

The Crystal Structure of α -Na₂Si₂O₅

BY A. K. PANT* AND D. W. J. CRUICKSHANK†

Chemistry Department, University of Glasgow, Glasgow W.2, Scotland

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Liebau's structure for α -Na₂Si₂O₅ is corrected. New data have been used in a refinement which gives the dimensions of the silicate sheet as Si-O(bridging) = 1.643, 1.638, 1.609 ± 0.004 Å and Si-O(non-bridging) = 1.578 Å. The two Si-O-Si angles are 138.9 and 160.0 ± 0.15°. Each Na forms 5 Na-O links in the range 2.29–2.60 Å. The structure is interpreted by the Pauling-Zachariasen method of the balancing of valences and in terms of π -bonding effects.

Introduction

As part of his study of the $A_m(\text{Si}_2\text{O}_5)_n$ structures, Liebau (1961*a*) reported some preliminary work and discussion on the structure of α -Na₂Si₂O₅. He determined the x and y parameters from a sharpened $P(UV0)$ Patterson projection and refined them, at first in the space group $Pcnb$, by two-dimensional Fourier syntheses and difference maps using 64 independent non-zero F_o 's. Although the extinctions observed by him were characteristic for the space group $Pcnb$, Donnay & Donnay (1953) had earlier observed some weak $0kl$ reflexions with odd l values, implying thereby that the real symmetry of the crystal could be $Pmnb$ or $P2_1nb$. Towards the end of the $Pcnb$ refinement Liebau (1961*a*) considered that the oxygen atom at the centre of symmetry should deviate from the special position, thus avoiding an Si-O-Si angle of 180°. His further refinement was therefore carried out in the space group $P2_1nb$, and led to a residual R of 16.5% for the 64 observed $hk0$ reflexions.

With these x and y parameters Liebau built a model which corresponded with the sharpened $P(0VW)$ Patterson projection determined from 39 coefficients. However, he did not report the z parameters as they were not then exact, and he stated that further work was in progress. We have not found any later report on this work.

The present study was undertaken in order (*a*) to settle the problem of the possible 180° angle by collecting very high precision data, (*b*) to determine accurate bond lengths and angles, as these are relevant to the discussion of π -bonding in second-row elements (Cruickshank, 1961), and (*c*) to examine whether Pauling's (1929) valence balance principle is as successful in explaining the various bond lengths in this structure as it is for datolite, CaBSiO₄(OH) (Pant & Cruickshank, 1967).

Crystal data

α -Na₂Si₂O₅. $M = 182.16$. Orthorhombic, $a = 6.409 \pm 0.002$, $b = 15.422 \pm 0.004$, $c = 4.896 \pm 0.002$ Å; $V = 483.9$ Å³, $Z = 4$, $D_c = 2.50$ g.cm⁻³. $F(000) = 520$. Space group $Pcnb$ (no. 60). μ for Mo $K\alpha$ radiation = 8.4 cm⁻¹.

Experimental

Crystals of α -Na₂Si₂O₅ were kindly supplied by Dr F. P. Glasser. For the present work two very small crystals were selected: a cylindrical needle of length 0.3 mm and mean diameter 0.12 mm used for the c -axis, and a granular crystal of mean diameter 0.15 mm for the a -axis setting. These were mounted in glass fibres and were then dipped twice in collodion, which formed a protective coating against moisture and carbon dioxide.

The cell dimensions were redetermined from Weissenberg photographs using a method of least squares proposed by Speakman (1966) and are given under *Crystal Data*. They agree well with the previous values given by Donnay & Donnay (1953) and Liebau (1961*a*).

Although the systematic absences in the zero- and higher-layer Weissenberg photographs around the a and c axes with Cu $K\alpha$ radiation were generally consistent with the space group $Pcnb$, a few weak $0kl$ reflexions with l odd were present in an over-exposed a -axis photograph. These reflexions were quite different from other reflexions since they were much sharper. An additional a -axis Weissenberg photograph with *unfiltered* Cu K radiation showed that these reflexions were not accompanied by the usual $K\beta$ component, although the intensities of 011 and 031 were large enough to give rise to visible β components. They were therefore suspected to be Renninger (1937) reflexions, as was later confirmed from the geometry of the reciprocal lattice and sphere of reflexion. This conclusively proved that the actual space group is $Pcnb$, and not $Pmnb$ or $P2_1nb$ as supposed by Liebau (1961*a*).

Intensity measurements were made on a Hilger linear diffractometer (Arndt & Phillips, 1961) with Mo $K\alpha$ radiation, balanced Sr and Zr filters, and a scintillation counter with pulse height discrimination. With the c -

* Present address: Physics Department, McMaster University, Hamilton, Ontario, Canada.

† Present address: Chemistry Department, University of Manchester Institute of Science and Technology, Sackville Street, Manchester 1, England.

axis mounting $hk0$ through $hk6$ reflexions were measured; and, although no individual layer scaling is usually necessary with diffractometer data, $0kl$ and $1kl$ reflexions were also measured with the a -axis mounting to check that the $hk0$ through $hk6$ measurements were all in the same scale. Further, for both mountings, equivalent reflexions in two octants were measured and their means were taken. The intensities were corrected for Lorentz and polarization factors with programs written by J. G. Sime for the KDF9 computer. No absorption corrections were considered necessary. A comparison of the F_o 's of common reflexions from the two mountings showed that the intensity measurements had been very satisfactory; the ratios of the intensities of the common reflexions were consistent within 4-5%. It was, therefore, decided to include all the reflexions from the two axes and treat them as independent observations. A small number of reflexions obtained at values not significantly above the background were included at their observed values, which provided a simple way of treating 'unobserved' reflexions. Subsequent examination of F_o 's and F_c 's showed that this worked well for most of the reflexions; a few bad ones were later removed from the refinement. In this way, initially 892 (746 c -axis and 146 a -axis) structure amplitudes were obtained.

Determination of structure and refinement

Starting from near the x and y coordinates given by Liebau, four cycles of minimum-residual refinement (Bhuiya & Stanley, 1963) with a program written by K. W. Muir for the KDF9 computer led to a residual of 5.6% for the 70 $hk0$ reflexions. With these x and y parameters and the appropriate O...O and Si-O distances unsuccessful attempts were made to find the z parameters, but one Na-O distance always came out too short. As Liebau's (1961a) $P(0VW)$ Patterson projection also did not provide any clue, it was decided to compute a three-dimensional Patterson map. At this stage, however, it was realized that a simple translation of the whole structure along the y axis by one fourth of the cell edge, thereby moving an oxygen atom from a centre of symmetry on to a twofold axis, would not affect the $hk0$ reflexions and would give at the same time a reasonable value for the Na-O distance. z parameters were fixed from the expected geometry of the structure, and all the peaks in the three-dimensional Patterson map were then interpretable. Four cycles of minimum-residual refinement with the 50 $0kl$ reflexions led to $R=16.7\%$.

Least-squares refinement with the program written by J. G. F. Smith and D. W. J. Cruickshank for the KDF9 computer was then started. The form factors for the neutral atoms were taken from *International Tables for X-ray Crystallography* (1962). Initially unit weight was given to each reflexion. The first structure factor calculation with isotropic thermal parameters gave a residual $R=(\sum |\Delta|)/(\sum |F_o|)$ of 22.2%. Two cycles of the full-matrix least-squares refinement of the coordinates and individual thermal parameters together with two scale factors, one each for the two sets of data collected along the c and a axes, reduced R to 6.6%. Anisotropic thermal parameters were introduced at this stage and R came down to 4.6% with two full-matrix cycles; a third cycle did not produce any significant change.

A close scrutiny of the weighting analysis and the list of observed and calculated structure factors showed that unit weights were not quite satisfactory; the strong reflexions were less accurate, partly perhaps owing to extinction, and there were appreciable errors in low-angle reflexions, mainly due to setting errors in the diffractometer. A gross error was found in the 014 reflexion from the c -axis data; the $|F_o|$'s for the first and second sets were respectively 28 and 45 and the $|F_c|$ was 43. The following weighting scheme suggested by Muir (1967) was then used:

$$w = w(1) \times w(2),$$

where $w(1)=1$ if $\sin \theta/\lambda > p(1)$, otherwise $[(\sin \theta/\lambda)/p(1)]^2$; $w(2)=1$ if $|F_o| < p(2)$, otherwise $p(2)/|F_o|$. The following reflexions were given zero weight: 1,16,0; 122; 6,12,3; 014; 824; 105 from the first set, and 1,14,1; 1,14,3; 1,14,4 from the second set. These omissions were made because these reflexions had relatively very high Δ 's, probably because of errors in the estimation of the intensities or of overlap with Renninger reflexions. Three cycles of full-matrix least-squares refinement with $p(1)=0.4$ and $p(2)=60$ brought the residual down to 3.9%, with considerable improvements in the standard deviations. The refinement at this stage had fully converged and the weighting analysis was also quite satisfactory. It may be useful to add that there were no major shifts in the atomic or even thermal

Table 1. *Final fractional coordinates and e.s.d.'s*

	x	y	z
Na	0.09888 (15)	0.56036 (5)	0.23704 (16)
Si	0.10516 (9)	0.34298 (3)	0.29624 (9)
O(1)	0	$\frac{1}{2}$	0.23929 (42)
O(2)	0.17933 (25)	0.34786 (9)	0.61707 (26)
O(3)	-0.04692 (26)	0.42141 (9)	0.23945 (28)

Table 2. *Vibration tensor components and e.s.d.'s (\AA^2)*

	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{31}$	$2U_{12}$
Na	0.0153 (4)	0.0182 (4)	0.0130 (3)	-0.0015 (5)	0.0006 (6)	0.0016 (7)
Si	0.0104 (3)	0.0089 (2)	0.0056 (2)	0.0001 (3)	-0.0010 (3)	-0.0019 (4)
O(1)	0.0281 (13)	0.0156 (9)	0.0172 (9)	0	0	-0.0219 (19)
O(2)	0.0121 (7)	0.0219 (6)	0.0074 (5)	-0.0014 (9)	-0.0009 (9)	0.0054 (12)
O(3)	0.0165 (8)	0.0161 (6)	0.0129 (6)	0.0008 (9)	-0.0034 (10)	0.0068 (12)

parameters with the introduction of this weighting scheme. The actual largest shift was $\sim 0.005 \text{ \AA}$ in z for O(1) (e.s.d. 0.002 \AA).

The final atomic parameters and standard deviations are given in Table 1, and the vibration parameters and their standard deviations in Table 2. The e.s.d.'s are those given by the inversion of the full matrix. The observed structure amplitudes and those calculated with the parameters of Tables 1 and 2 are given in Table 3.

Discussion of the structure

Crystal structure

The projections of the structure on the (001), (100) and (010) planes are shown in Figs. 1, 2 and 3 respectively. It can be clearly seen that $\alpha\text{-Na}_2\text{Si}_2\text{O}_5$ contains two-dimensional corrugated layers of tetrahedra of the formula $[\text{Si}_2\text{O}_5]_n^{2n-}$ extending in the (010) planes, the channels running along the [001] direction. These layers contain rings of six $[\text{SiO}_4]^{4-}$ tetrahedra (Fig. 3), which are the loops of six in Zoltai's (1960) classification of the tetrahedral structures. In each tetrahedron one oxygen atom is linked to a single silicon atom and three form bridges between two silicon atoms, giving a mean oxygen coordination of 1.75 silicon atoms; this is the sharing coefficient in Zoltai's classification. The various layers are held together through the sodium atoms. The monoclinic $\beta\text{-Na}_2\text{Si}_2\text{O}_5$ (Grund, 1954) and the stable form at room temperature of $\text{Li}_2\text{Si}_2\text{O}_5$ (Liebau, 1961*b*) also have very similar packing arrangements, in spite of the fact that the space groups are all different.

There are striking similarities between the symmetries of the metasilicate chain in Na_2SiO_3 (McDonald & Cruickshank, 1967) and each metasilicate part (if

we may so call it) of the sheet in $\alpha\text{-Na}_2\text{Si}_2\text{O}_5$. In Na_2SiO_3 the metasilicate chains are parallel to the short axis (c) and have symmetry $mc2_1$ with two tetrahedra in the repeat unit; the mirror plane is normal to the long axis (a), the 2_1 axis is parallel to the short c axis and the c -glide is normal to the b axis. The silicon and the bridging oxygen lie in the mirror plane. The metasilicate parts of $\alpha\text{-Na}_2\text{Si}_2\text{O}_5$ also show strong $cm2_1$ pseudo-symmetry: there is a perfect c -glide normal to the a axis ($\frac{1}{2}, y, z$); an approximate mirror plane normal to the b axis is $(x, 0.345, z)$ and this practically passes through the silicon atoms Si and Si' and the bridging oxygen atoms O(2) and O(2'); the line of intersection of the glide and mirror planes is an approximate two-fold screw axis ($\frac{1}{2}, 0.345, z$) (Fig. 1). The slight distortions in the symmetries are perhaps due to the facts that in Na_2SiO_3 the two oxygen atoms related by the mirror symmetry are both non-bridging, whereas in $\alpha\text{-Na}_2\text{Si}_2\text{O}_5$ one is bridging and the other is non-bridging.

The sodium and oxygen coordination

Each sodium atom is coordinated to five oxygen atoms, four of which are at a mean distance of 2.347 \AA and the fifth at 2.600 \AA . The various bond lengths and angles at sodium are given in Table 4. The estimated standard deviations are 0.002 \AA for the lengths and 0.06° for the angles. The polyhedron of five oxygen atoms is a distorted trigonal bipyramid in which O(3''') is associated with the largest distortions, Na-O(3''') being the longest Na-O link. For sodium to achieve a coordination of five, O(3) must also be five-coordinate. The bond lengths and angles at oxygen atoms are also given in Table 4. In Na_2SiO_3 (McDonald &

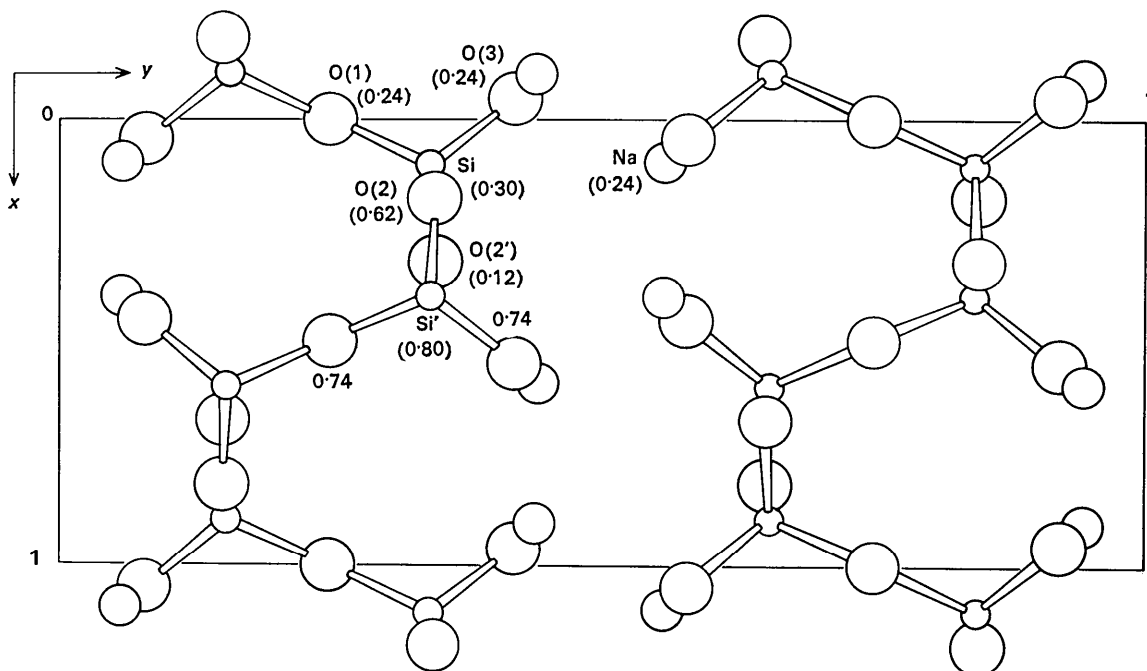


Fig. 1. Projection of the structure along [001].

Cruickshank, 1967) the sodium and oxygen atoms have a very similar coordination scheme.

The silicate sheet

The bond lengths and angles of the silicate sheet are given in Table 4. The estimated standard deviations are 0.002 Å for the lengths and 0.09° for the angles. As pointed out by Cruickshank (1964), since the U_{ij} 's for the oxygen atoms are slightly greater than those for silicon atoms, some corrections to the Si-O bonds are necessary to allow for errors due to rotational motions. However, a rigorous analysis, apart from being

difficult, is not warranted in the present study since it is not expected to produce corrections in lengths of more than 0.005 Å. A slight increase in the values of the e.s.d.'s of the bond lengths and angles will perhaps take account of these uncertainties; standard deviations of 0.004 Å in the lengths and 0.15° in angles are probably generous estimates.

The bridging Si-O bonds, of mean length 1.630 Å, are appreciably different from the non-bridging bond of length 1.578 Å; such a difference is expected in terms of the $d-p$ π -bonding theory suggested by Cruickshank (1961). As pointed out by McDonald & Cruick-

Table 4. Bond lengths and angles

Bond		Angle	
Na-O(2'')	2.386 Å	O(2'')-Na-O(3''')	62.94°
Na-O(3)	2.338	O(3)-Na-O(2'')	104.10
Na-O(3')	2.373	O(3)-Na-O(3')	93.29
Na-O(3'')	2.290	O(3)-Na-O(3''')	92.46
Na-O(3''')	2.600	O(3')-Na-O(2'')	96.84
		O(3')-Na-O(3''')	159.77
Si-O(1)	1.609	O(3'')-Na-O(2'')	130.76
Si-O(2)	1.643	O(3'')-Na-O(3)	120.56
Si-O(2')	1.638	O(3'')-Na-O(3')	100.02
Si-O(3)	1.578	O(3'')-Na-O(3''')	93.68
Angle		Bond	
O(1)-Si-O(2)	109.13°	O(1)-O(2)	2.650 Å
O(1)-Si-O(2')	107.54	O(1)-O(2')	2.619
O(1)-Si-O(3)	113.20	O(1)-O(3)	2.661
O(2)-Si-O(2')	105.42	O(2)-O(2')	2.610
O(2)-Si-O(3)	108.18	O(2)-O(3)	2.609
O(2')-Si-O(3)	113.03	O(2')-O(3)	2.683
Angle		Angle	
Si-O(1)-Si'	160.04°	Si-O(3)-Na''	134.22°
Si-O(2)-Si'''	138.93	Si-O(3)-Na	117.17
Si''-O(2)-Na'	119.81	Si-O(3)-Na'''	110.53
Si-O(2)-Na'	95.58	Si-O(3)-Na'	89.33
		Na-O(3)-Na''	106.49
		Na'''-O(3)-Na''	84.02
		Na'-O(3)-Na''	79.06
		Na-O(3)-Na'''	86.71
		Na-O(3)-Na'	87.54
		Na'-O(3)-Na'''	159.77

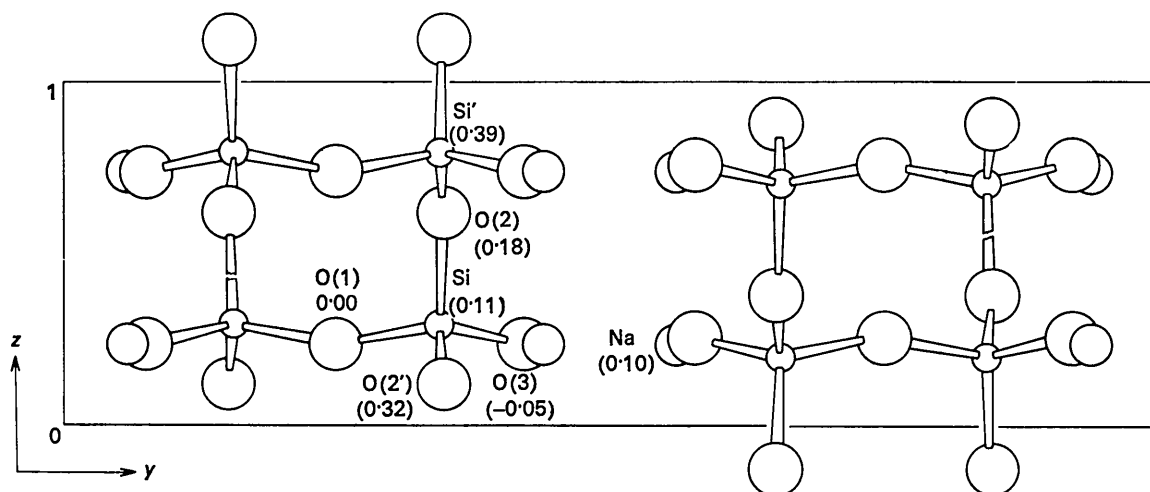


Fig. 2. Projection of the structure along [100].

shank (1967) and by Pant & Cruickshank (1967) large differences occur infrequently in silicates because (a) of the tendency of the silicate ion to shed its negative charge, and with this some of its π -bonding potential, by forming partial covalent bonds to the cations, and (b) X-O-X angles are usually large in silicates, which causes bridging bonds to gain strength at the expense of peripheral bonds. However, in the presence of rather an electropositive cation an appreciable difference should be observed.

In the present case the bridging bond Si-O(1), 1.609 Å, is significantly shorter than the mean, 1.641 Å, of the other two bridging bonds Si-O(2) and Si-O(2'); this is to be correlated with the larger angle of 160° at O(1), as compared with 139° at O(2). The point becomes quite clear from the dimensions observed in a number of other silicates which have recently been refined reasonably accurately. In datolite, $\text{CaBSiO}_4(\text{OH})$ (Pant & Cruickshank, 1967), Si-O(bridging) = 1.668 ± 0.007 , Si-O(non-bridging) = 1.563 ± 0.012 Å and Si-O(bridging)-B $\sim 125^\circ$. In Na_2SiO_3 (McDonald & Cruickshank, 1967) the dimensions are 1.672 ± 0.005 , 1.592 ± 0.004 Å and $\sim 134^\circ$. In omphacite (Clark & Papike, 1967) they are 1.660 ± 0.010 , 1.604 ± 0.010 Å and $\sim 135^\circ$. In β - $\text{Na}_2\text{Si}_2\text{O}_5$ the final dimensions from a new three-dimensional study by one of us (A.K.P.) are 1.639 ± 0.002 , 1.580 ± 0.005 Å and 136° .

There are appreciable distortions of the angles at Si; the largest angle is O(1)-Si-O(3) = 113.2° and the smallest is O(2)-Si-O(2') = 105.4° . By plotting the mean lengths of any pair of bonds forming an angle at Si against O...O, the present results fit the general silicon-oxygen curve given by McDonald & Cruickshank (1967); O(2)...O(2') is actually 0.05 Å less than O(1)...O(3), whereas the mean of Si-O(2) and Si-O(2'), 1.64 Å, is longer than the mean of Si-O(1) and Si-O(3), 1.59 Å. This evidently implies, as pointed out by McDonald & Cruickshank (1967), that the repulsive forces between pairs of bridging oxygens are much less than those between the external oxygen atoms.

General discussion

Once the tentative structure was fixed, it became clear that the Si-O(1)-Si group could not be linear. The value of the angle obtained from the final coordinates, 160° , is considerably different from 180° . Earlier Liebau (1961a), who maintained that a linear Si-O-Si group was improbable, had reduced the symmetry of the space group from $Pcnb$ to $P2_1nb$ in an attempt to reduce the value of the angle from 180° . The conclusion was, however, drawn from an incomplete and incorrect structure determination. From the present study it is conclusively proved that the space group of α - $\text{Na}_2\text{Si}_2\text{O}_5$ is $Pcnb$ and not $Pmnb$ or $P2_1nb$.

As in datolite (Pant & Cruickshank, 1967), the variations in the various bond distances can be explained on the basis of the Pauling-Zachariasen method of the balancing of valences. If we assign bond strengths of 1.00 to tetrahedral Si-O bonds and $\frac{1}{2}$ to an Na-O link,

we see that O(2) is 'overbonded' (2.2) [Si-O(2) = 1.641 Å], O(3) is 'underbonded' (1.8) [Si-O(3) = 1.578 Å], and O(1) is balanced [Si-O(1) = 1.609 Å], as it is bonded to two silicon atoms only and is not involved in any link to sodium. The valences get balanced in the actual structure by the lengthening of the Si-O(2) bonds and the shortening of the Si-O(3) bonds and by variations in the Na-O links. However, a comparison with Na_2SiO_3 shows that there are perhaps also other factors which are involved in the variations in the Si-O lengths. By assigning bond strengths of 1.00 to an Si-O and $\frac{1}{2}$ to an Na-O link, we find that in Na_2SiO_3 O(2) is 'overbonded' (2.2) [Si-O(2) = 1.672 Å] and O(1) is 'underbonded' (1.8) [Si-O(1) = 1.592]. Although the amounts of overbonding and underbonding in the pertinent atoms of both structures are exactly equal, there are unequal changes in the Si-O bond lengths; the differences in the Si-O(bridging)-Si angles are probably responsible for this.

The Si-O mean length of 1.616 Å in α - $\text{Na}_2\text{Si}_2\text{O}_5$ is 0.016 Å shorter than the mean of 1.632 Å in Na_2SiO_3 . This difference is in the direction indicated by Smith & Bailey's (1963) analysis of the variation of mean length with sharing coefficient.

We have mentioned both the $d-p$ π -bonding theory for Si-O bonds and the method of the balancing of valences. As discussed by Pant & Cruickshank (1967) the two theories are not exclusive, for π -bonding in Si-O bonds may be part of the mechanism whereby valency balance is achieved.

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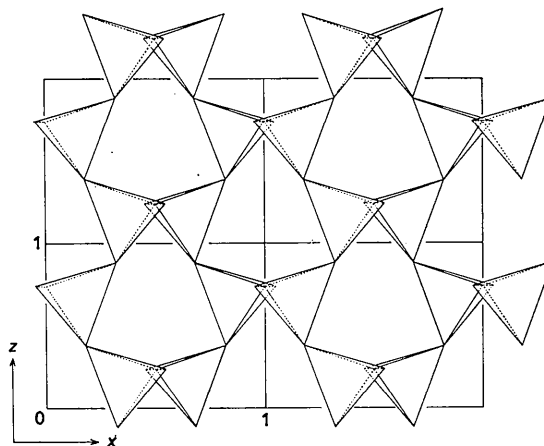


Fig. 3. Projection of the structure (4 unit cells) along [010] showing sheets formed by condensation of puckered rings of six tetrahedra.

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Fokussierende Monochromatoren für Einkristallverfahren?

VON H. JAGODZINSKI

Institut für Kristallographie der Universität, 8 München 2, Luisenstrasse 37/II, Deutschland

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Quantitative X-ray intensity measurements are often hindered by small crystals. It is shown that the usual film and diffractometer techniques are inconvenient in this case. The use of cylindrically bent monochromators and fine focus-tubes in a special position with a small crystal of arbitrary shape (needles are advantageous) leads to optimal intensities and resolution powers. This method forms a reliable basis for quantitative measurements for film and counter techniques as well.

Einleitung

Die Verwendung fokussierender Monochromatoren für Beugungsaufnahmen an Einkristallen ist dann allgemein üblich, wenn ein diffuser Untergrund geringer Intensität gemessen werden soll. Es wird dann die Messung meist mit Filmmethoden durchgeführt, weil die gleichzeitige Aufnahme des gesamten Schnitts der Ewald-Kugel mit dem reziproken Raum erhebliche Verkürzungen der Messzeit mit sich bringt. Die Verwendung von gebogenen Monochromatoren anstelle von ebenen für die quantitative Messung der scharfen Bragg-Reflexe mit Film oder Zählrohr ist jedoch keineswegs üblich; sie wird nach Woitschach (1956) für Röntgenstrahlen sogar als unzweckmässig angesehen. Azaroff (1957) empfiehlt dagegen gebogene Monochromatoren für Aufnahmen nach der Buegerschen Präzessionsmethode, während Ladell & Spielberg (1966) sich in einer ausführlichen Veröffentlichung auch mit der Monochromator-Geometrie für Einkristalldiffraktometer auseinandersetzen. Allerdings werden die Fokussierungseigenschaften in diesen Arbeiten nur am Rande diskutiert. Auf die zahlreichen Veröffentlichungen, die den Einsatz von gebogenen Monochromatoren in der Pulverdiffraktometrie behandeln, soll hier nicht eingegangen werden; man vergleiche dazu den Artikel über Monochromatoren in den *International Tables for X-ray Crystallography* (1962). Für Neutronenspektrometer gibt es eine Reihe von Arbeiten [vgl. z.B. Dachs & Stehr (1962)], die jedoch mehr den Gedanken einer hohen Integralintensität bei op-

timaler Auflösung verfolgen und die nutzbare Kristallgröße ausser Acht lassen.

Im folgenden soll gezeigt werden, dass die Anwendung fokussierender Monochromatoren besonders für sehr kleine Kristalle entscheidende Vorteile bietet, wenn die Geometrie des Aufnahmeverfahrens optimal gewählt wird; auch für die Messung mit Zählrohren ergeben sich dabei wichtige Vorteile des Intensitätsverhältnisses I_R/I_U (I_R = Intensität des Bragg-Reflexes, I_U = Intensität des kontinuierlichen Untergrundes).

Das integrale Reflexionsvermögen bei Drehaufnahmen

Normale Verfahren mit gefilterter oder ungefilterter Strahlung

Im folgenden werden wir die Absorption vernachlässigen, was die Allgemeinheit der untenstehenden Erörterungen nicht beeinträchtigt. Der Versuchskristall K (Fig. 1) werde um seine vertikale Achse gedreht, die Netzebenennormale liege senkrecht zur Drehachse. In erster Näherung (für kleine Öffnungswinkel) streut beim Durchdrehen des Kristalls das Volumenelement dV die integrale Intensität IdV in einen bestimmten Beugungswinkelbereich

$$IdV = F \varepsilon_x^0 \varepsilon_x^0 dV \int_{\lambda_0}^{\lambda_0 + \Delta\lambda} i(\lambda) d\lambda = F dV \varepsilon_x^0 \varepsilon_x^0 i \Delta\lambda, \quad (1)$$

mit

F = Flächenhelligkeit der Strahlungsquelle R (konstant angenommen)
 ε_x^0 = axialer Öffnungswinkel