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A refinement of the structure of anorthite *,[1]

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Auszug

Für eine Verfeinerung der Struktur von Anorthit wurden Kristalle vom Val Plasmeda, Tirol, Österreich verwendet. Der erreichte R-Wert beträgt 6,0%. Die erhaltenen Atomparameter und wichtige Bindungslängen und -winkel werden angegeben.

Abstract

A refinement of the structure of anorthite has been completed on crystals from Val Plasmeda, Tyrol, Austria. Atomic parameters and significant bond lengths and angles are reported. The residual error index R is 6.0%.

Introduction

The structure of anorthite has been reexamined using crystals from Val Pasmeda, Tyrol, Austria (U.S. National Museum C2354). The composition of this material was determined with the electron probe microanalyzer to be An_{100} (P. H. RIBBE, personal communication). All crystals examined showed c and d reflections indicative of the low-structure type.

Experimental

An approximately cubic fragment of dimensions $0.15 \times 0.13 \times 0.20$ mm was selected for examination. Cell dimensions were determined by

* *Dedicated to Professor F. Laves on the occasion of his 65th birthday.*

[1] Investigation performed, in part, under the auspices of the National Aeronautics and Space Administration.

the method of least squares from single-crystal observations of scattering angle. These data yielded the following:

$$a = 8.173 \pm 0.001 \text{ Å} \qquad \alpha = 93.113 \pm 0.006°$$
$$b = 12.869 \pm 0.001 \qquad \beta = 115.913 \pm 0.006$$
$$c = 14.165 \pm 0.001 \qquad \gamma = 91.261 \pm 0.006$$

cell volume = 1337.735 Å^3

space group $P\bar{1}$.

Intensity data were collected by means of an automated four-circle diffractometer using the θ-2θ scan method with crystal-monochromatized Mo$K\alpha$ radiation; a total of 7836 observations were recorded. Absorption corrections were made by approximating the crystal volume with six bounding planes, then applying an integration procedure (LARSON, CROMER and ROOF, 1964).

Refinement

The analysis was begun using the atomic coordinates derived by KEMPSTER, MEGAW and RADOSLOVICH (1962; MEGAW *et al.*, 1962) for anorthite from Monte Somma, Vesuvius. The parameters were refined by iterative least-squares calculations, employing both isotropic and anisotropic temperature factors. Hartree scattering factors were employed (CROMER, LARSON and WABER, 1963). The program written by L. FINGER of the Geophysical Laboratory was used for all least-squares computations. Because of the large number of atoms, all parameters could not be refined simultaneously.

With the inclusion of anisotropic thermal parameters for oxygen and calcium atoms, the measurement of agreement between observed and calculated $|F|$ values was as follows:

$$R\,[\equiv \Sigma\,(|F_o| - s\,|F_c|)^2 \,/\, \Sigma\,|F_o|^2] = 0.06\,.$$

The observations were weighted in inverse proportion to a variance defined as:

$$\sigma^2\,(F^2) = s\,(A^{-1}LP)^2\,[\sigma_n^2 + (0.02\,N)^2])$$

where s is a scale factor, A^{-1} is an absorption correction, LP is the Lorentz and polarization correction, and σ_n^2 is the statistical variance of N, the net count.

Table 1. *Atomic fractional coordinates of anorthite*
(Least-squares standard errors in the last significant figure are given in parentheses)

Atom	x	y	z	B
$O_A(1000)$	0.0269(4)	0.1242(3)	0.9960(4)	0.730(4) Å^2
$O_A(1z00)$	0.9812(4)	0.1257(3)	0.4835(3)	0.714(4)
$O_A(10i0)$	0.4875(4)	0.6241(4)	0.4868(4)	0.661(4)
$O_A(1zi0)$	0.5169(3)	0.6247(3)	0.9966(4)	0.754(5)
$O_A(2000)$	0.5744(4)	0.9913(3)	0.1434(4)	0.607(3)
$O_A(2z00)$	0.5720(4)	0.9897(4)	0.6379(4)	0.665(3)
$O_A(20i0)$	0.0731(3)	0.4875(4)	0.6354(4)	0.628(3)
$O_A(2zi0)$	0.0734(3)	0.4932(3)	0.1386(4)	0.796(4)
$O_B(0000)$	0.8154(5)	0.1018(4)	0.0806(4)	0.648(3)
$O_B(0z00)$	0.8124(4)	0.0968(4)	0.6057(4)	0.745(4)
$O_B(00i0)$	0.3325(4)	0.5957(3)	0.6047(4)	0.808(4)
$O_B(0zi0)$	0.2854(4)	0.6034(3)	0.0798(4)	0.813(4)
$O_B(m000)$	0.8175(5)	0.8554(4)	0.1443(3)	1.192(5)
$O_B(mz00)$	0.8113(4)	0.8518(4)	0.6034(4)	0.857(4)
$O_B(m0i0)$	0.2987(4)	0.3559(3)	0.6115(4)	0.799(4)
$O_B(mzi0)$	0.3419(4)	0.3587(3)	0.1333(3)	1.140(4)
$O_C(0000)$	0.0141(4)	0.2796(3)	0.1351(4)	1.028(4)
$O_C(0z00)$	0.0205(4)	0.2909(3)	0.6474(4)	0.841(4)
$O_C(00i0)$	0.5094(3)	0.7769(3)	0.6344(4)	0.824(3)
$O_C(0zi0)$	0.5092(4)	0.7965(3)	0.1510(3)	0.714(4)
$O_C(m000)$	0.0008(2)	0.6806(3)	0.1044(2)	0.662(3)
$O_C(mz00)$	0.0089(3)	0.6899(4)	0.6013(3)	0.539(3)
$O_C(m0i0)$	0.5165(4)	0.1788(3)	0.6101(3)	0.569(3)
$O_C(mzi0)$	0.5071(3)	0.1963(3)	0.0975(3)	0.905(5)
$O_D(0000)$	0.1826(3)	0.1059(2)	0.1917(3)	0.755(4)
$O_D(0z00)$	0.2155(3)	0.1025(2)	0.6847(4)	0.652(4)
$O_D(00i0)$	0.6989(3)	0.6079(4)	0.6790(4)	0.893(5)
$O_D(0zi0)$	0.6908(4)	0.6043(3)	0.2019(2)	0.703(4)
$O_D(m000)$	0.2038(2)	0.8740(3)	0.2107(2)	0.686(3)
$O_D(mz00)$	0.1709(2)	0.8564(4)	0.7197(3)	1.097(4)
$O_D(m0i0)$	0.6884(3)	0.3628(4)	0.7332(4)	1.123(4)
$O_D(mzi0)$	0.7006(3)	0.3697(4)	0.1970(2)	1.060(4)
$T_1(0000)$	0.0092(2)	0.1592(1)	0.1044(1)	0.662(3)
$T_1(0z00)$	0.0066(2)	0.1610(1)	0.6112(1)	0.609(5)
$T_1(00i0)$	0.5062(2)	0.6560(1)	0.6042(1)	0.631(4)
$T_1(0zi0)$	0.4984(2)	0.6658(1)	0.1128(1)	0.605(3)
$T_1(m000)$	0.9912(2)	0.8152(1)	0.1176(1)	0.598(4)
$T_1(mz00)$	0.0061(2)	0.8154(1)	0.6135(1)	0.558(3)
$T_1(m0i0)$	0.5073(2)	0.3145(1)	0.6212(1)	0.622(5)
$T_1(mzi0)$	0.5041(2)	0.3204(1)	0.1099(1)	0.613(4)

Table 1. *(Continued)*

Atom	x	y	z	B
$T_2(0000)$	0.6485(2)	0.1130(1)	0.1519(1)	0.637(5)
$T_2(0z00)$	0.6814(2)	0.1034(1)	0.6646(1)	0.596(3)
$T_2(00i0)$	0.1907(2)	0.6110(1)	0.6674(1)	0.664(4)
$T_2(0zi0)$	0.1713(2)	0.6067(1)	0.1495(1)	0.670(6)
$T_2(m000)$	0.6742(2)	0.8829(1)	0.1876(1)	0.624(5)
$T_2(mz00)$	0.6809(2)	0.8719(1)	0.6725(1)	0.572(4)
$T_2(m0i0)$	0.1762(2)	0.3789(1)	0.6734(1)	0.666(3)
$T_2(mzi0)$	0.1852(2)	0.3775(1)	0.1816(1)	0.657(5)
Ca(000)	0.2651(2)	0.9864(1)	0.0867(1)	1.203(6)
Ca(z00)	0.2692(2)	0.0312(1)	0.5435(1)	0.798(4)
Ca($0i$0)	0.7737(2)	0.5359(1)	0.5412(1)	0.865(4)
Ca(zi0)	0.7634(2)	0.5052(1)	0.0747(1)	1.432(6)

Table 2. *Anisotropic thermal vibration parameters**
(Estimated standard deviations in the last significant figure in parentheses)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
$O_A(1000)$	0.0032(6)	0.0012(3)	0.0010(3)	− 0.0003(5)	0.0009(5)	0.0001(3)
$O_A(1z00)$	0.0038(6)	0.0013(3)	0.0006(3)	− 0.0002(5)	0.0008(5)	− 0.0002(2)
$O_A(10i0)$	0.0027(5)	0.0010(3)	0.0014(3)	0.0001(4)	0.0010(5)	0.0001(3)
$O_A(1zi0)$	0.0046(4)	0.0015(3)	0.0012(3)	− 0.0001(5)	0.0018(5)	− 0.0002(3)
$O_A(2000)$	0.0018(4)	0.0008(3)	0.0014(3)	− 0.0001(4)	0.0004(5)	− 0.0001(2)
$O_A(2z00)$	0.0017(5)	0.0012(3)	0.0012(3)	0.0003(5)	0.0003(5)	0.0003(3)
$O_A(20i0)$	0.0020(6)	0.0009(3)	0.0015(3)	0.0001(4)	0.0005(5)	0.0003(3)
$O_A(2zi0)$	0.0017(6)	0.0013(3)	0.0015(3)	− 0.0005(5)	0.0005(5)	− 0.0001(3)
$O_B(0000)$	0.0031(5)	0.0009(3)	0.0015(3)	− 0.0002(4)	0.0012(5)	− 0.0002(3)
$O_B(0z00)$	0.0056(6)	0.0009(3)	0.0016(3)	− 0.0002(5)	0.0023(5)	− 0.0002(2)
$O_B(00i0)$	0.0003(3)	0.0013(3)	0.0018(4)	0.0001(5)	0.0017(5)	− 0.0001(3)
$O_B(0zi0)$	0.0033(3)	0.0013(3)	0.0023(3)	− 0.0002(5)	0.0020(5)	− 0.0004(3)
$O_B(m000)$	0.0037(6)	0.0022(4)	0.0032(4)	− 0.0001(5)	0.0029(6)	− 0.0007(3)
$O_B(mz00)$	0.0062(6)	0.0010(3)	0.0010(3)	0.0003(5)	0.0014(5)	0.0005(2)
$O_B(m0i0)$	0.0045(5)	0.0009(3)	0.0018(3)	− 0.0001(5)	0.0014(5)	0.0002(3)
$O_B(mzi0)$	0.0061(6)	0.0016(3)	0.0027(4)	− 0.0001(5)	0.0027(6)	0.0002(3)
$O_C(0000)$	0.0058(5)	0.0016(3)	0.0016(4)	− 0.0002(5)	0.0022(5)	0.0001(3)
$O_C(0z00)$	0.0044(3)	0.0019(3)	0.0018(3)	0.0004(5)	0.0021(5)	0.0002(3)
$O_C(00i0)$	0.0037(7)	0.0012(3)	0.0017(3)	− 0.0000(5)	0.0013(5)	0.0003(3)
$O_C(0zi0)$	0.0037(6)	0.0012(3)	0.0009(3)	0.0001(5)	0.0009(5)	0.0001(2)

* Coefficients in the expression:

$$\exp\left[-\left(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23}\right)\right] .$$

Table 2. *(Continued)*

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
$O_C(m000)$	0.0024(8)	0.0012(3)	0.0015(3)	− 0.0005(4)	0.0005(4)	− 0.0004(2)
$O_C(mz00)$	0.0017(9)	0.0012(3)	0.0009(3)	− 0.0004(4)	0.0003(4)	− 0.0001(2)
$O_C(m0i0)$	0.0042(9)	0.0007(3)	0.0014(3)	− 0.0001(4)	0.0015(4)	0.0001(2)
$O_C(mzi0)$	0.0039(8)	0.0014(3)	0.0017(3)	0.0003(4)	0.0008(4)	− 0.0001(2)
$O_D(0000)$	0.0048(6)	0.0014(3)	0.0009(3)	− 0.0003(4)	0.0007(5)	0.0001(3)
$O_D(0z00)$	0.0034(5)	0.0013(4)	0.0009(4)	0.0006(4)	0.0005(3)	0.0001(2)
$O_D(00i0)$	0.0040(6)	0.0013(4)	0.0013(3)	0.0001(3)	0.0006(2)	− 0.0002(3)
$O_D(0zi0)$	0.0038(5)	0.0009(3)	0.0010(3)	0.0003(3)	0.0002(4)	0.0001(2)
$O_D(m000)$	0.0032(6)	0.0015(4)	0.0014(5)	0.0000(3)	0.0009(4)	− 0.0003(2)
$O_D(mz00)$	0.0071(5)	0.0015(3)	0.0019(3)	− 0.0004(4)	0.0015(4)	− 0.0001(2)
$O_D(m0i0)$	0.0049(5)	0.0017(3)	0.0011(3)	− 0.0003(4)	0.0002(4)	− 0.0001(2)
$O_D(mzi0)$	0.0042(4)	0.0014(4)	0.0014(3)	0.0003(4)	0.0002(2)	− 0.0001(2)
Ca(000)	0.0038(3)	0.0029(1)	0.0021(1)	− 0.0003(1)	0.0016(1)	− 0.0009(1)
Ca(z00)	0.0032(2)	0.0014(1)	0.0015(1)	0.0003(1)	0.0011(1)	− 0.0004(1)
Ca($0i$0)	0.0032(2)	0.0015(1)	0.0014(1)	0.0005(1)	0.0007(1)	− 0.0003(1)
Ca(zi0)	0.0030(3)	0.0031(1)	0.0024(1)	0.0005(1)	0.0008(1)	− 0.0014(1)

Table 3. *Principal axes of thermal ellipsoids*

Atom	Axis	Root-mean-square displacement	Atom	Axis	Root-mean-square displacement
$O_A(1000)$	1	0.0805 Å	$O_A(2000)$	1	0.0687 Å
	2	0.0922		2	0.0842
	3	0.1059		3	0.1190
$O_A(1z00)$	1	0.0609	$O_A(2z00)$	1	0.0643
	2	0.0990		2	0.0957
	3	0.1102		3	0.1142
$O_A(10i0)$	1	0.0816	$O_A(20i0)$	1	0.0738
	2	0.0912		2	0.0803
	3	0.1054		3	0.1205
$O_A(1zi0)$	1	0.0637	$O_A(2zi0)$	1	0.0606
	2	0.1079		2	0.1103
	3	0.1229		3	0.1176
$O_B(0000)$	1	0.0810	$O_B(m000)$	1	0.0562
	2	0.0850		2	0.1232
	3	0.1165		3	0.1768
$O_B(0z00)$	1	0.0741	$O_B(mz00)$	1	0.0645
	2	0.0845		2	0.1032
	3	0.1353		3	0.1305

Table 3. *(Continued)*

Atom	Axis	Root-mean-square displacement	Atom	Axis	Root-mean-square displacement
$O_B(00i0)$	1	0.0741 Å	$O_B(m0i0)$	1	0.0811 Å
	2	0.1035		2	0.1103
	3	0.1245		3	0.1220
$O_B(0zi0)$	1	0.0713	$O_B(mzi0)$	1	0.0981
	2	0.0972		2	0.1181
	3	0.1451		3	0.1527
$O_C(0000)$	1	0.0845	$O_C(m000)$	1	0.0678
	2	0.1135		2	0.1012
	3	0.1358		3	0.1255
$O_C(0z00)$	1	0.0769	$O_C(mz00)$	1	0.0620
	2	0.0979		2	0.0928
	3	0.1281		3	0.1055
$O_C(00i0)$	1	0.0889	$O_C(m0i0)$	1	0.0749
	2	0.1037		2	0.0907
	3	0.1190		3	0.1143
$O_C(0zi0)$	1	0.0839	$O_C(mzi0)$	1	0.1005
	2	0.0976		2	0.1059
	3	0.1023		3	0.1286
$O_D(0000)$	1	0.0873	$O_D(m000)$	1	0.0919
	2	0.1045		2	0.0933
	3	0.1257		3	0.1249
$O_D(0z00)$	1	0.0833	$O_D(mz00)$	1	0.1083
	2	0.0934		2	0.1255
	3	0.1176		3	0.1435
$O_D(00i0)$	1	0.0892	$O_D(m0i0)$	1	0.0873
	2	0.1071		2	0.1206
	3	0.1237		3	0.1365
$O_D(0zi0)$	1	0.0827	$O_D(mzi0)$	1	0.0929
	2	0.0879		2	0.1043
	3	0.1236		3	0.1415
Ca(000)	1	0.0896	Ca(0i0)	1	0.0847
	2	0.1089		2	0.0964
	3	0.1759		3	0.1324
Ca(z00)	1	0.0790	Ca(zi0)	1	0.0855
	2	0.0996		2	0.0999
	3	0.1302		3	0.2018

Table 4. *Tetrahedral interatomic distances*
(Estimated standard deviations in the last significant figure in parentheses)

$T_1(0000)$	$-O_A(1000)$	1.645(2) Å	$T_1(0z00)$	$-O_A(1z00)$	1.760(2) Å
	$O_B(0000)$	1.619(2)		$O_B(0z00)$	1.743(2)
	$O_C(0000)$	1.582(2)		$O_C(0z00)$	1.709(2)
	$O_D(0000)$	1.616(2)		$O_D(0z00)$	1.776(2)
	Mean:	1.616		Mean:	1.747
$T_1(00i0)$	$-O_A(10i0)$	1.632(2)	$T_1(0zi0)$	$-O_A(1zi0)$	1.772(2)
	$O_B(00i0)$	1.606(2)		$O_B(0zi0)$	1.755(2)
	$O_C(00i0)$	1.588(2)		$O_C(0zi0)$	1.727(2)
	$O_D(00i0)$	1.626(2)		$O_D(0zi0)$	1.767(2)
	Mean:	1.613		Mean:	1.755
$T_1(mz00)$	$-O_A(1z00)$	1.647(2)	$T_1(m000)$	$-O_A(1000)$	1.777(2)
	$O_B(mz00)$	1.617(2)		$O_B(m000)$	1.705(2)
	$O_C(mz00)$	1.617(2)		$O_C(m000)$	1.738(2)
	$O_D(mz00)$	1.571(2)		$O_D(m000)$	1.779(2)
	Mean:	1.613		Mean:	1.750
$T_1(mzi0)$	$-O_A(1zi0)$	1.644(2)	$T_1(m0i0)$	$-O_A(10i0)$	1.777(2)
	$O_B(mzi0)$	1.583(2)		$O_B(m0i0)$	1.747(2)
	$O_C(mzi0)$	1.599(2)		$O_C(m0i0)$	1.752(2)
	$O_D(mzi0)$	1.626(2)		$O_D(m0i0)$	1.702(2)
	Mean:	1.613		Mean:	1.745
$T_2(0z00)$	$-O_A(2z00)$	1.635(2)	$T_2(0000)$	$-O_A(2000)$	1.760(2)
	$O_B(0z00)$	1.620(2)		$O_B(0000)$	1.769(2)
	$O_C(m0i0)$	1.606(2)		$O_C(mzi0)$	1.740(2)
	$O_D(m000)$	1.605(2)		$O_D(mz00)$	1.698(2)
	Mean:	1.617		Mean:	1.742
$T_2(0zi0)$	$-O_A(2zi0)$	1.617(2)	$T_2(00i0)$	$-O_A(20i0)$	1.769(2)
	$O_B(0zi0)$	1.628(2)		$O_B(00i0)$	1.751(2)
	$O_C(m000)$	1.614(2)		$O_C(mz00)$	1.754(2)
	$O_D(m0i0)$	1.574(2)		$O_D(mzi0)$	1.727(2)
	Mean:	1.608		Mean:	1.750
$T_2(m000)$	$-O_A(2000)$	1.644(2)	$T_2(mz00)$	$-O_A(2z00)$	1.755(2)
	$O_B(m000)$	1.581(2)		$O_B(mz00)$	1.748(2)
	$O_C(0zi0)$	1.607(2)		$O_C(00i0)$	1.716(2)
	$O_D(0z00)$	1.629(2)		$O_D(0000)$	1.757(2)
	Mean:	1.615		Mean:	1.744

Table 4. *(Continued)*

$T_2(m0i0)-O_A(20i0)$	1.641(2) Å	$T_2(mzi0)-O_A(2zi0)$	1.759(2) Å
$O_B(m0i0)$	1.618(2)	$O_B(mzi0)$	1.713(2)
$O_C(0z00)$	1.586(2)	$O_C(0000)$	1.735(2)
$O_D(0zi0)$	1.616(2)	$O_D(00i0)$	1.774(2)
Mean:	1.615	Mean:	1.745
Grand mean:	1.614	Grand mean:	1.747

Table 5. *Bond angles at tetrahedral sites*

	O_A-O_B	O_A-O_C	O_A-O_D	O_B-O_C	O_B-O_D	O_C-O_D
$T_1(0000)$	100.90°	118.07°	101.40°	111.73°	113.80°	110.44°
$T_1(00i0)$	103.09	116.38	102.05	110.92	113.56	110.51
$T_1(mz00)$	100.78	113.70	108.85	111.38	113.45	108.61
$T_1(mzi0)$	106.15	112.27	102.08	113.14	112.06	110.54
$T_2(0z00)$	105.34	101.24	110.17	112.51	111.79	114.83
$T_2(0zi0)$	109.19	102.50	110.99	112.86	107.14	114.10
$T_2(m000)$	111.89	104.43	108.95	112.98	107.26	111.33
$T_2(m0i0)$	108.79	106.37	107.89	112.60	108.75	112.27
$T_1(0z00)$	99.75	117.51	98.98	112.77	115.60	111.25
$T_1(0zi0)$	97.25	121.03	97.16	113.20	116.44	110.66
$T_1(m000)$	107.57	112.19	99.12	114.34	111.15	111.40
$T_1(m0i0)$	99.28	113.08	108.52	113.59	113.26	108.83
$T_2(0000)$	108.87	104.115	107.84	112.63	108.08	115.02
$T_2(00i0)$	100.96	99.94	107.64	112.74	115.95	116.74
$T_2(mz00)$	108.59	105.69	103.15	110.45	111.95	116.30
$T_2(mzi0)$	110.32	105.24	107.35	111.99	108.71	113.09

Table 6. *Coordination of calcium* (within 3 Å)
(Estimated standard deviations in the last significant figure in parentheses)

$Ca(000)-O_A(2000)$	2.292(2) Å	$Ca(z00)-O_A(2z00)$	2.333(2) Å
$O_B(0000)$	2.378(2)	$O_D(0z00)$	2.372(2)
$O_D(0000)$	2.390(2)	$O_B(0z00)$	2.443(2)
$O_A(1000)$	2.515(2)	$O_B(mz00)$	2.494(2)
$O_D(m000)$	2.538(2)	$O_A(1z00)$	2.496(2)
$O_A(1000)$	2.608(2)	$O_C(m0i0)$	2.559(2)
Mean:	2.454	$O_A(1z00)$	2.733(2)
		Mean:	2.490

Table 6. *(Continued)*

$Ca(0i0)-O_A(20i0)$	2.336(2)	$Ca(zi0)-O_A(2zi0)$	2.300(2)
$O_B(00i0)$	2.426(2)	$O_B(0zi0)$	2.405(2)
$O_D(00i0)$	2.434(2)	$O_D(0zi0)$	2.440(2)
$O_A(10i0)$	2.448(2)	$O_A(1zi0)$	2.454(2)
$O_B(m0i0)$	2.494(2)	$O_A(1zi0)$	2.616(2)
$O_C(mz00)$	2.563(2)	$O_D(mzi0)$	2.717(2)
$O_A(10i0)$	2.817(2)	$O_C(m000)$	2.834(2)
Mean:	2.503	Mean:	2.525

Atomic coordinates and thermal vibration parameters derived from the final least-squares cycle are listed in Tables 1 and 2. The atom notation of MEGAW (1956) is used. Significant details of the structure are recorded in Tables 4—7. Figure 1 illustrates a portion of the structure bounded by the planes $y = \pm 0.3$.

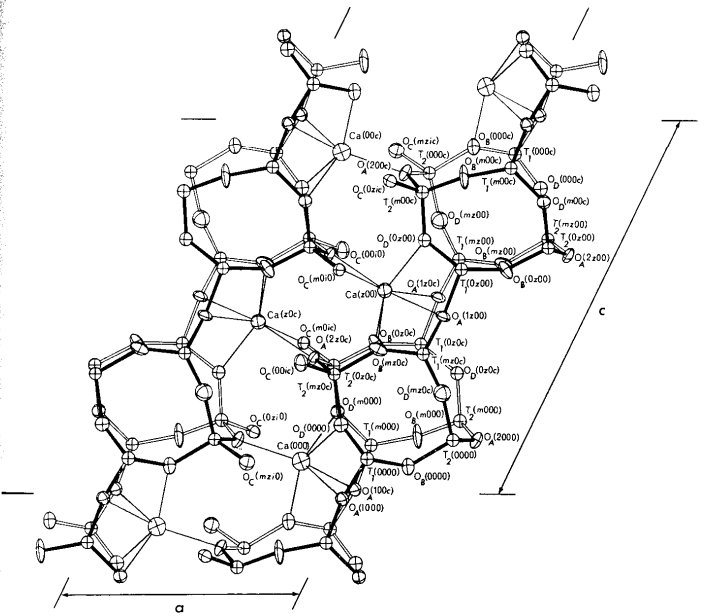

Fig. 1

Table 7. T–O–T *angles in the fourfold rings*

Atom	Angle	Atom	Angle
$O_B(0000)$	129.41 Å	$O_B(0z00)$	138.79 Å
$O_D(0000)$	136.45	$O_D(0z00)$	123.67
$O_B(mz0c)$	144.07	$O_B(m00c)$	169.97
$O_D(mz0c)$	165.21	$O_D(m00c)$	139.70
Mean:	143.78	Mean:	143.03
$O_B(m0i0)$	145.76	$O_B(mzi0)$	165.67
$O_D(m0i0)$	165.08	$O_D(mzi0)$	136.14
$O_B(0zic)$	126.88	$O_B(00ic)$	137.61
$O_D(0zic)$	135.01	$O_D(00ic)$	127.15
Mean:	143.18	Mean:	141.64

Conclusions

The atomic coordinates derived are not significantly different from those previously determined. The anomalous Al—O bond lengths and tetrahedral distortions in AlO_4 tetrahedra have been confirmed.

References

D. T. CROMER, A. C. LARSON and J. T. WABER (1963), Hartree scattering factors for elements 2 through 98 and for several ions. Los Alamos Scientific Laboratory, LA-2987.

C. J. E. KEMPSTER, H. D. MEGAW and E. W. RADOSLOVICH (1962), The structure of anorthite, $CaAl_2Si_2O_8$. I. Structure analysis. Acta Crystallogr. **15**, 1005–1017.

A. C. LARSON, D. T. CROMER and B. B. ROOF (1964), An integrated series of crystallographic computer programs. II. Processing collected intensity data. Los Alamos Scientific Laboratory, LA-3043.

H. D. MEGAW (1956), Notation for the feldspar structure. Acta Crystallogr. **9**, 56–60.

H. D. MEGAW, C. J. E. KEMPSTER and E. W. RADOSLOVICH (1962), The structure of anorthite, $CaAl_2Si_2O_8$. II. Description and discussion. Acta Crystallogr. **15**, 1017–1035.