

The crystal structure of alamosite, PbSiO_3 ¹

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Auszug

Alamosit PbSiO_3 hat die Raumgruppe $P2/n$ und für die reduzierte Zelle die Gitterkonstanten $a = 11,23 \text{ \AA}$, $b = 7,08 \text{ \AA}$, $c = 12,26 \text{ \AA}$, $\beta = 113^\circ 15'$; die Zelle enthält 12 PbSiO_3 . Die Struktur wurde auf Grund von dreidimensionalen Zählrohrmessungen bestimmt. Im Lauf der Verfeinerung konvergierte R gegen 11,1% bei Berücksichtigung aller Interferenzen. Die Alamositstruktur ist in einzigartiger Weise aus Tetraederketten parallel $[\bar{1}01]$ aufgebaut, wobei die Translationsperiode in dieser Richtung zwölf Tetraeder umfaßt. Die drei Pb-Atome, die nicht durch Symmetrie verbunden sind, werden von drei oder vier O-Atomen umgeben; die drei nächsten O-Atome liegen stets auf der einen Seite vom Pb-Atom, was auf kovalente Bindung hinweist. Abwechselnd aufeinanderfolgende benachbarte Pb- und O-Atome bilden Spiralen um $[010]$, die annähernd die Symmetrie 3_1 haben.

Abstract

Alamosite, PbSiO_3 , has space group $P2/n$ with cell parameters for the reduced cell $a = 11.23 \text{ \AA}$, $b = 7.08 \text{ \AA}$, $c = 12.26 \text{ \AA}$, and $\beta = 113^\circ 15'$, with $Z = 12$. The structure has been determined using three-dimensional counter-diffractometer data. Refinement converged with $R = 11.1\%$, including a number of reflections omitted due to extinction effects. The structure of alamosite is unique in that it consists partially of chains of tetrahedra extending parallel to $[\bar{1}0\bar{1}]$ with a lattice translation repeat of twelve tetrahedra. The three independent Pb atoms are coordinated by 3 or 4 oxygen atoms, in each case the nearest oxygen neighbors being distributed on one side of the Pb atom, indicating covalency in Pb—O bonding. The Pb atoms and their coordinating oxygen atoms are related by an approximation to a 3_1 screw axis parallel to $[010]$ so that they form a continuous spiral of bonded Pb, O atoms.

Introduction

MACKAY (1952) determined that alamosite, PbSiO_3 , has space group $P2/c$ or Pc , and unit-cell parameters $a = 11.28 \text{ \AA}$, $b = 7.08 \text{ \AA}$,

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$c = 13.06 \text{ \AA}$, and $\beta = 120^\circ$. Following the suggestion of PALACHE and MERWIN (1909), he compared the properties of alamosite with those of the monoclinic form of CaSiO_3 , parawollastonite, for possible evidence of isotypy. The lack of correspondence suggested a difference in structure. The 3 : 1 ratio of O : Si indicates that alamosite should have a structure based on a silicate chain or ring. MACKAY noted that the presence of rings is more probable since alamosite has a pseudo-hexagonal cell and indices of refraction indicating "anisotropic structure units." PREWITT and PEACOR (1964), in a review of chain metasilicate structures, showed that such structures with cations larger than Ca, such as Pb, were unlikely to be based on silicate chains.

Unit cell and space group

Specimens of alamosite from Alamos, Sonora, Mexico were kindly provided by Dr. C. FRONDEL from the Harvard mineralogical collection, catalogue number 84459. The unit-cell parameters determined for this material are $a = 11.23 \text{ \AA}$, $b = 7.08 \text{ \AA}$, $c = 12.95 \text{ \AA}$, and $\beta = 119^\circ 34'$. Systematic extinctions were found which verified that alamosite has space group $P2/c$ or Pc , as determined by MACKAY. The cell parameters for the $P2/n$ or Pn setting have been used throughout our results, however, since this corresponds with the reduced cell. Parameters for this cell are $a = 11.23 \text{ \AA}$, $b = 7.08 \text{ \AA}$, $c = 12.26 \text{ \AA}$, and $\beta = 113^\circ 15'$. MACKAY noted that a test for piezoelectricity was negative and that many accidental absences occur on single-crystal photographs. He therefore suggested that the centrosymmetric group is probably the correct one. MACKAY also determined that the calculated cell contents are 12.3 formula weights of PbSiO_3 , using data of PALACHE and MERWIN. We confirmed the value $Z = 12$, departures from the integral value being ascribable, in part, to error in specific-gravity determination.

Structure determination

Alamosite occurs as aggregates of radiating fibrous crystals, with fiber axis [010], and with a perfect (010) cleavage. Our type material suffered from serious lineage-structure effects with reflections broadened irregularly parallel to (010). Three-dimensional data were therefore obtained by planimetry recorded peaks, using a crystal rotated about the b axis, with $\text{CuK}\alpha$ radiation and a scintillation counter with pulse-height analysis, followed by correction for Lorentz-polarization factors.

The function $P(uw)$ was then calculated. From a computation of predicted relative peak heights it was clear that all peaks except Pb—Pb peaks were close to the background level. The projection symmetry was $P2$ with 6PbSiO_3 per cell. No large peaks were found in special positions, so the Pb atoms were assumed to be distributed in three general positions (rank 4 in $P2/n$; rank 2 in this projection). Using the conjugate-peak relation (BUERGER, 1959), two probable single-weight Pb—Pb inversion peaks were readily located. Each was used for the construction of an $M_2(xz)$ function. Only three large peaks were found in this function and it was assumed that they corresponded to three Pb atoms in general positions. Structure factors were calculated on this basis and the relatively low R factor verified this decision. All attempts to locate Si and O atoms in projection through the $M_4(xz)$, $\rho(xz)$ and $\Delta\rho(xz)$ functions failed, however.

The three-dimensional Patterson function, $P(uvw)$ was therefore calculated. The coordinates u, w of Pb—Pb vectors were known from the analyses of the two-dimensional function. Examination of $P(uvw)$ readily resulted in identification of Pb—Pb inversion vectors, and the y coordinates of the Pb atoms were determined. Reasonable agreement between values of F'_o and F_o , using only Pb atoms, verified these results. A Fourier synthesis, $\rho(xyz)$ was then prepared using those large values of F'_o with signs assumed to be unambiguously determined. Only three nonequivalent peaks of approximately equal height were present with heights significantly above background, in addition to those corresponding to Pb. The cell contents are consistent with 3 Si atoms in general positions. In addition, interpeak distances were $3 \pm 0.2 \text{ \AA}$, which is in the range of known Si—Si distances across bridging oxygen atoms. These peaks were therefore assumed to correspond to Si atoms. Oxygen-atom positions were then predicted assuming ideal tetrahedral oxygen coordination about Si, on the basis that adjacent Si atoms were linked through bridging oxygens. Refinement carried out using all Pb, Si and O positions failed to converge, however. A difference Fourier synthesis $\Delta\rho(xyz)$ readily suggested adjustments in some oxygen positions. Refinement was continued to convergence with $R = 10.4\%$, excluding reflections with $F'_o = 0$.

At this time an unusually perfect crystal of alamosite was separated which showed a major improvement over the first in perfection of reflections. The intensity data were therefore redetermined. Some crystal imperfection was still detectable in diffractometer scans

however, so intensity data were again determined through the planimetry of recorded peaks. $\text{CuK}\alpha$ radiation was again used and the data corrected for the Lorentz-polarization factor and absorption. Due to the large absorption factor, absorption had to be precisely accounted for; this was accomplished by using the IBM program ABSRP kindly provided by C. W. BURNHAM, taking care to define the crystal vertices to within about $\pm .003$ mm. The crystal shape was easily defined since the crystal was a prism mounted for rotation about b and bounded by $\{h0l\}$ faces and $\{010\}$ cleavages, 0.17 mm long with principal diameters of about 0.06 and 0.03 mm.

Refinement was continued with the new data using the weighting scheme recommended by CRUICKSHANK (1965), with corrections for anomalous scattering. Following convergence, with only the atomic coordinates and the single scale factor varying, it became evident that the data were subject to a secondary-extinction error, since large structure factors consistently had $F_o < F_c$. Since a precise extinction correction could not readily be made, due to the complexity of the crystal shape, refinement was continued with the rejection of about 50 reflections for which a significant extinction error was indicated. The refinement rapidly converged with final cycles of refinement of atom coordinates and the single scale factor alternating

Table 1. *Refined coordinates and isotropic temperature factors of alamosite*
(Standard deviations are given in parentheses)

| Atom | x | y | z | B |
|-------|---------------|---------------|---------------|-----------|
| Pb(1) | .5447 (1) | .0667 (2) | .6739 (1) | .65 (2) |
| Pb(2) | .4096 (1) | .3857 (2) | .8469 (1) | .53 (2) |
| Pb(3) | .2989 (1) | .3041 (2) | .0999 (1) | .57 (2) |
| Si(1) | .6180 (7) | .1254 (12) | .1539 (6) | .35 (11) |
| Si(2) | .5292 (7) | .4070 (12) | .3914 (6) | .44 (12) |
| Si(3) | .7122 (6) | .1824 (12) | .9616 (6) | .20 (11) |
| O(1) | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | .77 (47) |
| O(2) | $\frac{3}{4}$ | .2249 (48) | $\frac{1}{4}$ | .74 (44) |
| O(3) | .6418 (23) | .2458 (40) | .4576 (2) | 1.49 (36) |
| O(4) | .6581 (18) | .0597 (33) | .0419 (18) | .57 (31) |
| O(5) | .5070 (17) | .2875 (31) | .1071 (17) | .34 (32) |
| O(6) | .5758 (21) | .9442 (37) | .2132 (19) | 1.10 (36) |
| O(7) | .4041 (19) | .2935 (33) | .3036 (18) | .73 (34) |
| O(8) | .4209 (19) | .4265 (34) | .6710 (18) | .77 (34) |
| O(9) | .6269 (22) | .3728 (36) | .9159 (20) | 1.22 (35) |
| O(10) | .7139 (17) | .0497 (32) | .8538 (16) | .25 (29) |

Table 2. Observed and final calculated structure factors

| h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} |
|---------|------------------|------------------|----------|------------------|------------------|---------|------------------|------------------|----------|------------------|------------------|
| 0 0 2 | 112.53 | 133.57 | 8 0 -2 | 63.42 | 81.00 | 2 1 3 | 64.08 | 65.87 | 6 1 -1 | 280.89 | 306.41 |
| 4 | 265.61 | 491.20 | 0 | 211.03 | 228.82 | 4 | 34.01 | 38.33 | 0 | 84.13 | 87.28 |
| 6 | 178.29 | 230.59 | 2 | 0.00 | 5.90 | 5 | 173.95 | 187.26 | 1 | 21.35 | 8.69 |
| 8 | 59.29 | 55.40 | 4 | 55.69 | 54.12 | 6 | 29.05 | 28.01 | 2 | 244.24 | 241.31 |
| 10 | 30.23 | 29.44 | 5 | 80.32 | 81.45 | 7 | 17.99 | 13.99 | 3 | 235.38 | 234.61 |
| 12 | 214.66 | 202.12 | 9 0 -13 | 83.44 | 89.26 | 8 | 28.66 | 21.54 | 4 | 64.64 | 59.39 |
| 1 0 -13 | 29.60 | 19.20 | -11 | 316.48 | 349.41 | 9 | 90.95 | 75.12 | 5 | 32.80 | 19.24 |
| -11 | 247.87 | 311.95 | -9 | 237.23 | 248.17 | 10 | 144.58 | 127.46 | 6 | 124.10 | 111.93 |
| -9 | 210.27 | 246.60 | -7 | 185.50 | 205.55 | -11 | 35.55 | 29.54 | 7 | 52.38 | 49.77 |
| -7 | 194.56 | 256.03 | -5 | 223.15 | 246.16 | -12 | 45.19 | 43.82 | 8 | 20.84 | 17.39 |
| -5 | 217.59 | 296.58 | -3 | 72.28 | 78.79 | 3 1 -14 | 98.05 | 84.03 | 9 | 47.49 | 36.04 |
| -3 | 171.72 | 211.23 | -1 | 94.74 | 94.03 | -13 | 139.89 | 121.29 | 7 1 -14 | 43.52 | 52.85 |
| 1 | 111.78 | 160.32 | 1 | 238.54 | 254.59 | -12 | 109.21 | 114.60 | -13 | 56.64 | 41.11 |
| 3 | 142.76 | 205.36 | 3 | 323.95 | 331.15 | -11 | 105.75 | 109.93 | -12 | 191.63 | 197.13 |
| 5 | 99.89 | 116.32 | 5 | 173.74 | 198.48 | -10 | 200.84 | 233.09 | -11 | 52.87 | 31.31 |
| 7 | 62.96 | 65.32 | 10 0 -12 | 41.18 | 43.23 | -9 | 149.82 | 158.85 | -10 | 151.32 | 156.04 |
| 9 | 107.62 | 114.32 | -10 | 50.34 | 28.97 | -8 | 181.88 | 198.76 | -9 | 35.30 | 32.32 |
| 11 | 25.58 | 7.06 | -8 | 143.44 | 146.64 | -7 | 162.12 | 171.76 | -8 | 248.40 | 272.20 |
| 13 | 263.84 | 257.35 | -6 | 70.96 | 81.74 | -6 | 245.64 | 296.95 | -7 | 30.21 | 16.38 |
| 2 0 -14 | 88.27 | 91.70 | -4 | 199.49 | 224.54 | -5 | 113.77 | 109.76 | -6 | 152.87 | 158.63 |
| -12 | 47.81 | 61.04 | -2 | 14.75 | 11.07 | -4 | 74.89 | 69.17 | -5 | 27.33 | 26.15 |
| -10 | 213.46 | 252.18 | 0 | 170.80 | 158.80 | -3 | 43.64 | 39.26 | -4 | 97.46 | 97.12 |
| -8 | 173.52 | 207.96 | 2 | 142.79 | 140.32 | -2 | 141.13 | 164.36 | -3 | 91.75 | 93.14 |
| -6 | 281.27 | 300.73 | 4 | 135.57 | 114.93 | 1 | 248.34 | 302.95 | -2 | 57.59 | 31.68 |
| -4 | 280.72 | 467.15 | 11 0 -13 | 0.00 | 13.42 | 0 | 35.39 | 28.22 | -1 | 31.43 | 30.75 |
| -2 | 87.49 | 82.06 | -11 | 21.58 | 12.46 | 1 | 235.14 | 272.50 | 0 | 69.44 | 68.37 |
| 0 | 124.79 | 151.09 | -9 | 104.05 | 101.07 | 2 | 0.00 | 6.76 | 1 | 167.74 | 173.28 |
| 2 | 330.93 | 417.24 | -7 | 213.57 | 213.21 | 3 | 169.23 | 155.32 | 2 | 150.35 | 140.97 |
| 4 | 244.12 | 338.68 | -5 | 0.00 | 16.51 | 4 | 194.76 | 176.44 | 3 | 191.34 | 192.68 |
| 6 | 275.52 | 328.64 | -3 | 343.94 | 403.53 | 5 | 377.57 | 388.01 | 4 | 114.52 | 103.16 |
| 8 | 375.14 | 418.19 | -1 | 74.66 | 68.73 | 6 | 36.97 | 25.18 | 5 | 37.56 | 31.83 |
| 10 | 28.26 | 25.99 | 1 | 223.31 | 226.16 | 7 | 94.76 | 81.04 | 6 | 211.42 | 195.02 |
| 12 | 253.42 | 242.78 | 3 | 124.97 | 132.96 | 8 | 163.69 | 144.85 | 7 | 158.74 | 145.33 |
| 13 | 25.26 | 8.31 | 12 0 -12 | 169.76 | 196.89 | -9 | 153.47 | 139.35 | -8 | 116.99 | 103.83 |
| 5 0 -11 | 158.88 | 189.12 | -10 | 169.69 | 165.51 | 10 | 143.73 | 132.76 | 8 1 -14 | 129.75 | 123.09 |
| -9 | 166.20 | 177.84 | -8 | 200.66 | 214.00 | 11 | 137.25 | 121.80 | -13 | 139.08 | 139.94 |
| -7 | 151.97 | 160.00 | -6 | 77.11 | 74.90 | 12 | 49.75 | 42.84 | -12 | 85.28 | 79.99 |
| -5 | 92.41 | 51.31 | -4 | 12.67 | 2.68 | 4 1 -14 | 25.44 | 25.72 | -11 | 97.14 | 104.16 |
| -3 | 349.66 | 536.70 | -2 | 47.89 | 39.96 | -13 | 112.00 | 115.30 | -10 | 112.64 | 102.31 |
| -1 | 129.90 | 144.80 | 0 | 142.70 | 139.86 | -12 | 180.29 | 168.77 | -9 | 35.94 | 30.67 |
| 1 | 358.04 | 512.83 | 13 0 -9 | 127.95 | 144.53 | -11 | 106.18 | 118.03 | -8 | 285.94 | 310.73 |
| 3 | 26.81 | 19.18 | -7 | 97.34 | 100.89 | -10 | 201.09 | 209.68 | -7 | 119.89 | 125.05 |
| 5 | 202.67 | 182.87 | -5 | 12.23 | 12.20 | -9 | 212.18 | 242.63 | -6 | 101.52 | 100.09 |
| 7 | 108.90 | 90.51 | -3 | 23.51 | 10.95 | 1 | 351.54 | 351.54 | -5 | 84.08 | 84.26 |
| 9 | 122.43 | 110.70 | -1 | 190.75 | 200.15 | -7 | 23.28 | 21.61 | -4 | 223.93 | 228.98 |
| 11 | 130.36 | 108.46 | 0 1 -13 | 70.76 | 72.28 | -6 | 258.86 | 305.59 | -3 | 30.96 | 31.00 |
| 13 | 23.04 | 21.93 | -12 | 36.21 | 18.31 | -5 | 178.79 | 178.94 | -2 | 232.75 | 262.90 |
| 4 0 -12 | 89.54 | 81.75 | -9 | 192.89 | 195.05 | -4 | 225.95 | 244.16 | -1 | 86.75 | 65.14 |
| -10 | 25.64 | 32.86 | -10 | 29.89 | 11.75 | -3 | 116.60 | 109.58 | 1 | 93.24 | 84.26 |
| -8 | 108.17 | 96.60 | -9 | 134.71 | 143.67 | -2 | 91.92 | 94.93 | 2 | 155.11 | 151.23 |
| -6 | 205.86 | 223.78 | -8 | 159.91 | 176.29 | -1 | 50.99 | 48.65 | 3 | 186.64 | 167.75 |
| -4 | 169.28 | 181.70 | -7 | 246.77 | 330.54 | 0 | 131.74 | 142.80 | 4 | 131.38 | 124.42 |
| -2 | 435.15 | 614.99 | -6 | 120.76 | 132.24 | 1 | 114.29 | 115.41 | 5 | 156.29 | 152.22 |
| 0 | 20.67 | 12.32 | -5 | 159.63 | 183.46 | 2 | 116.60 | 109.58 | 6 | 59.33 | 53.87 |
| 2 | 403.27 | 479.81 | -4 | 135.76 | 155.54 | 3 | 193.22 | 182.77 | 7 | 179.10 | 164.39 |
| 4 | 190.61 | 172.68 | -3 | 160.50 | 204.61 | 4 | 72.02 | 64.10 | 9 1 -14 | 56.84 | 67.66 |
| 6 | 0.00 | 23.03 | -2 | 103.74 | 111.94 | 6 | 42.52 | 35.68 | -13 | 127.77 | 124.22 |
| 8 | 103.88 | 94.22 | 1 1 -12 | 53.85 | 30.27 | 7 | 236.22 | 228.95 | -12 | 75.13 | 69.77 |
| 10 | 268.57 | 265.09 | -13 | 78.16 | 66.19 | 8 | 101.78 | 91.61 | -11 | 37.22 | 30.96 |
| 11 | 297.81 | 322.32 | -12 | 175.64 | 175.49 | 9 | 202.05 | 190.47 | -10 | 23.92 | 6.52 |
| 5 0 -13 | 187.64 | 192.10 | -11 | 0.00 | 7.90 | 10 | 13.99 | 3.79 | -9 | 53.61 | 48.64 |
| -9 | 287.83 | 317.81 | -10 | 67.92 | 75.43 | 11 | 91.37 | 85.22 | -8 | 158.08 | 163.50 |
| -7 | 359.49 | 474.00 | -9 | 142.08 | 132.90 | -14 | 199.10 | 195.58 | -7 | 74.81 | 71.75 |
| -5 | 154.76 | 155.66 | -8 | 22.68 | 9.61 | -13 | 47.89 | 32.42 | -6 | 67.07 | 63.42 |
| -3 | 185.31 | 206.64 | -7 | 213.59 | 264.43 | -12 | 35.05 | 42.59 | -5 | 50.33 | 55.02 |
| -1 | 55.56 | 57.37 | -6 | 88.53 | 95.29 | -11 | 0.00 | 4.63 | -4 | 282.14 | 314.34 |
| 1 | 162.24 | 175.32 | -5 | 55.06 | 55.78 | -10 | 88.69 | 77.14 | -3 | 76.34 | 88.56 |
| 3 | 157.52 | 146.49 | -4 | 186.93 | 217.73 | -9 | 75.46 | 76.66 | -2 | 0.00 | 2.75 |
| 5 | 252.42 | 245.36 | -3 | 258.47 | 383.96 | -8 | 58.63 | 61.14 | -1 | 33.98 | 12.21 |
| 7 | 25.93 | 27.19 | -2 | 0.00 | 10.40 | -7 | 59.78 | 51.61 | 0 | 294.17 | 303.99 |
| 9 | 155.09 | 144.44 | 1 | 52.46 | 60.38 | -6 | 197.29 | 193.09 | 1 | 26.81 | 34.47 |
| 11 | 147.63 | 159.29 | 2 | 0.00 | 13.38 | -5 | 215.77 | 230.54 | 2 | 43.16 | 43.28 |
| 12 | 105.27 | 111.04 | 3 | 184.97 | 265.35 | -4 | 0.00 | 4.17 | 3 | 62.89 | 59.71 |
| -10 | 42.88 | 40.87 | 4 | 178.79 | 242.32 | -3 | 100.09 | 95.73 | 4 | 124.66 | 107.78 |
| -8 | 192.71 | 202.23 | 5 | 181.26 | 235.74 | -2 | 316.08 | 370.66 | 5 | 130.92 | 122.61 |
| -6 | 61.98 | 57.17 | 6 | 101.63 | 114.11 | -1 | 194.60 | 202.10 | 6 | 61.56 | 47.59 |
| -4 | 131.50 | 154.71 | 7 | 21.62 | 18.70 | 0 | 29.55 | 22.68 | 10 1 -13 | 85.12 | 92.57 |
| -2 | 31.56 | 33.26 | 8 | 141.00 | 148.95 | 1 | 253.18 | 277.10 | -12 | 159.80 | 162.64 |
| 0 | 147.71 | 168.77 | 9 | 241.03 | 260.44 | 2 | 255.83 | 251.74 | -11 | 164.95 | 167.13 |
| 2 | 271.73 | 277.82 | 10 | 191.98 | 172.55 | 3 | 32.53 | 21.11 | -10 | 23.75 | 21.02 |
| 4 | 286.91 | 296.14 | 11 | 187.10 | 165.48 | 4 | 21.49 | 16.07 | -9 | 130.26 | 129.78 |
| 6 | 349.73 | 346.39 | 12 | 58.23 | 47.37 | 5 | 137.28 | 127.81 | -8 | 142.10 | 140.40 |
| 8 | 126.78 | 112.32 | 13 | 74.87 | 76.81 | 6 | 126.57 | 112.04 | -7 | 183.76 | 186.50 |
| 10 | 209.86 | 211.45 | 2 1 -14 | 148.79 | 125.37 | 7 | 255.16 | 254.43 | -6 | 204.49 | 219.00 |
| -11 | 193.74 | 197.03 | -13 | 98.03 | 84.76 | 8 | 112.63 | 103.10 | -5 | 0.00 | 6.76 |
| -9 | 104.64 | 100.47 | -12 | 216.16 | 220.53 | 9 | 99.27 | 83.93 | -4 | 65.76 | 64.83 |
| -7 | 196.17 | 203.53 | -11 | 82.09 | 86.06 | 10 | 16.70 | 6.63 | -3 | 124.69 | 131.05 |
| -5 | 367.12 | 457.07 | -10 | 0.00 | 20.82 | 6 1 -14 | 139.73 | 138.09 | -2 | 184.96 | 201.08 |
| -3 | 15.16 | 15.34 | -9 | 64.88 | 69.63 | -13 | 0.00 | 5.77 | -1 | 36.14 | 38.83 |
| -1 | 395.79 | 515.51 | -8 | 195.00 | 220.42 | -12 | 159.39 | 153.07 | 0 | 238.49 | 248.52 |
| 1 | 129.55 | 129.78 | -7 | 116.29 | 125.40 | -11 | 145.22 | 146.78 | 1 | 93.20 | 92.54 |
| 3 | 137.56 | 121.44 | -6 | 121.30 | 119.91 | -10 | 267.27 | 284.09 | 2 | 25.28 | 25.62 |
| 5 | 85.04 | 85.47 | -5 | 25.61 | 22.90 | -9 | 153.56 | 149.79 | 3 | 61.29 | 52.63 |
| 7 | 88.78 | 78.41 | -4 | 18.82 | 9.42 | -8 | 46.72 | 34.20 | 4 | 181.11 | 174.01 |
| 9 | 116.56 | 123.07 | -3 | 231.23 | 309.13 | -7 | 50.05 | 46.02 | 5 | 23.42 | 17.36 |
| 11 | 143.92 | 142.16 | -2 | 55.09 | 47.31 | -6 | 114.71 | 110.04 | 11 1 -12 | 111.56 | 115.60 |
| 13 | 158.33 | 171.97 | -1 | 43.69 | 41.03 | -5 | 237.00 | 275.85 | -11 | 127.00 | 126.74 |
| -8 | 72.09 | 68.40 | 0 | 86.62 | 88.70 | -4 | 218.58 | 242.75 | -10 | 195.57 | 209.32 |
| -6 | 68.44 | 61.68 | 1 | 312.94 | 403.50 | -3 | 34.36 | 37.84 | -9 | 62.64 | 69.94 |
| -4 | 211.45 | 221.19 | 2 | 154.29 | 143.59 | -2 | 180.74 | 186.88 | -8 | 115.60 | 111.87 |

Table 2. (Continued)

| h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} |
|----------|------------------|------------------|---------|------------------|------------------|----------|------------------|------------------|---------|------------------|------------------|
| 11 1 -7 | 116.27 | 111.78 | 3 2 -10 | 166.32 | 185.89 | 7 2 -11 | 172.68 | 182.20 | 12 2 -6 | 165.28 | 173.19 |
| -6 | 101.42 | 107.49 | -9 | 194.29 | 218.74 | -10 | 84.48 | 82.81 | -5 | 117.08 | 120.72 |
| -5 | 70.45 | 78.08 | -8 | 37.65 | 18.26 | -9 | 0.00 | 18.97 | -4 | 15.58 | 4.27 |
| -4 | 82.68 | 85.01 | -7 | 77.82 | 75.44 | -8 | 80.74 | 80.98 | -3 | 212.41 | 206.45 |
| -3 | 31.52 | 15.45 | -6 | 305.61 | 420.33 | -7 | 212.13 | 237.81 | -2 | 108.47 | 110.12 |
| -2 | 56.62 | 55.85 | -5 | 149.11 | 161.45 | -6 | 74.30 | 72.67 | -1 | 106.37 | 112.17 |
| -1 | 20.29 | 2.09 | -4 | 147.33 | 147.48 | -5 | 38.65 | 35.11 | 0 | 36.54 | 24.53 |
| 0 | 82.35 | 73.21 | -3 | 58.69 | 50.72 | -4 | 127.62 | 141.34 | 13 2 -8 | 64.77 | 72.49 |
| 1 | 48.40 | 35.69 | -2 | 274.00 | 382.53 | -3 | 66.92 | 69.21 | -7 | 87.33 | 89.51 |
| 2 | 105.04 | 102.83 | -1 | 70.46 | 73.97 | -2 | 32.95 | 30.88 | -6 | 153.64 | 149.07 |
| 3 | 26.88 | 32.93 | 0 | 223.58 | 246.59 | -1 | 57.09 | 52.01 | -5 | 84.92 | 80.31 |
| 12 1 -11 | 27.30 | 20.55 | 1 | 92.18 | 94.65 | 0 | 26.50 | 8.78 | -4 | 102.19 | 97.08 |
| -10 | 185.06 | 189.69 | 2 | 51.04 | 44.50 | 1 | 172.97 | 174.39 | -3 | 147.84 | 150.80 |
| -9 | 22.80 | 32.77 | 3 | 178.25 | 162.03 | 2 | 0.00 | 10.41 | 0 3 2 | 51.81 | 51.64 |
| -8 | 0.00 | 0.71 | 4 | 153.98 | 135.25 | 3 | 116.28 | 110.53 | 3 | 80.55 | 87.57 |
| -7 | 127.04 | 139.87 | 5 | 195.15 | 174.88 | 4 | 201.73 | 201.20 | 4 | 202.90 | 276.32 |
| -6 | 232.28 | 265.23 | 6 | 325.64 | 313.31 | 5 | 152.53 | 144.36 | 5 | 210.23 | 285.07 |
| -5 | 0.00 | 8.55 | 7 | 50.45 | 46.98 | 6 | 54.41 | 52.31 | 6 | 19.66 | 19.32 |
| -4 | 146.24 | 151.13 | 8 | 138.53 | 121.28 | 7 | 117.09 | 102.69 | 7 | 129.91 | 145.42 |
| -3 | 164.76 | 154.70 | 9 | 59.05 | 48.15 | 8 | 224.77 | 212.30 | 8 | 23.24 | 16.99 |
| -2 | 70.87 | 76.28 | 10 | 254.58 | 238.36 | 8 2 -14 | 20.49 | 32.57 | 9 | 39.92 | 36.32 |
| -1 | 11.74 | 5.53 | 11 | 35.28 | 31.75 | -13 | 217.79 | 227.52 | 10 | 68.08 | 80.67 |
| 0 | 156.17 | 161.90 | -14 | 0.00 | 5.67 | -12 | 42.51 | 44.65 | 11 | 155.52 | 110.05 |
| 1 | 149.03 | 135.49 | -13 | 220.63 | 207.61 | -11 | 44.40 | 40.85 | 12 | 110.27 | 100.63 |
| 13 1 -10 | 96.48 | 107.57 | -12 | 57.78 | 66.05 | -10 | 0.00 | 11.05 | 1 3 -13 | 64.07 | 53.77 |
| -9 | 78.86 | 79.40 | -11 | 248.13 | 279.83 | -9 | 218.42 | 244.29 | -11 | 98.30 | 92.57 |
| -8 | 53.07 | 53.81 | -10 | 115.28 | 120.01 | -8 | 191.55 | 197.82 | -10 | 237.63 | 262.59 |
| -7 | 17.27 | 20.21 | -9 | 27.82 | 14.98 | -7 | 164.38 | 156.29 | -9 | 151.33 | 174.54 |
| -6 | 202.37 | 211.29 | -8 | 131.36 | 135.01 | -6 | 53.15 | 53.83 | -8 | 80.02 | 79.10 |
| -5 | 101.00 | 99.19 | -7 | 212.46 | 225.62 | -5 | 0.00 | 5.29 | -7 | 173.46 | 206.56 |
| -4 | 36.96 | 38.30 | -6 | 174.04 | 183.05 | -4 | 177.52 | 186.88 | -6 | 205.33 | 236.22 |
| -3 | 87.62 | 102.06 | -5 | 159.64 | 204.68 | -3 | 189.02 | 192.46 | -5 | 81.37 | 87.36 |
| -2 | 187.58 | 188.30 | -4 | 205.19 | 223.49 | -2 | 64.66 | 64.12 | -4 | 57.19 | 57.31 |
| 0 2 2 | 144.58 | 181.10 | -3 | 149.70 | 170.63 | -1 | 257.94 | 305.94 | -3 | 150.70 | 165.64 |
| 3 | 61.00 | 66.22 | -2 | 87.54 | 91.85 | 0 | 21.61 | 7.86 | -2 | 66.09 | 67.00 |
| 4 | 46.58 | 43.63 | -1 | 160.45 | 160.01 | 1 | 84.88 | 72.66 | 1 | 150.69 | 179.91 |
| 5 | 107.43 | 120.75 | 0 | 21.90 | 12.46 | 2 | 119.53 | 105.40 | 0 | 0.00 | 4.42 |
| 6 | 221.46 | 294.13 | 1 | 295.92 | 349.03 | 3 | 282.42 | 283.23 | 3 | 90.06 | 98.43 |
| 7 | 77.85 | 83.73 | 2 | 25.51 | 5.61 | 4 | 73.49 | 70.69 | 4 | 160.73 | 192.95 |
| 8 | 106.77 | 109.95 | 3 | 127.27 | 114.16 | 5 | 54.18 | 50.94 | 5 | 83.83 | 87.88 |
| 9 | 181.84 | 219.47 | 4 | 263.28 | 245.45 | 6 | 190.94 | 167.85 | 6 | 71.36 | 72.98 |
| 10 | 133.36 | 132.05 | 5 | 202.74 | 172.41 | 7 | 131.82 | 114.44 | 7 | 119.32 | 120.65 |
| 11 | 201.55 | 182.52 | 6 | 0.00 | 0.00 | 8 | 94.74 | 97.31 | 8 | 46.27 | 45.21 |
| 12 | 78.60 | 65.56 | 7 | 67.39 | 58.61 | 9 2 -13 | 99.73 | 91.92 | 9 | 84.66 | 82.54 |
| 13 | 181.35 | 161.46 | 8 | 216.00 | 198.00 | -11 | 26.50 | 19.53 | 10 | 0.00 | 5.96 |
| 1 2 -13 | 96.55 | 94.24 | 9 | 86.61 | 81.52 | -10 | 29.80 | 29.81 | 11 | 45.90 | 47.31 |
| -12 | 142.62 | 142.49 | -10 | 72.44 | 64.12 | -9 | 51.51 | 44.79 | 12 | 128.59 | 110.15 |
| -11 | 47.37 | 42.65 | -11 | 72.10 | 63.59 | -8 | 143.60 | 130.60 | 2 3 -13 | 37.88 | 41.86 |
| -10 | 99.98 | 95.31 | 5 2 -14 | 76.41 | 85.55 | -7 | 60.94 | 60.86 | -12 | 91.62 | 96.18 |
| -9 | 0.00 | 23.31 | -13 | 62.68 | 38.93 | -6 | 80.63 | 78.31 | -11 | 131.59 | 129.69 |
| -8 | 198.90 | 240.67 | -12 | 59.32 | 57.05 | -5 | 145.63 | 146.38 | -10 | 159.58 | 164.74 |
| -7 | 140.97 | 147.21 | -11 | 27.82 | 36.61 | -4 | 27.82 | 36.61 | -9 | 151.33 | 174.54 |
| -6 | 125.07 | 134.16 | -10 | 65.84 | 68.50 | -3 | 182.58 | 202.50 | -8 | 104.03 | 104.11 |
| -5 | 31.74 | 31.12 | -9 | 60.59 | 56.15 | -2 | 0.00 | 13.77 | -7 | 140.34 | 143.07 |
| -4 | 68.81 | 68.56 | -8 | 25.72 | 18.43 | -1 | 159.37 | 164.14 | -6 | 202.90 | 232.34 |
| -3 | 233.47 | 223.97 | -7 | 74.40 | 66.96 | 0 | 192.01 | 195.97 | -5 | 248.55 | 312.64 |
| -2 | 233.15 | 358.47 | -6 | 28.92 | 23.60 | 1 | 128.05 | 124.51 | -4 | 86.27 | 81.79 |
| 1 | 158.25 | 203.58 | -5 | 220.31 | 218.92 | 2 | 69.35 | 68.99 | -3 | 132.31 | 137.33 |
| 2 | 197.00 | 305.21 | -4 | 95.74 | 102.06 | 3 | 20.76 | 7.15 | -2 | 72.46 | 72.51 |
| 3 | 42.03 | 40.54 | -3 | 104.35 | 119.77 | 4 | 151.14 | 143.46 | -1 | 101.36 | 110.62 |
| 4 | 288.44 | 472.50 | -2 | 196.56 | 218.67 | 5 | 55.93 | 44.20 | 0 | 0.00 | 0.88 |
| 5 | 37.27 | 38.25 | -1 | 269.49 | 297.00 | 6 | 19.45 | 20.98 | 2 | 108.10 | 98.20 |
| 6 | 26.65 | 24.99 | 0 | 164.50 | 190.75 | 10 2 -13 | 83.49 | 78.61 | 3 | 283.14 | 324.98 |
| 7 | 107.60 | 112.49 | 1 | 91.79 | 89.39 | -12 | 43.79 | 39.24 | 4 | 196.53 | 204.60 |
| 8 | 222.70 | 247.38 | 2 | 356.30 | 389.02 | -11 | 189.10 | 196.57 | 5 | 28.50 | 23.85 |
| 9 | 97.93 | 84.75 | 3 | 46.62 | 35.74 | -10 | 140.19 | 152.55 | 6 | 113.52 | 104.26 |
| 10 | 183.65 | 156.40 | 4 | 46.87 | 42.68 | -9 | 50.07 | 0.66 | 7 | 368.30 | 368.24 |
| 11 | 212.43 | 196.48 | 5 | 37.70 | 31.48 | -8 | 73.04 | 69.84 | 8 | 237.16 | 220.54 |
| 12 | 19.58 | 5.83 | 6 | 262.41 | 267.31 | -7 | 262.96 | 280.22 | 9 | 137.85 | 119.56 |
| 2 2 -14 | 87.90 | 72.38 | 7 | 120.71 | 113.35 | -6 | 56.29 | 54.08 | 10 | 116.67 | 106.32 |
| -13 | 151.40 | 131.98 | 8 | 161.37 | 151.35 | -5 | 173.11 | 186.62 | 11 | 140.53 | 128.48 |
| -12 | 160.54 | 151.26 | 9 | 112.61 | 97.83 | -4 | 104.95 | 104.21 | 3 3 -13 | 40.33 | 39.14 |
| -11 | 96.73 | 97.27 | 10 | 36.41 | 34.26 | -3 | 152.89 | 157.93 | -12 | 55.24 | 54.37 |
| -10 | 52.71 | 38.91 | 6 2 -14 | 100.07 | 93.05 | -2 | 15.46 | 17.14 | -11 | 106.55 | 114.70 |
| -9 | 87.77 | 83.93 | -13 | 67.72 | 69.81 | -1 | 151.59 | 152.29 | -10 | 171.27 | 187.67 |
| -8 | 42.95 | 35.26 | -12 | 124.70 | 122.40 | 0 | 194.99 | 190.75 | -9 | 40.71 | 37.78 |
| -7 | 225.76 | 282.66 | -11 | 124.76 | 114.91 | 1 | 99.71 | 100.34 | -8 | 131.24 | 131.82 |
| -6 | 16.11 | 7.49 | -10 | 118.04 | 111.31 | 2 | 20.33 | 9.93 | -7 | 91.75 | 88.99 |
| -5 | 128.79 | 135.94 | -9 | 304.60 | 341.79 | 3 | 12.20 | 6.94 | -6 | 53.96 | 49.57 |
| -4 | 59.34 | 104.98 | -8 | 46.83 | 52.20 | 4 | 103.80 | 99.92 | -5 | 47.59 | 44.36 |
| -3 | 217.37 | 284.20 | -7 | 114.80 | 118.01 | 11 2 -12 | 180.83 | 184.51 | -4 | 205.50 | 235.11 |
| -2 | 162.52 | 171.06 | -6 | 19.59 | 16.98 | -11 | 106.88 | 103.94 | -3 | 215.78 | 220.19 |
| -1 | 149.29 | 171.28 | -5 | 364.90 | 444.52 | -10 | 29.60 | 29.72 | -2 | 180.79 | 196.89 |
| 0 | 258.36 | 329.86 | -4 | 51.11 | 48.95 | -9 | 153.53 | 159.07 | -1 | 22.80 | 23.61 |
| 1 | 169.13 | 177.35 | -3 | 243.97 | 276.69 | -8 | 108.15 | 92.32 | 0 | 82.02 | 73.02 |
| 2 | 211.01 | 205.97 | -2 | 223.55 | 233.59 | -7 | 70.39 | 73.24 | 1 | 201.82 | 215.56 |
| 3 | 54.55 | 11.00 | -1 | 208.18 | 204.84 | -6 | 34.10 | 28.70 | 2 | 126.82 | 117.38 |
| 4 | 125.80 | 126.40 | 0 | 78.09 | 76.66 | -5 | 107.11 | 114.94 | 3 | 24.72 | 10.42 |
| 5 | 100.61 | 100.07 | 1 | 126.99 | 124.70 | -4 | 41.27 | 50.98 | 4 | 0.00 | 8.33 |
| 6 | 37.39 | 22.27 | 2 | 187.47 | 187.69 | -3 | 18.56 | 6.30 | 5 | 204.13 | 179.15 |
| 7 | 38.14 | 38.37 | 3 | 77.23 | 74.00 | -2 | 15.56 | 6.30 | 6 | 0.00 | 3.75 |
| 8 | 46.76 | 35.96 | 4 | 90.87 | 85.76 | -1 | 84.32 | 79.77 | 7 | 146.91 | 130.49 |
| 9 | 58.40 | 37.60 | 5 | 36.71 | 33.79 | 0 | 95.76 | 87.13 | 8 | 104.36 | 89.48 |
| 10 | 124.90 | 108.85 | 6 | 19.59 | 10.14 | 1 | 38.45 | 26.14 | 9 | 68.51 | 60.50 |

Table 2. (Continued)

| h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} | h k l | F _{obs} | F _{cal} |
|--------|------------------|------------------|----------|------------------|------------------|---------|------------------|------------------|----------|------------------|------------------|
| 4 5 -9 | 41.28 | 35.08 | 8 5 0 | 161.61 | 152.38 | 2 4 -8 | 156.26 | 182.23 | 6 4 1 | 193.15 | 205.99 |
| -8 | 45.54 | 48.65 | 1 | 124.78 | 117.06 | -7 | 63.04 | 65.20 | 2 | 62.44 | 62.85 |
| -7 | 81.98 | 89.20 | 2 | 19.31 | 17.38 | -6 | 23.91 | 47.61 | 3 | 197.31 | 193.78 |
| -6 | 179.54 | 190.40 | 3 | 73.58 | 73.27 | -5 | 31.58 | 23.25 | 4 | 84.79 | 79.21 |
| -5 | 0.00 | 3.93 | 4 | 46.96 | 43.13 | -4 | 189.62 | 228.95 | 5 | 57.11 | 45.67 |
| -4 | 112.35 | 105.02 | 5 | 78.77 | 80.03 | -3 | 189.14 | 231.72 | 6 | 136.11 | 130.32 |
| -3 | 259.50 | 315.19 | 6 | 41.27 | 36.50 | -2 | 158.03 | 162.48 | 7 | 27.17 | 20.06 |
| -2 | 243.69 | 283.04 | 9 5 -13 | 89.03 | 95.65 | 0 | 133.31 | 145.81 | 7 4 -12 | 158.75 | 157.75 |
| -1 | 229.41 | 258.68 | -12 | 128.64 | 128.26 | 1 | 281.57 | 316.40 | -11 | 172.08 | 174.00 |
| 0 | 0.00 | 3.01 | -11 | 202.77 | 209.43 | 2 | 239.97 | 232.61 | -10 | 114.82 | 111.66 |
| 1 | 239.56 | 237.24 | -10 | 247.84 | 265.53 | 3 | 57.41 | 57.07 | -9 | 21.39 | 22.87 |
| 2 | 235.48 | 256.42 | -9 | 111.60 | 107.09 | 4 | 0.00 | 11.22 | -8 | 170.70 | 176.65 |
| 3 | 314.40 | 321.07 | -8 | 28.49 | 21.47 | 5 | 90.35 | 73.31 | -7 | 189.32 | 195.80 |
| 4 | 19.91 | 2.48 | -7 | 146.49 | 158.92 | 6 | 133.51 | 123.51 | -6 | 126.78 | 129.41 |
| 5 | 33.60 | 29.92 | -6 | 201.01 | 219.81 | 7 | 41.55 | 34.00 | -5 | 119.11 | 126.74 |
| 6 | 61.43 | 55.27 | -5 | 48.60 | 43.63 | 8 | 146.94 | 133.91 | -4 | 99.23 | 98.22 |
| 7 | 87.95 | 84.48 | -4 | 186.07 | 190.58 | 9 | 109.42 | 92.74 | -3 | 87.66 | 84.21 |
| 8 | 56.91 | 47.62 | -3 | 0.00 | 10.30 | 10 | 0.00 | 4.46 | -2 | 74.22 | 68.56 |
| 9 | 163.84 | 148.27 | -2 | 54.74 | 58.34 | 11 | 122.27 | 151.31 | -1 | 121.35 | 122.34 |
| 10 | 137.09 | 121.53 | -1 | 43.09 | 54.53 | 3 4 -13 | 33.55 | 36.92 | 0 | 22.20 | 23.70 |
| 11 | 174.40 | 162.64 | 0 | 146.52 | 150.03 | -12 | 168.11 | 159.81 | 1 | 84.34 | 77.89 |
| 12 | 114.00 | 111.13 | 1 | 76.35 | 69.81 | -11 | 119.51 | 110.05 | 2 | 255.78 | 239.27 |
| 13 | 220.95 | 222.65 | 2 | 247.33 | 242.65 | -10 | 132.40 | 104.97 | 3 | 239.16 | 242.42 |
| 14 | 146.57 | 135.89 | 3 | 174.43 | 150.60 | -9 | 154.61 | 172.96 | 4 | 39.75 | 28.88 |
| 15 | 103.11 | 93.31 | 4 | 25.17 | 22.29 | -8 | 181.15 | 205.82 | 5 | 163.27 | 138.21 |
| 16 | 214.63 | 222.36 | 5 | 100.66 | 93.71 | -7 | 53.46 | 51.27 | 6 | 204.87 | 180.08 |
| 17 | 308.83 | 327.53 | 10 5 -12 | 74.29 | 82.10 | -6 | 33.51 | 27.35 | 8 4 -12 | 102.71 | 85.68 |
| 18 | 141.25 | 131.90 | -12 | 247.33 | 242.65 | -5 | 132.40 | 104.97 | -11 | 56.27 | 59.99 |
| 19 | 82.12 | 74.95 | -10 | 80.08 | 79.42 | -4 | 63.29 | 62.92 | -10 | 42.47 | 39.00 |
| 20 | 158.40 | 162.42 | -9 | 34.88 | 32.08 | -3 | 84.80 | 73.21 | -9 | 171.42 | 174.71 |
| 21 | 115.01 | 112.06 | -8 | 54.96 | 54.52 | 0 | 271.64 | 300.81 | -8 | 103.53 | 95.36 |
| 22 | 46.54 | 43.84 | -7 | 99.99 | 100.79 | 1 | 175.90 | 184.62 | -7 | 287.39 | 267.66 |
| 23 | 87.72 | 87.81 | -6 | 42.65 | 40.54 | 2 | 64.72 | 56.97 | -6 | 85.06 | 75.97 |
| 24 | 55.87 | 52.17 | -5 | 33.60 | 22.29 | 3 | 40.36 | 27.27 | -5 | 114.57 | 112.77 |
| 25 | 110.03 | 117.52 | -4 | 100.27 | 110.23 | 4 | 342.37 | 331.90 | -4 | 44.69 | 47.44 |
| 26 | 75.32 | 77.97 | -3 | 79.83 | 83.62 | 5 | 176.42 | 155.29 | -3 | 234.65 | 270.55 |
| 27 | 49.74 | 45.98 | -2 | 42.60 | 41.97 | 6 | 138.32 | 129.08 | -2 | 145.25 | 132.61 |
| 28 | 0.00 | 12.50 | -1 | 49.08 | 31.86 | 7 | 113.77 | 97.45 | -1 | 39.16 | 29.99 |
| 29 | 60.68 | 175.89 | 0 | 130.77 | 121.66 | 8 | 88.09 | 66.74 | 0 | 24.68 | 2.18 |
| 30 | 167.45 | 152.27 | 1 | 20.02 | 4.35 | 9 | 81.69 | 73.69 | 1 | 51.70 | 47.75 |
| 31 | 121.71 | 108.21 | 2 | 75.90 | 64.71 | 10 | 75.27 | 66.26 | 2 | 169.30 | 160.20 |
| 32 | 68.39 | 60.39 | 3 | 141.78 | 129.47 | 4 4 -13 | 17.36 | 15.41 | 3 | 15.09 | 13.84 |
| 33 | 100.52 | 90.51 | 4 | 21.31 | 17.28 | -12 | 184.71 | 177.26 | 4 | 87.03 | 71.33 |
| 34 | 119.89 | 105.97 | 5 | 65.69 | 62.81 | -11 | 106.92 | 91.15 | 5 | 206.40 | 197.11 |
| 35 | 42.47 | 34.78 | -9 | 0.00 | 2.49 | -10 | 68.05 | 57.82 | 9 4 -12 | 60.90 | 61.34 |
| 36 | 108.88 | 102.12 | -8 | 204.22 | 204.32 | -9 | 214.78 | 234.70 | -11 | 81.41 | 80.17 |
| 37 | 50.15 | 54.53 | -7 | 178.46 | 173.21 | -8 | 127.33 | 132.12 | -10 | 23.16 | 27.28 |
| 38 | 64.15 | 62.72 | -6 | 62.13 | 59.88 | -7 | 81.41 | 69.86 | -9 | 122.69 | 126.65 |
| 39 | 87.33 | 77.10 | -5 | 42.54 | 42.00 | -6 | 132.23 | 128.04 | -8 | 53.17 | 52.79 |
| 40 | 170.41 | 170.91 | -4 | 240.43 | 260.04 | -5 | 322.56 | 386.21 | -7 | 0.00 | 17.77 |
| 41 | 129.76 | 130.47 | -3 | 200.57 | 204.16 | -4 | 0.00 | 12.73 | -6 | 14.69 | 1.40 |
| 42 | 0.00 | 0.99 | -2 | 198.47 | 203.92 | -3 | 32.49 | 33.13 | -5 | 147.66 | 149.05 |
| 43 | 23.03 | 20.72 | -1 | 25.47 | 16.29 | 2 | 121.49 | 136.10 | -4 | 193.10 | 220.02 |
| 44 | 77.38 | 77.21 | 0 | 116.38 | 108.09 | -1 | 164.45 | 177.01 | -3 | 113.02 | 122.45 |
| 45 | 104.26 | 109.61 | 1 | 165.37 | 156.92 | 0 | 130.90 | 147.25 | -2 | 39.33 | 40.79 |
| 46 | 37.73 | 36.99 | 2 | 161.06 | 160.31 | 1 | 32.11 | 20.60 | -1 | 85.30 | 77.04 |
| 47 | 178.20 | 184.95 | -8 | 61.75 | 65.20 | 2 | 46.14 | 44.98 | 0 | 163.61 | 165.68 |
| 48 | 57.26 | 52.50 | -7 | 64.55 | 64.81 | 3 | 154.20 | 145.28 | 1 | 165.22 | 155.94 |
| 49 | 118.74 | 116.27 | -6 | 107.50 | 109.49 | 4 | 220.62 | 209.74 | 2 | 13.87 | 10.55 |
| 50 | 155.90 | 142.83 | -5 | 39.54 | 27.50 | 5 | 168.65 | 151.48 | 3 | 23.06 | 21.71 |
| 51 | 95.28 | 95.36 | -4 | 14.64 | 6.94 | 6 | 58.98 | 55.47 | 4 | 49.29 | 53.64 |
| 52 | 124.12 | 112.31 | -3 | 15.09 | 5.04 | 7 | 157.24 | 143.78 | 10 4 -11 | 9.09 | 17.82 |
| 53 | 121.44 | 269.03 | -2 | 56.44 | 50.57 | 8 | 185.64 | 163.54 | -10 | 154.18 | 142.03 |
| 54 | 212.32 | 203.27 | -1 | 32.76 | 38.04 | 9 | 185.64 | 162.83 | -9 | 156.71 | 162.88 |
| 55 | 67.10 | 58.33 | 0 4 2 | 87.51 | 96.64 | 5 4 -13 | 123.95 | 117.28 | -8 | 25.21 | 23.35 |
| 56 | 130.70 | 119.72 | 3 | 190.41 | 238.30 | -12 | 48.77 | 53.37 | -7 | 34.00 | 30.28 |
| 57 | 132.26 | 129.91 | 4 | 145.83 | 165.86 | -11 | 23.11 | 17.84 | -6 | 163.83 | 149.03 |
| 58 | 205.96 | 195.60 | 5 | 100.00 | 114.98 | -10 | 36.01 | 23.21 | -5 | 70.11 | 71.23 |
| 59 | 0.00 | 22.05 | 6 | 165.36 | 195.39 | -9 | 114.51 | 101.53 | -4 | 42.95 | 31.56 |
| 60 | 132.27 | 82.78 | 7 | 189.92 | 227.30 | -8 | 51.66 | 50.42 | -3 | 92.19 | 92.08 |
| 61 | 47.83 | 41.76 | 8 | 0.00 | 4.68 | -7 | 143.65 | 140.82 | -2 | 103.86 | 100.95 |
| 62 | 69.54 | 66.71 | 9 | 0.00 | 8.84 | -6 | 215.62 | 224.94 | -1 | 232.41 | 248.51 |
| 63 | 37.90 | 24.09 | 10 | 172.22 | 164.73 | -5 | 24.71 | 15.92 | 0 | 75.10 | 65.46 |
| 64 | 229.95 | 254.38 | 11 | 129.53 | 108.83 | -4 | 172.73 | 192.78 | 1 | 173.12 | 169.17 |
| 65 | 209.88 | 225.57 | 12 | 83.48 | 73.96 | -3 | 227.98 | 258.36 | -2 | 19.66 | 18.93 |
| 66 | 193.54 | 203.07 | -12 | 72.67 | 64.29 | -2 | 259.52 | 308.51 | 11 4 -9 | 86.70 | 89.59 |
| 67 | 44.29 | 46.94 | -11 | 129.02 | 121.26 | -1 | 133.23 | 126.54 | -8 | 37.99 | 41.75 |
| 68 | 204.20 | 204.03 | -10 | 30.76 | 35.26 | 0 | 133.49 | 144.11 | -7 | 82.04 | 86.31 |
| 69 | 194.40 | 209.21 | -9 | 68.57 | 66.47 | 1 | 182.31 | 173.96 | -6 | 168.66 | 184.78 |
| 70 | 267.67 | 304.14 | -8 | 133.49 | 143.59 | 2 | 68.37 | 59.88 | -5 | 25.98 | 15.75 |
| 71 | 27.01 | 22.98 | -7 | 131.14 | 138.61 | 3 | 167.46 | 152.97 | -4 | 0.00 | 15.90 |
| 72 | 23.62 | 10.03 | -6 | 191.73 | 238.83 | 4 | 49.31 | 41.23 | -3 | 103.07 | 97.12 |
| 73 | 175.48 | 169.67 | -5 | 86.13 | 92.46 | 5 | 63.56 | 54.08 | -2 | 24.30 | 15.82 |
| 74 | 128.79 | 117.06 | -4 | 159.77 | 184.19 | 6 | 126.86 | 124.04 | -1 | 95.85 | 93.74 |
| 75 | 44.03 | 32.20 | -3 | 70.23 | 67.52 | 7 | 114.83 | 104.11 | 0 | 136.47 | 132.18 |
| 76 | 48.60 | 50.77 | -2 | 259.04 | 374.16 | 8 | 234.64 | 224.74 | 12 4 -6 | 25.42 | 21.82 |
| 77 | 33.18 | 25.70 | 2 | 130.36 | 155.65 | 9 | 0.00 | 13.28 | -5 | 187.98 | 208.70 |
| 78 | 19.50 | 14.87 | 3 | 156.60 | 178.60 | -12 | 0.00 | 9.88 | -4 | 125.60 | 111.42 |
| 79 | 50.37 | 56.94 | 4 | 37.34 | 34.52 | -11 | 224.67 | 229.29 | 0 5 2 | 31.77 | 30.36 |
| 80 | 144.51 | 139.40 | 5 | 148.59 | 169.32 | -10 | 123.68 | 109.19 | 3 | 52.09 | 51.99 |
| 81 | 92.14 | 93.22 | 6 | 145.80 | 171.67 | -9 | 109.84 | 97.39 | 4 | 46.50 | 47.32 |
| 82 | 0.00 | 3.82 | 7 | 113.81 | 119.13 | -8 | 111.82 | 101.62 | 5 | 85.94 | 92.23 |
| 83 | 147.15 | 156.54 | 8 | 0.00 | 10.52 | -7 | 67.82 | 71.65 | 6 | 67.26 | 71.65 |
| 84 | 33.25 | 25.90 | 9 | 162.66 | 145.12 | -6 | 117.60 | 123.60 | | | |

Table 2. (Continued)

| h | k | l | F _{obs} | F _{cal} | h | k | l | F _{obs} | F _{cal} | h | k | l | F _{obs} | F _{cal} | h | k | l | F _{obs} | F _{cal} |
|-----|---|-----|------------------|------------------|-----|---|-----|------------------|------------------|----|---|-----|------------------|------------------|----|---|-----|------------------|------------------|
| 1 | 5 | -8 | 129.32 | 134.69 | 4 | 5 | 5 | 34.17 | 14.71 | 9 | 5 | -9 | 44.68 | 30.38 | 4 | 6 | -6 | 62.65 | 51.70 |
| -7 | | | 0.00 | 10.58 | 6 | | | 96.16 | 86.26 | -8 | | | 19.84 | 17.56 | -5 | | | 139.76 | 131.68 |
| -6 | | | 38.70 | 30.00 | 7 | | | 45.50 | 35.52 | -7 | | | 123.96 | 112.90 | -4 | | | 168.01 | 181.70 |
| -5 | | | 45.56 | 42.00 | 8 | | | 194.71 | 179.32 | -6 | | | 35.23 | 40.39 | -3 | | | 219.20 | 253.55 |
| -4 | | | 91.71 | 99.43 | 5 | 5 | -12 | 91.91 | 77.44 | -5 | | | 132.32 | 127.93 | -2 | | | 36.32 | 7.24 |
| -3 | | | 16.17 | 9.65 | -11 | | | 127.74 | 132.24 | -4 | | | 34.29 | 40.14 | -1 | | | 240.93 | 266.46 |
| -2 | | | 161.97 | 190.81 | -10 | | | 28.08 | 25.36 | -3 | | | 97.70 | 84.23 | 0 | | | 19.46 | 16.17 |
| -1 | | | 133.34 | 137.44 | -9 | | | 89.70 | 77.46 | -2 | | | 54.22 | 52.66 | 1 | | | 172.73 | 186.90 |
| 0 | | | 51.91 | 56.83 | -8 | | | 53.83 | 56.72 | -1 | | | 141.86 | 148.17 | 2 | | | 80.28 | 83.65 |
| 1 | | | 223.70 | 298.55 | -7 | | | 20.50 | 19.28 | 0 | | | 18.10 | 13.58 | 3 | | | 194.10 | 192.31 |
| 2 | | | 166.85 | 208.69 | -6 | | | 105.92 | 68.76 | 1 | | | 103.68 | 95.07 | 4 | | | 167.22 | 167.44 |
| 3 | | | 192.88 | 248.27 | -5 | | | 76.58 | 67.71 | 2 | | | 75.00 | 81.20 | 5 | | | 28.94 | 26.52 |
| 4 | | | 51.91 | 56.83 | -4 | | | 99.62 | 101.86 | 10 | 5 | -8 | 157.38 | 160.14 | 6 | | | 22.80 | 16.94 |
| 5 | | | 212.48 | 214.60 | -3 | | | 176.69 | 207.73 | -7 | | | 161.61 | 166.35 | 7 | | | 23.95 | 23.52 |
| 6 | | | 132.36 | 116.26 | -2 | | | 44.36 | 45.69 | -6 | | | 234.51 | 268.75 | 5 | 6 | -10 | 63.37 | 65.41 |
| 7 | | | 126.30 | 113.39 | -1 | | | 65.67 | 58.09 | -5 | | | 93.35 | 85.16 | -9 | | | 46.37 | 41.66 |
| 8 | | | 155.26 | 128.55 | 0 | | | 131.93 | 150.43 | -4 | | | 77.09 | 72.20 | -8 | | | 262.08 | 290.10 |
| 9 | | | 100.61 | 82.93 | 1 | | | 280.68 | 314.99 | -3 | | | 81.18 | 81.87 | -5 | | | 133.75 | 133.52 |
| 10 | | | 95.04 | 89.74 | 2 | | | 151.01 | 144.82 | -2 | | | 188.96 | 188.05 | -6 | | | 51.15 | 43.24 |
| -9 | | | 0.00 | 12.31 | 3 | | | 161.65 | 152.09 | -1 | | | 157.11 | 153.97 | -5 | | | 102.71 | 112.27 |
| -8 | | | 97.07 | 99.24 | 4 | | | 67.39 | 63.38 | 0 | 6 | 3 | 141.13 | 169.49 | -4 | | | 158.42 | 173.05 |
| -7 | | | 149.80 | 170.52 | 5 | | | 264.85 | 255.20 | 4 | | | 56.85 | 61.06 | -5 | | | 106.52 | 112.91 |
| -6 | | | 207.66 | 259.15 | 6 | | | 184.00 | 172.42 | 5 | | | 176.07 | 215.71 | -7 | | | 47.65 | 47.11 |
| -5 | | | 76.90 | 83.69 | 7 | | | 94.70 | 92.39 | 6 | | | 160.29 | 193.98 | -1 | | | 161.43 | 177.80 |
| -4 | | | 143.09 | 154.38 | 6 | 5 | -11 | 115.28 | 109.86 | 7 | | | 39.30 | 34.43 | 0 | | | 53.12 | 59.74 |
| -3 | | | 36.03 | 34.68 | -10 | | | 126.31 | 124.09 | 8 | | | 89.35 | 78.01 | 1 | | | 47.92 | 39.58 |
| -2 | | | 184.63 | 189.24 | -9 | | | 151.39 | 152.93 | 9 | | | 21.34 | 4.89 | 2 | | | 39.30 | 32.44 |
| -1 | | | 115.14 | 114.47 | -8 | | | 211.72 | 235.19 | 1 | | | 60.06 | 51.74 | 3 | | | 53.95 | 59.36 |
| 0 | | | 85.64 | 85.21 | -7 | | | 34.42 | 29.69 | -8 | | | 25.32 | 25.18 | 4 | | | 182.11 | 179.36 |
| 1 | | | 113.44 | 88.88 | -6 | | | 163.50 | 164.88 | -7 | | | 28.37 | 26.62 | 5 | | | 0.00 | 3.92 |
| 2 | | | 65.65 | 61.64 | -5 | | | 158.79 | 163.84 | -6 | | | 213.81 | 266.63 | 6 | 6 | -10 | 61.95 | 51.10 |
| 3 | | | 178.89 | 174.02 | -4 | | | 238.18 | 269.35 | -5 | | | 20.10 | 13.95 | 6 | 6 | -10 | 58.11 | 54.33 |
| 4 | | | 32.46 | 26.10 | -3 | | | 113.60 | 123.63 | -4 | | | 23.33 | 16.68 | 7 | | | 0.00 | 7.79 |
| 5 | | | 24.60 | 8.35 | -2 | | | 62.71 | 53.03 | 3 | | | 0.00 | 8.86 | 8 | | | 24.07 | 20.73 |
| 6 | | | 100.36 | 87.66 | -1 | | | 24.46 | 23.81 | 4 | | | 61.76 | 64.15 | 7 | | | 108.75 | 103.62 |
| 7 | | | 104.59 | 91.09 | 0 | | | 159.66 | 105.08 | 5 | | | 48.45 | 51.14 | 6 | | | 20.22 | 18.94 |
| 8 | | | 71.54 | 62.38 | 1 | | | 72.74 | 68.71 | 6 | | | 32.43 | 29.57 | -5 | | | 0.00 | 13.18 |
| 9 | | | 69.21 | 57.94 | 2 | | | 23.92 | 14.27 | 7 | | | 87.43 | 72.43 | -4 | | | 0.00 | 4.16 |
| 10 | | | 22.08 | 25.25 | 3 | | | 96.27 | 88.34 | 8 | | | 28.54 | 23.06 | -3 | | | 0.00 | 4.53 |
| -9 | | | 37.91 | 12.47 | 4 | | | 25.18 | 22.39 | 9 | | | 24.31 | 25.49 | -2 | | | 143.82 | 161.12 |
| -8 | | | 140.89 | 146.79 | 5 | | | 59.07 | 52.24 | 2 | 6 | -10 | 27.66 | 26.22 | -1 | | | 0.00 | 7.72 |
| -7 | | | 110.26 | 105.93 | 6 | | | 18.42 | 13.32 | -9 | | | 205.85 | 217.56 | 0 | | | 76.15 | 76.08 |
| -6 | | | 138.83 | 187.14 | 7 | 5 | -11 | 186.09 | 193.71 | -8 | | | 60.20 | 51.49 | 1 | | | 195.65 | 198.10 |
| -5 | | | 140.48 | 150.14 | -10 | | | 25.05 | 12.74 | -7 | | | 25.71 | 24.00 | 2 | | | 83.95 | 83.83 |
| -4 | | | 201.87 | 237.94 | -9 | | | 42.51 | 50.97 | -6 | | | 45.03 | 44.94 | 3 | | | 19.05 | 7.94 |
| -3 | | | 40.21 | 36.35 | -8 | | | 25.35 | 17.55 | -5 | | | 201.79 | 241.84 | 4 | | | 88.30 | 84.18 |
| -2 | | | 130.04 | 138.62 | -7 | | | 179.16 | 188.13 | -4 | | | 154.15 | 179.50 | 5 | 7 | -9 | 0.00 | 4.77 |
| -1 | | | 144.82 | 150.07 | -6 | | | 75.23 | 89.10 | -3 | | | 72.09 | 73.06 | -9 | | | 0.00 | 0.00 |
| 0 | | | 199.02 | 226.13 | -5 | | | 104.22 | 114.61 | -2 | | | 187.89 | 170.88 | 7 | 6 | -9 | 170.80 | 184.42 |
| 1 | | | 140.15 | 140.15 | -4 | | | 102.39 | 104.79 | 3 | | | 296.72 | 294.70 | 6 | | | 180.68 | 189.87 |
| 2 | | | 27.45 | 34.31 | -3 | | | 133.35 | 143.74 | 4 | | | 60.36 | 47.20 | -5 | | | 87.85 | 95.17 |
| 3 | | | 37.18 | 37.00 | -2 | | | 31.11 | 19.15 | 5 | | | 35.08 | 25.33 | 4 | | | 195.64 | 198.96 |
| 4 | | | 26.12 | 20.55 | -1 | | | 46.80 | 45.34 | 6 | | | 85.50 | 71.74 | -3 | | | 50.96 | 50.62 |
| 5 | | | 157.58 | 145.15 | 0 | | | 94.14 | 101.84 | 7 | | | 306.62 | 297.18 | -2 | | | 167.60 | 193.16 |
| 6 | | | 105.03 | 99.92 | 1 | | | 34.04 | 31.89 | 8 | | | 96.10 | 95.16 | -1 | | | 39.56 | 36.14 |
| 7 | | | 151.50 | 134.01 | 2 | | | 109.66 | 103.52 | 3 | 6 | -10 | 138.70 | 127.78 | 0 | | | 223.93 | 236.25 |
| 8 | | | 218.90 | 211.76 | 3 | | | 0.00 | 7.77 | -9 | | | 158.38 | 157.50 | 1 | | | 131.70 | 139.17 |
| 9 | | | 30.22 | 26.01 | 4 | | | 45.07 | 41.19 | 8 | | | 78.25 | 79.34 | 2 | | | 94.60 | 88.50 |
| 10 | | | 70.76 | 64.32 | 5 | | | 156.10 | 140.96 | 7 | | | 66.22 | 70.57 | 3 | | | 58.48 | 55.05 |
| 4 | 5 | -12 | 286.85 | 291.29 | 6 | 5 | -11 | 59.01 | 57.01 | -6 | | | 43.73 | 39.64 | 8 | 6 | -8 | 90.03 | 94.63 |
| -11 | | | 151.55 | 152.38 | -10 | | | 178.95 | 181.75 | -5 | | | 94.61 | 97.64 | -7 | | | 131.39 | 135.86 |
| -10 | | | 75.11 | 64.64 | -9 | | | 135.00 | 153.24 | -4 | | | 152.07 | 163.25 | -6 | | | 46.29 | 49.62 |
| -9 | | | 37.80 | 33.07 | -8 | | | 45.37 | 42.91 | -3 | | | 85.72 | 83.15 | -5 | | | 103.74 | 90.40 |
| -8 | | | 156.10 | 208.24 | -7 | | | 122.70 | 116.30 | -2 | | | 159.63 | 186.44 | -4 | | | 83.81 | 93.37 |
| -7 | | | 54.56 | 53.85 | -6 | | | 43.93 | 46.39 | 0 | | | 168.34 | 182.48 | -3 | | | 118.87 | 111.21 |
| -6 | | | 26.46 | 19.32 | -5 | | | 19.90 | 17.74 | 1 | | | 47.35 | 47.17 | -2 | | | 0.00 | 24.32 |
| -5 | | | 131.90 | 123.02 | -4 | | | 0.00 | 3.59 | 2 | | | 164.26 | 160.58 | -1 | | | 117.71 | 118.13 |
| -4 | | | 33.07 | 48.47 | -3 | | | 194.24 | 170.44 | 3 | | | 96.32 | 99.19 | 0 | | | 17.37 | 22.90 |
| -3 | | | 108.67 | 112.93 | -2 | | | 203.67 | 232.43 | 4 | | | 141.88 | 130.44 | 1 | | | 76.53 | 64.06 |
| -2 | | | 84.26 | 92.50 | -1 | | | 139.11 | 145.28 | 5 | | | 68.12 | 62.72 | 9 | 6 | -7 | 0.00 | 4.37 |
| -1 | | | 40.76 | 36.61 | 0 | | | 180.56 | 100.47 | 6 | | | 59.44 | 55.55 | -6 | | | 140.83 | 130.06 |
| 0 | | | 137.97 | 148.34 | 1 | | | 0.00 | 9.09 | 7 | | | 0.00 | 5.52 | -5 | | | 141.96 | 151.23 |
| 1 | | | 116.37 | 120.64 | 2 | | | 250.46 | 236.52 | 4 | 6 | -10 | 76.97 | 72.29 | -7 | | | 59.06 | 58.38 |
| 2 | | | 145.94 | 142.16 | 3 | | | 152.68 | 145.91 | -9 | | | 34.75 | 37.74 | -3 | | | 125.51 | 139.51 |
| 3 | | | 76.34 | 72.18 | 4 | | | 128.63 | 121.46 | -8 | | | 110.08 | 113.61 | -2 | | | 77.64 | 67.03 |
| 4 | | | 184.20 | 171.62 | 9 | 5 | -10 | 38.50 | 53.85 | -7 | | | 110.41 | 103.24 | -1 | | | 88.42 | 86.79 |

with cycles of isotropic temperature-factor refinement. The final values of the conventional R factor are: 11.1% including reflections with $F_0 = 0$ and those rejected as affected by extinction; 8.7% excluding the latter; 8.3% also excluding reflections with $F_0 = 0$. Refinement of anisotropic temperature factors was not attempted since the accuracy of the data was not sufficiently high to permit the determination of meaningful values. Values of the isotropic temperature factors and atom coordinates are given in Table 1, and of the structure factors in Table 2.

Description of the alamosite structure

Figure 1 is a representation of the structure of alamosite projected on (010). The dominant structural feature is a chain of silica tetrahedra which extends parallel to $[10\bar{1}]$. This chain has a lattice-translation repeat of twelve tetrahedra. There are four independent bridging oxygen atoms in the chain, O(1)—O(4), with O(1) at an inversion center and O(2) on a two-fold axis. Thus, units of the chain which are three tetrahedra long form the symmetry-repeated chain unit.

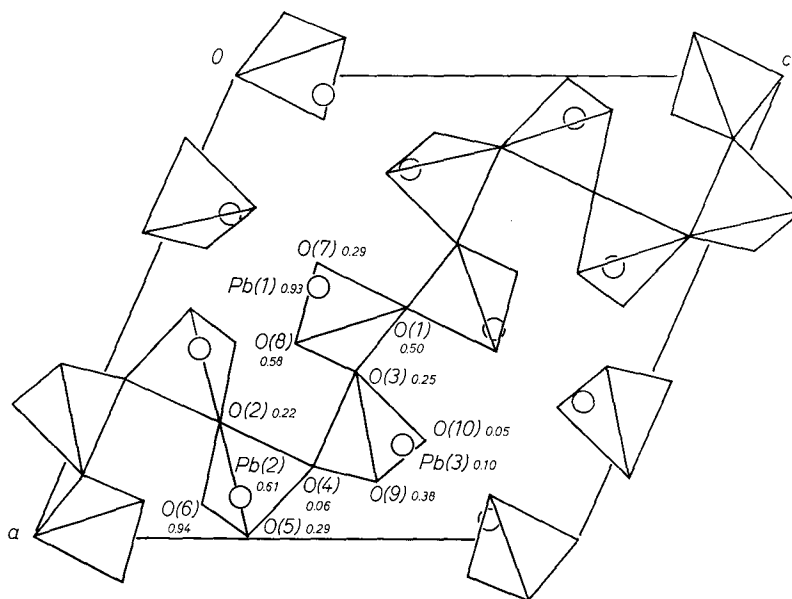


Fig. 1. Projection of the structure of alamosite, space group $P2/n$, on (010). Oxygen atoms are represented by tetrahedron vertices, and Pb atoms by circles

PREWITT and PEACOR (1964) have reviewed the general nature of metasilicate chain structures. All are based on an approximation to closest packing. No analogy to the structures of these phases (pyroxenes and pyroxenoids) is evident in the alamosite structure and thus it has a unique structural configuration.

Values of silicon-oxygen distances are given in Table 3, and values of tetrahedral oxygen-oxygen distances and oxygen-silicon-oxygen angles in Table 4. All values were calculated using the IBM program ORFFE written and kindly made available by BUSING and LEVY. Estimated standard deviations were calculated using the full least-squares variance-covariance matrix and estimated lattice-