Discussion. The general features of the structure (Fig. 1) are the same as those determined by Rundqvist (1965). The interatomic distances (Table 2) are almost the same as those previously established by Rundqvist but the thermal motion factors are positive definite. The Mo—P distances range from 2·375 to 3·002 Å. All the atoms are located in the mirror planes of the unit cell. One observes three types of P polyhedra around the Mo atoms: two MoP$_6$ octahedra around Mo(2) and M(3), two MoP$_5$ triangular bipyramids around Mo(1) and Mo(7), and four MoP$_5$ square pyramids around Mo(4), Mo(5), Mo(6) and Mo(8). The structure can be described as layers of corner-, edge- and face-sharing MoP$_6$ and MoP$_5$ polyhedra parallel to the (010) plane (Fig. 1). Two successive layers share the edges of their polyhedra. Around the P atoms one observes two types of Mo polyhedra: one triangular prism around P(3) and five mono-capped triangular prisms around the others (Fig. 2). This ratio explains the fact that the asymmetric unit formula is Mo$_8$P$_6$ instead of Mo$_4$P$_3$.

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Structure of Intermediate Albite, NaAlSi$_3$O$_8$

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Abstract. $M_r = 262{\cdot}22$, triclinic, $C\bar{1}$, $a = 8{\cdot}149\,(1)$, $b = 12{\cdot}840\,(1)$, $c = 7{\cdot}120\,(1)$ Å, $\alpha = 93{\cdot}83\,(1)$, $\beta = 116{\cdot}47\,(1)$, $\gamma = 89{\cdot}51\,(1)°$, $V = 665{\cdot}2\,(3)$ Å^3, $Z = 4$, $D_x = 2{\cdot}62$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 9{\cdot}0$ cm^{-1}, $F(000) = 520$, $T = 294\,(1)$ K, $R = 0{\cdot}030$ for 2055 unique reflections with $I > 3\sigma(I)$ of 2303 total unique data. Mean tetrahedral bond lengths (Å) and estimated average Al/(Al + Si) occupancies are: $T_1$0 1·677, 0·51 Al; T_1m 1·631, 0·15 Al; $T_2$0 1·632, 0·16 Al, T_2m 1·633, 0·17 Al.

Introduction. The K feldspar (KAlSi$_3$O$_8$) and Na feldspar (NaAlSi$_3$O$_8$) minerals are isostructural (space group $C\bar{1}$) in their completely ordered ('low') modifications: the Al atom is ordered into a particular tetrahedral (T) site (designated $T_1$0), with Si in the other three nonequivalent T sites (*i.e.* T_1m, $T_2$0, T_2m). Both K and Na end members may have completely disordered 'high' (= high temperature) modifications, with $t \equiv$ Al/(Al + Si) = 0·25 in all four T sites, but at room temperature the K feldspar is monoclinic ($C2/m$) and the Na feldspar is triclinic ($C\bar{1}$). [The unconventional space group preserves a common unit-cell orientation for all alkali feldspars.]

In nature, series of both monoclinic (with $t_1 0 = t_1 m$ and $t_2 0 = t_2 m$) and triclinic (with $t_1 0 > t_1 m \geq t_2 0 \sim t_2 m$) K-rich feldspars are well documented (Kroll & Ribbe, 1983, 1987), but K-free Na feldspar ('albite') has only been reported in its ordered form, as though a first-order transformation occurred during cooling (see discussions by Ribbe, 1983; Smith, 1983). This is not the case, however, as Goldsmith & Jenkins (1985) demonstrated in their studies at high pressures of the equilibrium Al,Si order–disorder relations in albite. They found that the 'low ↔ high' albite conversion takes place continuously, without change in symmetry, over the range ~925–1125 K. Salje (1985) and Salje, Kuscholke, Wruck & Kroll (1985) predicted the thermodynamic properties of albite with a two-parameter Landau-type free-energy expression, confirming the conclusions of Goldsmith & Jenkins (1985).

Su, Ribbe, Bloss & Goldsmith (1986) investigated a suite of albite single crystals with degrees of Al,Si order ranging from low (ordered) to high (~90% dis-

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ordered). They found that refractive indices and extinction angles, $X' \wedge [100]$ on (010) and $X' \wedge [100]$ on (001), varied linearly with the reciprocal-lattice angles α^* and γ^* measured on X-ray precession photographs. They also reported the empirical equation

$$\Delta t_1 \simeq (t_1 0 - t_1 m) = -0{\cdot}353 + 2{\cdot}121 \sin^2 V_x, \quad (1)$$

which relates half the optic axial angle $2V_x$ to the difference in Al/(Al+Si) content of the $T_1 0$ and $T_1 m$ tetrahedral sites. For triclinic feldspars, especially those in which $t_1 m \sim t_2 0 \sim t_2 m$, Δt_1 is useful as a relative measure of long-range Al,Si order, because values range from 1·0 for complete order to 0·0 for complete disorder. Equation (1) was derived from the relation between the optic axial angle and γ^* for albites and the relation

$$\Delta t_1 = \frac{\gamma^* - 44{\cdot}778 - 0{\cdot}50246\alpha^*}{6{\cdot}646 - 0{\cdot}05061\alpha^*} \quad (2)$$

for alkali feldspars whose crystal structures are known (Kroll & Ribbe, 1987).

Experimental. For this refinement we chose one of the colorless crystals (MAB176) from the suite studied by Su *et al.* (1986). It is a cleavage fragment of a natural albite (Clear Creek, California) which had been embedded in reagent-grade Na_2CO_3, sealed in a gold capsule and then heated for 19 d at 1050 K in a piston cylinder device maintained at 1·7 GPa.

Crystal 0·21 × 0·18 × 0·14 mm; Enraf–Nonius CAD-4 computer-controlled κ-axis diffractometer, graphite monochromator; cell dimensions from 25 reflections, $22 < 2\theta < 54°$; scan type ω–2θ. Absorption: ψ scans (North, Phillips & Mathews, 1968), relative transmission coefficients ranged from 0·915 to 0·999; subsequently improved by method of Walker & Stuart (1983); max. $(\sin\theta)/\lambda = 0{\cdot}746$ Å^{-1}. Index range: $-12 \le h \le 12$, $-19 \le k \le 19$, $-10 \le l \le 10$. Three standard reflections, linear decay from 0·968 to 1·020, intensities adjusted accordingly; 4606 data, 2303 unique, 248 unobserved, $I < 3\sigma(I)$, $R_{\rm int} = 0{\cdot}014$; starting coordinates from oligoclase, $Na_{0.83}K_{0.01}Ca_{0.16}Al_{1.16}Si_{2.84}O_8$ (Phillips, Colville & Ribbe, 1971); refined by full-matrix least squares minimizing $\sum w(|F_o| - |F_c|)^2$, $w = 1/[\sigma(F_o)^2 + (0{\cdot}005F_o)^2 + 4{\cdot}5]$ (Killean & Lawrence, 1969), 119 parameters; anisotropic thermal parameters; isotropic extinction $g = 2{\cdot}4\,(2) \times 10^{-6}$; final $R = 0{\cdot}030$, $wR = 0{\cdot}036$; max. shift to e.s.d. = 0·00; max. and min. of ΔF synthesis 0·14 (10) and −0·16 (10) e Å^{-3}; e.s.d. of observation of unit weight = 1·32, atomic scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974); anomalous-dispersion effects were included in F_c (Ibers & Hamilton, 1964); values of f' and f'' from *International Tables for X-ray Crystallography* (1974); computer programs *SDP*/VAX (Frenz, 1978).

Table 1. *Positional and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

Anisotropically refined atoms are given in the form of the equivalent isotropic displacement parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

	x	y	z	$B_{\rm eq}$(Å^2)
Na	0·2721 (2)	0·0017 (2)	0·1385 (2)	6·82 (3)
$T_1 0$	0·00880 (6)	0·16574 (4)	0·21242 (7)	0·764 (8)
$T_1 m$	0·00427 (6)	0·81603 (4)	0·23167 (7)	0·777 (8)
$T_2 0$	0·69086 (6)	0·10857 (4)	0·31795 (7)	0·778 (8)
$T_2 m$	0·68395 (6)	0·87870 (4)	0·35626 (7)	0·750 (8)
$O_A 1$	0·0052 (2)	0·1338 (1)	0·9780 (2)	1·50 (3)
$O_A 2$	0·5920 (2)	0·9924 (1)	0·2791 (2)	1·17 (2)
$O_B 0$	0·8178 (2)	0·1086 (1)	0·1949 (2)	1·53 (3)
$O_B m$	0·8188 (2)	0·8476 (1)	0·2496 (2)	1·73 (3)
$O_C 0$	0·0153 (2)	0·2939 (1)	0·2757 (2)	1·40 (2)
$O_C m$	0·0218 (2)	0·6888 (1)	0·2211 (2)	1·41 (3)
$O_D 0$	0·1991 (2)	0·1110 (1)	0·3876 (2)	1·36 (2)
$O_D m$	0·1868 (2)	0·8672 (1)	0·4305 (2)	1·51 (3)

Table 2. *Distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

$T_1 0$—$O_A 1$	1·679 (1)	Na—$O_A 2$	2·345 (2)
—$O_B 0$	1·676 (1)	—$O_D 0$	2·462 (2)
—$O_C 0$	1·672 (1)	—$O_B 0$	2·489 (2)
—$O_D 0$	1·682 (1)	—$O_A 1$	2·626 (2)
		—$O_A 1$	2·650 (2)
$T_1 m$—$O_A 1$	1·635 (1)	—$O_C m$	3·014 (2)
—$O_B m$	1·619 (1)	—$O_D m$	3·094 (3)
—$O_C m$	1·639 (1)	—$O_C 0$	3·245 (2)
—$O_D m$	1·632 (1)	—$O_B m$	3·286 (3)
$T_2 0$—$O_A 2$	1·648 (1)	$T_1 0$—$O_A 1$—$T_1 m$	142·69 (9)
—$O_B 0$	1·627 (1)	$T_2 0$—$O_A 2$—$T_2 m$	129·84 (8)
—$O_C m$	1·630 (1)	$T_1 0$—$O_B 0$—$T_2 0$	140·41 (9)
—$O_D m$	1·624 (1)	$T_1 m$—$O_B m$—$T_2 m$	159·38 (10)
		$T_1 0$—$O_C 0$—$T_2 m$	130·27 (8)
$T_2 m$—$O_A 2$	1·648 (1)	$T_1 m$—$O_C m$—$T_2 0$	134·71 (9)
—$O_B m$	1·625 (1)	$T_1 0$—$O_D 0$—$T_2 m$	134·87 (8)
—$O_C 0$	1·625 (1)	$T_1 m$—$O_D m$—$T_2 0$	150·53 (10)
—$O_D 0$	1·635 (1)		

After initial convergence, mean T—O bond lengths were calculated for each tetrahedral site and used to estimate the Al/(Al+Si) contents [Kroll & Ribbe, 1983; equation (3) below]. These values were then used to adjust the scattering factors in the final stages of refinement.

Discussion. Final atomic coordinates are listed in Table 1, and principal bond distances and angles are listed in Table 2.*

There is a pronounced anisotropy of the Na atom in all albites. Winter, Ghose & Okamura (1977) have suggested that the anisotropy in low albite is attributable solely to thermal disorder. The anisotropy in high

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*Lists of structure factors, anisotropic thermal parameters, distances and angles and further experimental details have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51512 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

albite, which is substantially greater, is due to positional disorder as well (Prewitt, Sueno & Papike, 1976; Winter, Okamura & Ghose, 1979). Although no split-atom models are tested in this study, comparison of the B_{eq} value of sodium in this intermediate albite (6·82 Å^2) with unpublished results for a low albite (2·59 Å^2) and a high albite (7·49 Å^2) from the same suite suggests that positional disorder is present in this structure.

This structure determination is the first of an albite with any other than a completely ordered (Harlow & Brown, 1980; Smith, Artioli & Kvick, 1986) or nearly disordered (Prewitt *et al.*, 1976; Winter *et al.*, 1979) Al, Si arrangement. As such, it presents the first test of the numerous models that have been devised to estimate Al/(Al + Si) contents of tetrahedral sites from lattice parameters or other physical properties of albites.

Kroll & Ribbe (1983) established a method for calculating the average Al/(Al + Si) content (t_i) of individual tetrahedral sites (T_i) using the results of 44 modern structure analyses of K,Na,Ca feldspars:

$$\begin{aligned} t_i = {} & 0{\cdot}25(1 + n_{\rm An}) \\ & + (\langle T_i\text{—O}\rangle - \langle\langle T\text{—O}\rangle\rangle)/\text{constant}, \end{aligned} \qquad (3)$$

where t_i is the Al content or site occupancy of the T_i tetrahedral site (*i.e.* t_i = number of Al atoms occupying T_i tetrahedra divided by the number of T_i tetrahedra), $n_{\rm An}$ (=0·00 in MAB176) is the mole fraction of the anorthite ($CaAl_2Si_2O_8$) content, (T_i—O) is the mean of four (Al,Si)—O bond lengths for the T_i tetrahedron, and $\langle\langle T\text{—O}\rangle\rangle$ is the grand mean of all nonequivalent T—O bond lengths in the unit cell. The denominator of the second term is $\langle\langle\text{Al—O}\rangle\rangle - \langle\langle\text{Si—O}\rangle\rangle$, and it is equal to 0·125 Å for K- and 0·130 Å for the Na-rich feldspars.

Using equation (3) and the T—O bond distances from Table 1, this albite is estimated to have $t_1 0 = 0{\cdot}510\,(6)$, $t_1 m = 0{\cdot}155\,(7)$, $t_2 0 = 0{\cdot}164\,(6)$, $t_2 m = 0{\cdot}171\,(6)$, and $\Delta t_1 = 0{\cdot}356\,(9)$. Taken at face value, this Al,Si distribution is consistent with all those observed for Na-rich plagioclase feldspars, $Na_{1-x}Ca_xAl_{1-x}Si_{3-x}O_8$ [*cf.* Table 1, p. 60 in Kroll & Ribbe (1983) and Table 4, p. 27 in Ribbe (1984)], even down to the detail that $t_1 m$ is slightly smaller than $t_2 0$ which in turn is smaller than $t_2 m$. If, as Kroll & Ribbe (1987, p. 493) suggest, we calculate Δt_1 using the following,

$$\Delta t_1 = t_1 0 - (t_1 m + t_2 0 + t_2 m)/3, \qquad (4)$$

the value becomes 0·347 (7) – slightly, but not significantly, smaller.

The reciprocal-lattice angles, α^* and γ^*, of this 'intermediate' (partially disordered) albite were determined to be 85·97 (1) and 88·64 (1)°, respectively. Both agree within 0·02° with those measured from precession photographs by Su *et al.* (1986). Using equation (2), the calculated value of Δt_1 is 0·290, not significantly different from $\Delta t_1 = 0{\cdot}288$ calculated from equation (1) using the optic axial angle ($2V_x = 66{\cdot}7°$) observed by Su *et al.* (1986) on this same crystal.

The question arises as to whether or not the value $\Delta t_1 \sim 0{\cdot}35$, estimated directly from mean bond distances using equation (3) or (4), is significantly different from $\Delta t_1 \sim 0{\cdot}29$, estimated from equations (1) and (2). If the assumptions on which equations (1) and (3) are based are correct and if all errors are assumed to be random and independently distributed, it is possible to estimate errors for Δt_1. Using bond lengths, the propagation of errors suggests $\Delta t_1 = 0{\cdot}356\,(9)$ [or 0·347 (7), if equation (4) is employed]. The errors for the coefficients in equation (1) given by Su *et al.* (1986) yield $\Delta t_1 = 0{\cdot}29\,(5)$. Given the uncertainties of the assumptions and the proximity of the upper range of the equation (1) values to the lower range of the equation (3) values, it is not possible to provide a definite answer to the question at this time. However, the details of this comparative study will be continued when the crystal structures of the entire suite of low–high albites are completed, and a suite of Δt_1 values is available for comparison.

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Atomic Substitution in $Cd_{1-x}Mn_xTe$ for $0{\cdot}1 \le x \le 0{\cdot}4$

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Abstract. Cadmium manganese telluride, $Cd_{1-x}Mn_xTe$ with $x = 0{\cdot}10$, $0{\cdot}25$ and $0{\cdot}40$ has $M_r = 234{\cdot}25$, $225{\cdot}63$ and $217{\cdot}02$, respectively. Each composition is cubic, $F\bar{4}3m$, $a_{0.10} = 6{\cdot}4531\ (20)$, $a_{0.25} = 6{\cdot}4396\ (10)$, $a_{0.40} = 6{\cdot}4163\ (22)$ Å, $V_{0.10} = 268{\cdot}7\ (5)$, $V_{0.25} = 267{\cdot}0\ (4)$, $V_{0.40} = 264{\cdot}2\ (5)$ Å^3, $Z = 4$, $D_m^{0.10} = 5{\cdot}91\ (5)$, $D_m^{0.40} = 5{\cdot}49\ (3)$ g cm^{-3}, $D_x^{0.10} = 5{\cdot}790$, $D_x^{0.25} = 5{\cdot}612$, $D_x^{0.40} = 5{\cdot}457$ g cm^{-3}, $\lambda(\text{Mo } K\alpha_1,\alpha_2) = 0{\cdot}709319$, $0{\cdot}713609$ Å, $\mu_{0.10} = 1{\cdot}806$, $\mu_{0.25} = 1{\cdot}767$, $\mu_{0.40} = 1{\cdot}734$ cm^{-1}, $T = 294\ (1)$ K. $R(F_m) = 0{\cdot}0108$ for $x = 0{\cdot}10$, $0{\cdot}0259$ for $x = 0{\cdot}25$ and $0{\cdot}0117$ for $x = 0{\cdot}40$, based upon 214, 188 and 205 independent averaged structure factors at the three respective compositions. Mn completely substitutes for Cd in the range $0{\cdot}1 \le x \le 0{\cdot}4$. The randomly distributed Cd and Mn atoms at the Cd site in the zinc-blende structure, and the Te atom, each undergo significantly anharmonic displacements that increase with increasing Mn content. The anharmonicity at both sites probably originates in static atomic displacements along the unit-cell body diagonals that conserve the ~0·05 Å difference between average Te—Cd and Te—Mn interatomic distances. The lattice constant follows Vegard's rule in the range $0 \le x \le 0{\cdot}4$.

Introduction. The semimagnetic semiconducting properties of $Cd_{1-x}Mn_xTe$ have led to numerous recent studies of this system (see, for example, Giebultowicz, Lebech, Buras, Minor, Kepa & Galazka, 1984). Pajaczkowska (1978) gave lattice constants for the resulting zinc-blende structure that ranged from 6·479 (1) Å with $x = 0{\cdot}05$ to 6·378 (2) Å with $x = 0{\cdot}7$. Triboulet & Didier (1981) confirm that solid solutions with zinc-blende structure form between $x = 0$ and 0·75. The distribution coefficient of Mn in the composition range $0{\cdot}1 \le x \le 0{\cdot}4$ is found to be close to unity (Bridenbaugh, 1985). Since large single crystals are readily grown throughout the stability range and the lattice constant can be chosen at will between 6·37 and 6·47 Å (Balzarotti, Motta, Kisiel, Zimnal-Starnawska, Czyzyk & Podgorny, 1985), $Cd_{1-x}Mn_xTe$ has become an attractive choice of substrate crystal for the epitaxic overgrowth of $Hg_{1-x}Cd_xTe$ and related (II)–(VI) compositions in the fabrication of infrared detectors. The growing importance of this system of materials led us to study the nature of the substitution that takes place as x is varied, with results as presented below.

Experimental. Large single-crystal boules of $Cd_{1-x}Mn_xTe$ were grown by the vertical Bridgman method using a multizone furnace. The temperature profiles in the hot and cold zones varied less than ±1 K over their entire length and were separated by a 5 cm long unheated loss section that created a thermal gradient of 25 K cm^{-1} at the growth interface. The growth rate varied from 1 to 2 cm h^{-1}. The ampoule used was 16 mm ID fused quartz; the inner surface was coated with pyrolytic graphite to prevent reaction by Mn and Cd. The first and last 20% of each growth boule, with compositions that correspond to $x = 0{\cdot}10$, $0{\cdot}25$ and $0{\cdot}40$, was discarded. The densities for compositions with $x = 0{\cdot}10$ and $0{\cdot}40$ were measured pycnometrically on samples with masses greater than 20 mg. A sphere of each composition was ground, with radius as in Table 1, and mounted in arbitrary orientation on a CAD-4 diffractometer. Radiation used was Mo $K\alpha$

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