of thomsonite at 13 K was undertaken in order to study this possible cation ordering. Structure determinations at very low temperatures also have the general advantage of giving results of higher precision and are less biased by thermal motions.

Experimental. The natural single crystal of thomsonite used here (also used by PSK) is of unknown locality (Cambridge University collection No. 2882), prismatic (001), bounded by {010}, {100}, $(1\bar{1}0)$, $(\bar{1}\bar{1}0)$, $(\bar{1}06)$ and $(10\bar{6})$, 1·7 × 3·1 × 8·2 mm, volume 42 mm^3, having the composition $Na_{1\cdot0}(Ca_{1\cdot85}Sr_{0\cdot10})Al_{5\cdot0}Si_{5\cdot0}O_{20}.6H_2O$ (PSK, from microprobe analysis).

Data were collected on a four-circle diffractometer at the Brookhaven National Laboratory High Flux Beam Reactor. The wavelength, 1·1588 (1) Å, was obtained with a Ge(220) monochromator calibrated against 32 2θ values from KBr at room temperature [$a = 6{\cdot}6000$ (1) Å]. The data-collection temperature, 13 K, was attained with a Displex CS–202. Unit-cell dimensions were determined from least-squares fitting of 64 2θ values, $41 < 2\theta < 64°$.

Intensity data were collected using $\omega/2\theta$ step scans in approximately one hemisphere of reciprocal space for $4 \leq 2\theta \leq 60°$ $(-7 \leq h \leq 10,\ |k| \leq 10,\ 0 \leq l \leq 11)$ using constant scan intervals $\Delta 2\theta = 3{\cdot}0°$ and in one quarter sphere for $60 \leq 2\theta \leq 112°$ $(-7 \leq h \leq 8,\ -18 \leq k \leq 0,\ 0 \leq l \leq 16)$ using $\Delta 2\theta = 1{\cdot}52° + 2{\cdot}51° \tan\theta$. 5040 symmetry-allowed reflections were collected. The background was calculated from the first and last tenths of a scan. Standard reflections (10,0,0 and $0\bar{6}8$) measured between every 50 reflections showed no systematic variations. Corrections were made for the Lorentz effect and for absorption (Gaussian integration, 8 × 8 × 8 grid, transmission factors in the range 0·70–0·94). Heavily exposed X-ray precession films showed no evidence of a superstructure or modulated structure.

The full-matrix least-squares refinements minimized $\sum w(F_o^2 - F_c^2)^2$ with $w = [\sigma^2(F_o^2) + (cF_o^2)^2]^{-1}$, $\sigma(F_o^2)$ from counting statistics and c (= 0·02) adjusted to give constant $\langle w(\Delta F^2)\rangle$ in different F_o^2 and $(\sin\theta)/\lambda$ intervals. The refinements were started with parameters (including H atoms) from PSK, retaining the non-standard space group *Pncn* used in previous investigations. 239 parameters were refined in the final least-squares cycles: one scale factor, positional and anisotropic thermal parameters on all atoms and occupancy factors on Ca/Na and Ca. Initial refinements of the Al, Si and water occupancy factors gave no significant deviation from unity, and they were kept constant in the final cycles. An isotropic extinction parameter, 0·67 (2) × 10^4, [type I, Lorentzian mosaicity (Becker & Coppens, 1974)] was refined in the initial cycles. Largest extinction correction factor, $y = 2{\cdot}44$ (on F_o^2). 24 reflections with $y > 1{\cdot}30$ were excluded in the final cycles together with 450 weak reflections having $F_o^2/F_c^2 > 5{\cdot}0$, the latter being affected by multiple scattering or Al scattering from the cryostat. Final $R(F^2) = 0{\cdot}0369$ [$R(F) = 0{\cdot}0392$], $wR(F^2) = 0{\cdot}06632$ and $S = 1{\cdot}50$ for 4513 (3004 unique) reflections. Final (parameter shift)/(e.s.d.) < 0·01. The largest residual peaks correspond to < 3% of the scattering power of a framework O atom. The internal agreement factor, $R_{\rm int}$, was 0·0172. Refinements in the non-centrosymmetric space groups *Pn*2*n* and $P2_122$ did not improve the *R* factors, but caused severe correlation between centrosymmetrically related parameters.

The neutron scattering length for Ca was taken from Ståhl, Kvick & Ghose (1987), the others from Koester, Rauch, Herkens & Schroeder (1981). The crystallographic computer programs have been described by Lundgren (1983). Final positional parameters and the isotropic mean value of the anisotropic temperature factor coefficients are given in Table 1.* Selected distances and angles are in Table 2. Fig. 1 shows an *ac* projection of thomsonite at 13 K, and Fig. 2 the water coordination.

Discussion. The framework at 13 K is generally very similar to that of the room-temperature structure (PSK). The observed *T*—O distances are slightly shorter at 295 K due to thermal motions: ⟨Si—O⟩ = 1·626 and 1·621 Å and ⟨Al—O⟩ = 1·748 and 1·744 Å at 13 and 295 K, respectively. The *T*—O—*T* angles are larger at 295 K. The average differences are larger when the *T*—O—*T* O atoms are involved in hydrogen bonding [0·47 (5)°] as compared to cation

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52808 (35 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final fractional coordinates* ($\times 10^5$) *and* B_{iso} (Å^2) *for thomsonite at* 13 K

$B_{\rm iso} = (4/3)\sum_i \sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	$B_{\rm iso}$
Ca/Na*	5834 (6)	50375 (9)	36020 (6)	0·56 (2)
Ca*	49916 (16)	47480 (10)	49915 (16)	0·53 (3)
Si(1)	25000	25000	68808 (9)	0·21 (2)
Al(1)	25000	75000	69025 (11)	0·22 (2)
Si(2)	11302 (6)	69465 (7)	50019 (6)	0·26 (2)
Al(2)	11948 (7)	30637 (8)	49585 (7)	0·23 (2)
Si(3)	30886 (6)	38484 (7)	37739 (6)	0·25 (2)
Al(3)	31012 (7)	62393 (8)	38013 (7)	0·26 (2)
O(1)	16923 (4)	31182 (5)	61795 (4)	0·43 (1)
O(2)	15866 (4)	69043 (5)	61417 (4)	0·43 (1)
O(3)	31377 (4)	33088 (5)	75611 (5)	0·43 (1)
O(4)	31301 (5)	65759 (5)	76235 (5)	0·44 (1)
O(5)	214 (5)	63666 (4)	50126 (6)	0·44 (1)
O(6)	18383 (4)	62910 (5)	42295 (5)	0·51 (1)
O(7)	19041 (4)	38525 (5)	41545 (5)	0·48 (1)
O(8)	10428 (4)	81256 (5)	46124 (5)	0·46 (1)
O(9)	11827 (4)	18080 (5)	45269 (5)	0·50 (1)
O(10)	35702 (4)	49933 (6)	38296 (4)	0·38 (1)
O*W*(1)	12620 (4)	50179 (7)	18922 (5)	0·90 (1)
O*W*(2)	38972 (4)	49775 (7)	63828 (4)	0·77 (1)
O*W*(3)	0	65045 (8)	75000	1·21 (2)
O*W*(4)	0	34407 (8)	75000	1.06 (2)
H(1)	15862 (10)	43726 (11)	66126 (11)	1·75 (3)
H(2)	15679 (11)	55944 (11)	66093 (11)	1·84 (3)
H(3)	36905 (12)	43779 (12)	67664 (12)	1·96 (3)
H(4)	37059 (12)	55568 (12)	68072 (12)	1·93 (3)
H(5)	4677 (11)	69191 (14)	71289 (12)	2·34 (3)
H(6)	5035 (11)	30212 (13)	71813 (13)	2·53 (4)

* For occupancy, see text.

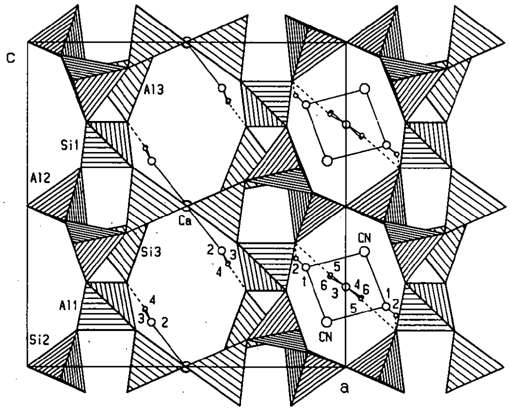

Fig. 1. An *ac* projection of thomsonite at 13 K. Largest circles cations (the CaNa site is denoted CN), intermediate circles water O atoms and smallest circles H atoms.

Table 2. *Selected distances* (Å) *and angles* (°) *in thomsonite at* 13 K

Si(1)—O(1)	1·6232 (9)	O(1)—Si(1)—O(1)	110·19 (8)
Si(1)—O(3)	1·6204 (9)	O(1)—Si(1)—O(3)	107·82 (3)
Mean	1·6218	O(1)—Si(1)—O(3)′	109·30 (3)
		O(3)—Si(1)—O(3)′	112·42 (8)
Al(1)—O(2)	1·7474 (10)	O(2)—Al(1)—O(2)	109·56 (9)
Al(1)—O(4)	1·7464 (10)	O(2)—Al(1)—O(4)	107·40 (3)
Mean	1·7469	O(2)—Al(1)—O(4)′	109·37 (3)
		O(4)—Al(1)—O(4)′	113·69 (9)
Si(2)—O(2)	1·6249 (10)	O(2)—Si(2)—O(5)	107·62 (6)
Si(2)—O(5)	1·6386 (10)	O(2)—Si(2)—O(6)	110·92 (6)
Si(2)—O(6)	1·6250 (10)	O(2)—Si(2)—O(8)	110·64 (6)
Si(2)—O(8)	1·6277 (12)	O(5)—Si(2)—O(6)	105·57 (6)
Mean	1·6290	O(5)—Si(2)—O(8)	112·18 (5)
		O(6)—Si(2)—O(8)	109·80 (6)
Al(2)—O(1)	1·7453 (12)	O(1)—Al(2)—O(5)	107·52 (6)
Al(2)—O(5)	1·7592 (11)	O(1)—Al(2)—O(7)	109·99 (6)
Al(2)—O(7)	1·7490 (12)	O(1)—Al(2)—O(9)	110·31 (6)
Al(2)—O(9)	1·7364 (13)	O(5)—Al(2)—O(7)	104·22 (6)
Mean	1·7475	O(5)—Al(2)—O(9)	113·46 (6)
		O(7)—Al(2)—O(9)	111·12 (6)
Si(3)—O(4)	1·6223 (11)	O(4)—Si(3)—O(7)	108·86 (5)
Si(3)—O(7)	1·6320 (10)	O(4)—Si(3)—O(9)	112·13 (6)
Si(3)—O(9)	1·6253 (10)	O(4)—Si(3)—O(10)	110·11 (6)
Si(3)—O(10)	1·6244 (11)	O(7)—Si(3)—O(9)	111·78 (6)
Mean	1·6260	O(7)—Si(3)—O(10)	110·64 (6)
		O(9)—Si(3)—O(10)	103·24 (5)
Al(3)—O(3)	1·7463 (12)	O(3)—Al(3)—O(6)	108·52 (6)
Al(3)—O(6)	1·7507 (11)	O(3)—Al(3)—O(8)	113·42 (6)
Al(3)—O(8)	1·7607 (11)	O(3)—Al(3)—O(10)	109·06 (6)
Al(3)—O(10)	1·7395 (13)	O(6)—Al(3)—O(8)	112·73 (6)
Mean	1·7493	O(6)—Al(3)—O(10)	111·29 (6)
		O(8)—Al(3)—O(10)	101·67 (6)
Si(1)—O(1)—Al(2)	138·90 (6)	Si(2)—O(6)—Al(3)	139·83 (6)
Al(1)—O(2)—Si(2)	140·61 (6)	Al(2)—O(7)—Si(3)	133·76 (6)
Si(1)—O(3)—Al(3)	136·83 (6)	Si(2)—O(8)—Al(3)	126·45 (5)
Al(1)—O(4)—Si(3)	137·20 (6)	Al(2)—O(9)—Si(3)	134·00 (6)
Si(2)—O(5)—Al(2)	127·45 (6)	Si(3)—O(10)—Al(3)	136·26 (5)
Ca/Na—O(5)	2·6543 (12)	Ca—O(8)	2·5808 (18)
Ca/Na—O(5)′	2·7123 (12)	Ca—O(8)′	3·1302 (17)
Ca/Na—O(6)	2·4646 (11)	Ca—O(9)	2·6219 (18)
Ca/Na—O(7)	2·4342 (11)	Ca—O(9)′	3·1746 (17)
Ca/Na—O*W*(1)	2·4334 (11)	Ca—O(10)	2·4374 (22)
Ca/Na—O*W*(1)′	2·5054 (10)	Ca—O(10)′	2·4708 (22)
Ca/Na—O*W*(3)	2·6017 (13)	Ca—O*W*(2)	2·3544 (22)
Ca/Na—O*W*(4)	2·5814 (13)	Ca—O*W*(2)′	2·3586 (22)
O*W*(1)—H(1)	0·9752 (17)	O*W*(2)—H(3)	0·9719 (17)
O*W*(1)—H(2)	0·9696 (17)	O*W*(2)—H(4)	0·9751 (17)
H(1)—O*W*(1)—H(2)	110·25 (13)	H(3)—O*W*(2)—H(4)	104·59 (14)
H(1)···O(1)	1·7410 (16)	H(3)···O(3)	1·8924 (17)
O*W*(1)···O(1)	2·6706 (11)	O*W*(2)···O(3)	2·8590 (10)
O*W*(1)—H(1)···O(1)	158·07 (13)	O*W*(2)—H(3)···O(3)	173·62 (14)
H(2)···O(2)	1·8192 (16)	H(4)···O(4)	1·8733 (17)
O*W*(1)···O(2)	2·7327 (11)	O*W*(2)···O)4)	2·8402 (10)
O*W*(1)—H(2)···O(2)	155·82 (13)	O*W*(2)—H(4)···O(4)	170·84 (14)
O(1)···O(2)	4·9462 (11)	O(3)···O(4)	4·2666 (13)
O*W*(3)—H(5)	0·9541 (17)	O*W*(4)—H(6)	0·9558 (17)
H(5)—O*W*(3)—H(5)′	110·86 (23)	H(6)—O*W*(4)—H(6)′	110·07 (23)
H(5)···O(2)	1·9647 (16)	H(6)···O(1)	2·0503 (17)
O*W*(3)···O(2)	2·7987 (7)	O*W*(4)···O(1)	2·8556 (7)
O*W*(3)—H(5)···O(2)	144·76 (16)	O*W*(4)—H(6)···O(1)	140·80 (16)
O(2)···O(2)	5·4991 (13)	O(1)···O(1)	5·6488 (13)

coordination [0·24 (3)°]. The same behaviour was observed for bikitaite (Ståhl, Kvick & Ghose, 1989) and scolecite (Kvick, Ståhl & Smith, 1985).

As mentioned above, refinements were unsuccessful in the non-centrosymmetric space groups *Pn*2*n* and $P2_122$, which would have allowed ordered Ca and NaCa sites. In determining the extra-framework cation-site composition, several factors have to be considered: (i) the refined occupancy factors, NaCa 0·984 (5) ($b = 4{\cdot}15$ fm) and Ca 1·004 (6) ($b = 4{\cdot}90$ fm); (ii) the chemical analysis; (iii) the refined occupancy of the water sites, as the fully occupied water sites indicate fully occupied cation sites; and (iv) the framework cation distribution, as the fully ordered framework cations require a balancing extra-framework cation charge of +5e per formula unit. In addition, the assumption that all Sr are in the Ca site led to the suggested extra-framework cation distribution of $(\mathrm{Na}_{1\cdot00}\mathrm{Ca}_{1\cdot00})$ and $(\mathrm{Ca}_{0\cdot88}\mathrm{Sr}_{0\cdot12})$. This site composition fulfils the charge-balancing and

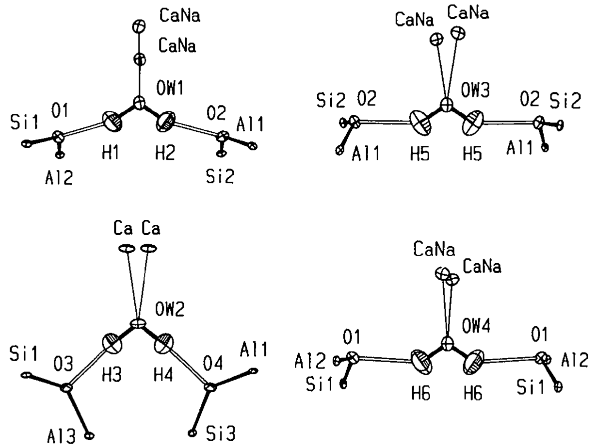

Fig. 2. The water coordination in thomsonite at 13 K. Thermal ellipsoids are scaled to include 75% probability. Only one of the Ca sites coordinating O*W*(2) is occupied.

occupancy requirements. It results in the calculated occupancy factors 0·998 and 1·007, which are within 3 e.s.d.'s of the refined values, and a composition that is within the limits of error of the microprobe analysis.

The NaCa coordination is changed very little between 13 and 295 K except for NaCa—O*W*(1): 2·433 (1) (13 *K*) and 2·452 (1) Å (295 K). The Ca coordination shows more significant changes. The Ca–Ca separation is larger at 13 K, 0·659 (2) Å as compared with 0·565 (2) Å at 295 K, resulting in a more asymmetric coordination at 13 K: Ca—O(8) and Ca—O(9) decrease by 0·031 Å while Ca—O(8)′ and Ca—O(9)′ increase by 0·047 Å on lowering the temperature to 13 K.

The shortest hydrogen bonds involving O*W*(1) and O*W*(2) become even shorter and increase their O*W*—H···O angles on cooling, while the opposite is true for the longer hydrogen bonds involving O*W*(3) and O*W*(4). The largest change is observed for H(5)···O(2), 1·965 (2) (13 K) to 1·945 (3) Å (295 K), and is accompanied by a large change in the water angle, 110·9 (2) (13 K) to 112·5 (4)° (295 K). The flexibility of the water angle is also demonstrated in the distribution of water angles in thomsonite, 104·6 (1) to 110·9 (2)°, which is highly correlated to the distance between the two hydrogen-bond acceptors (Kvick, 1986). A short acceptor–acceptor distance results in a small water angle as was also demonstrated in scolecite (Kvick *et al.*, 1985).

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Structure of Synthetic Dipotassium Zinc Tetrasilicate

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Abstract. $K_2ZnSi_4O_{10}$, $M_r = 415{\cdot}9$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}0676\ (8)$, $b = 14{\cdot}047\ (1)$, $c = 7{\cdot}0673\ (8)$ Å, $V = 999{\cdot}4\ (2)$ Å^3, $Z = 4$, $D_x = 2{\cdot}76$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 3{\cdot}85$ mm^{-1}, $F(000) = 816$, $T = 293$ K, final $R = 0{\cdot}048$ for 1656 independent reflections. The structure is built from a tectosilicate framework containing SiO_4 (mean Si—O 1·618 Å) and ZnO_4 (mean Zn—O 1·950 Å) tetrahedra and large cavities for K atoms. The SiO_4 tetrahedra form three-dimensional frameworks built up by ten-membered rings parallel to the (100) plane connected to other rings by

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