

The Crystal Structure of Latiumite, a New Type of Sheet Silicate

ELIO CANNILLO, A. DAL NEGRO, GIUSEPPE ROSSI

*C.N.R. Centro di Studio per la Cristallografia Strutturale,
c/o Istituto di Mineralogia, via Bassi 4, 27100 Pavia, Italy*

Abstract

The crystal structure of latiumite, $K_{0.85}Ca_3(Si_{2.15}Al_{2.85})O_{11}(SO_4)_{0.7}(CO_3)_{0.3}$; $a = 12.06$, $b = 5.08$, $c = 10.81$ Å, $\beta = 106^\circ$; space group $P2_1$, $Z = 2$, has been determined on an Albano specimen, using Weissenberg data. The isotropic least-squares refinement led to a final R-index of 0.08.

The main structural feature is the presence of double layers of (Si,Al) tetrahedra; the double layers, parallel to the cleavage plane (100), are connected to each other by Ca-atoms and SO_4^{2-} groups. The Si and Al atoms are ordered among the five symmetry independent tetrahedra. A pseudo-glide plane results in frequent twinning on (100).

Introduction

Latiumite was discovered by Tilley and Henry (1953) in some ejected blocks found in the 'peperino' of the Albano Hills near Rome. A tentative interpretation of the chemical analysis of latiumite (analyst J. H. Scoon) is given by the same authors (Table 1, columns 1 and 2).

The optical properties of latiumite are unusual: the optic axial angle is variable, sections with lower extinction angle being optically positive, those with higher extinction angles optically negative; mottled extinction is always present and zoning occurs frequently. Tilley and Henry explained these optical features with the assumption that the mineral is a solid solution series, but no correlation with chemical composition was made owing to the small number of chemical analyses.

A second Italian occurrence of latiumite was reported (Barbieri and Fornaseri, 1970) in metamorphic ejected blocks found in a pumice deposit near Pitigliano (Grosseto, Tuscany). The mineral from Pitigliano has different optical properties: the optic axial angle is constant, the optic sign is always negative, and the refractive indexes are lower. Unfortunately Barbieri and Fornaseri gave no chemical analysis of this latiumite.

Experimental

A small prismatic crystal of latiumite from Albano was used for recording the X-ray data. Weissenberg photographs (rotation axis b) of five reciprocal lattice layers were recorded with $CuK\alpha$ radiation

($\lambda_{\alpha_1} = 1.54051$ Å) using the multiple film technique. A total of 1350 reflections (84%) of the 1612 present in the $CuK\alpha$ limiting sphere were inspected; the intensities of 877 reflections were measured photometrically, the remainder being too weak to be conveniently measured.

Cell parameters were re-determined from Weissenberg and oscillation photographs: $a = 12.06 \pm 0.01$, $b = 5.08 \pm 0.02$, $c = 10.81 \pm 0.01$ Å, $\beta = 106.0^\circ$; these values are in fair agreement with those published by Tilley and Henry except for β (106° vs 108°).

The systematic absences of $0k0$ reflections with $k = 2n + 1$ restricted the choice of the space group to $P2_1/m$ or $P2_1$. In the course of the structure analysis the correct space group proved to be $P2_1$.

The measured intensities were corrected for Lorentz and polarization effects but no absorption correction was applied. The correction suggested by Sakurai (1962) for incomplete resolution of the $K\alpha$ doublet was applied with the replacement of γ for θ (Buerger's notation) in the interpolation formula.

Crystal Structure Analysis

The statistical averages and distribution of the normalized structure factors are given in Table 2 where they are compared with the theoretical values for both a centrosymmetric and a non-centrosymmetric distribution of atoms in the unit cell (Karle *et al.*, 1965). Since no conclusive indication as to space group can be drawn from Table 2 or from a piezoelectricity test, it was assumed initially that latiumite was centrosymmetric. An attempt was

TABLE 1. Chemical Composition of Latiumite

| | From chemical analyses* | | From structure analysis** | |
|--------------------------------|-------------------------|---------------|-----------------------------|-----------------|
| | Wt. % | Atoms to O=25 | Wt. % | Atoms to O=29.4 |
| SiO ₂ | 28.33 | 5.32 | 23.41 | 4.3 |
| Al ₂ O ₃ | 24.67 | 5.45 | 26.32 | 5.7 |
| Fe ₂ O ₃ | 0.50 | 0.07 | -- | -- |
| FeO | 0.55 | 0.09 | -- | -- |
| MnO | 0.02 | -- | -- | -- |
| MgO | 0.76 | 0.21 | -- | -- |
| CaO | 29.41 | 5.91 | 30.48 | 6.0 |
| Na ₂ O | 1.11 | 0.40 | -- | -- |
| K ₂ O | 7.20 | 1.73 | 7.25 | 1.7 |
| H ₂ O ⁺ | 0.27 | -- | -- | -- |
| SO ₃ | 5.42 | 0.76 | 10.15 | 1.4 |
| CO ₂ | 1.60 | 0.40 | 2.39 | 0.6 |
| Cl | 0.14 | 0.02 | -- | -- |
| | 99.98 | | 100.00 | |
| Less O=Cl | 0.03 | | | |
| D _{calc} | = 2.92*** | | D _{calc} = 2.88*** | |

*Analysis published by Tilley and Henry (1952), analyst J.H. Socon. The results are from two partial analyses: one of pure material for all the elements but SO₃, CO₂, Cl; the other using "a product containing a very small fraction of melilite which itself has been subject to analysis."

**Chemical analysis computed on the basis of the results of the structure determination.

***D_{obs} = 2.93 (From Tilley and Henry, 1952).

made to solve the crystal structure in space group $P2_1/m$ by the reiterative application of Sayre's equation using an unpublished program by Long (1965).

The set of signs with the highest consistency was used to compute an E map. The highest peaks appeared in the sections with y nearly equal to $1/4$ and $3/4$; a number of smaller peaks, doubled by the mirror plane, produced unreasonably short interatomic distances. These difficulties led to the consideration of space group $P2_1$. By assuming that the peaks at $y = 1/4$ and $y = 3/4$ corresponded to the 'heavy' atoms Si, Ca, K, and by suitably interpreting the peaks doubled by the mirror, it was possible to construct a structural model in $P2_1$. Success-

TABLE 2. Statistical Averages and Distribution of E for Latiumite

| | Experimental | Centric | Acentric |
|-----------------------------|--------------|---------|----------|
| $\langle E \rangle$ | 0.846 | 0.798 | 0.886 |
| $\langle E^2 - 1 \rangle$ | 0.886 | 0.969 | 0.736 |
| $\langle E^2 \rangle$ | 1.0 | 1.0 | 1.0 |
| E > 1 | 33.5 % | 32.0 % | 36.8 % |
| E > 2 | 3.4 % | 5.0 % | 1.8 % |
| E > 3 | 0.0 % | 0.3 % | 0.01 % |

TABLE 3. Atomic Coordinates and Isotropic Temperature Factors of Latiumite*

| Atom | Mult.** | x/a | y/b | z/c | B(Å ²) |
|--|----------|------------|-------------|------------|--------------------|
| T(1)=Si _{0.80} Al _{0.20} | | 0.3779 (4) | 0.7500 | 0.0710 (4) | 0.17 (8) |
| T(2)=Al | | .3816 (4) | .7581(27) | .3497 (5) | 0.00 (8) |
| T(3)=Si _{0.50} Al _{0.50} | | .3447 (4) | .2601(25) | .4784 (5) | 0.05 (8) |
| T(4)=Si _{0.85} Al _{0.15} | | .8239 (4) | .7103(23) | .3569 (5) | 0.13 (9) |
| T(5)=Al | | .6530 (4) | .7494(27) | .0840 (5) | 0.08 (8) |
| O(1) | | .6900(13) | .0804(43) | .0583(15) | 1.21(28) |
| O(2) | | .5165(10) | .7269(46) | .1035(12) | 0.75(22) |
| O(3) | | .3379(12) | .0631(41) | .0460(14) | 0.79(26) |
| O(4) | | .3389(11) | .6388(37) | .1934(13) | 0.41(24) |
| O(5) | | .3414(13) | .0920(42) | .3428(14) | 1.02(26) |
| O(6) | | .5299(11) | .7277(50) | .4097(13) | 0.95(23) |
| O(7) | | .3073(12) | .5754(40) | .4366(14) | 0.85(26) |
| O(8) | | .2426(12) | .1173(42) | .5358(13) | 0.80(25) |
| O(9) | | .9407(13) | .5519(42) | .3981(15) | 1.34(30) |
| O(10) | | .8350(12) | .0299(40) | .3540(14) | 0.68(26) |
| O(11) | | .7475(12) | .5974(40) | .2166(13) | 0.65(24) |
| Ca(1) | | .8866 (3) | .2581(23) | .1913 (3) | 0.33 (6) |
| Ca(2) | | .2025 (3) | .2549(22) | .1460 (4) | 0.82 (7) |
| Ca(3) | | .1166 (3) | .7384(23) | .4515 (3) | 0.22 (6) |
| K | 1.70 (5) | .5747 (5) | .2574(29) | .2748 (6) | 1.20(17) |
| S | 1.42 (5) | .0358 (5) | .7833(27) | .1387 (6) | 0.44(17) |
| O(12) | | .9119(14) | .8170(46) | .0803(17) | 2.16(37) |
| O(13) | 1.35(10) | .1059(17) | .3298(49) | .0461(20) | 0.49(60) |
| O(14) | | .0649(17) | .5317(50) | .2018(21) | 2.30(42) |
| O(15) | | .0703(16) | -0.0107(48) | .2388(19) | 1.75(38) |
| C*** | 0.60 | .01 | 0.77 | .17 | |

*Estimated standard deviations in parentheses.

**The multipliers which in the course of the refinement showed deviations from the expected values smaller than one standard deviation are omitted and have the theoretical value of 2.

***The parameters of this atom are those of the center of the triangle formed by O(12), O(14) and O(15). These parameters were not allowed to vary in the course of the refinement.

sive structure-factor calculations and three-dimensional Fourier syntheses revealed the atoms that were not detected on the E map and confirmed the structure. The positions of all the 'heavy' atoms were consistent with space group $P2_1/m$, thus explaining the initial success of the E map obtained with the centrosymmetric assumption.

Five cycles of full matrix least-squares refinement with individual isotropic temperature factors lowered the R-index to 0.081 for the 877 measured reflections. An attempt to use anisotropic temperature factors was unsuccessful, probably because of the unfavorable ratio of number of variables to number of observations. Consequently, the refinement was stopped at the last isotropic cycle. A secondary extinction correction (Zachariasen, 1963), introduced in the last two cycles of the refinement ($g = 1.53 \times 10^{-6}$), reduced R from 0.094 to 0.081.

Refinement was carried out using a locally modified version of the program ORFLS by Busing *et al* (1962). The scattering factors were for neutral atoms, taken from Hanson *et al* (1964).

TABLE 5. Interatomic Distances of Latiumite*

| | | | | | |
|-----------|----------|------------|----------|---------|----------|
| T(1)-O(1) | 1.65(2)Å | Ca(1)-O(1) | 2.57(2)Å | S-O(12) | 1.46(2)Å |
| O(2) | 1.62(1) | O(9) | 2.62(2) | O(13) | 1.50(2)Å |
| O(3) | 1.66(2) | O(10) | 2.33(2) | O(14) | 1.45(2) |
| O(4) | 1.62(1) | O(11) | 2.47(2) | O(15) | 1.48(2) |
| mean | 1.64 | O(12) | 2.60(2) | mean | 1.47 |
| T(2)-O(4) | 1.73(1) | O(13) | 2.62(2) | K-O(1) | 3.16(2) |
| O(5) | 1.76(2) | O(14) | 2.54(2) | O(2) | 2.98(2) |
| O(6) | 1.73(1) | O(15) | 2.53(2) | O(2)* | 3.24(2) |
| O(7) | 1.74(2) | mean | 2.53 | O(5) | 3.21(2) |
| mean | 1.74 | Ca(2)-O(3) | 2.40(1) | O(6) | 2.93(2) |
| T(3)-O(5) | 1.69(2) | O(4) | 2.51(2) | O(6)* | 3.18(2) |
| O(6) | 1.66(1) | O(5) | 2.46(2) | O(7) | 3.19(2) |
| O(7) | 1.69(2) | O(12) | 2.48(2) | O(8) | 3.15(2) |
| O(8) | 1.69(2) | O(13) | 2.55(2) | O(10) | 3.23(2) |
| mean | 1.68 | O(14) | 2.38(2) | O(11) | 2.91(2) |
| T(4)-O(8) | 1.65(1) | O(15) | 2.50(2) | mean | 3.12 |
| O(9) | 1.58(2) | mean | 2.47 | C-O | 1.37** |
| O(10) | 1.63(2) | Ca(3)-O(7) | 2.49(1) | | |
| O(11) | 1.65(2) | O(8) | 2.47(2) | | |
| mean | 1.63 | O(9) | 2.25(2) | | |
| T(5)-O(1) | 1.78(2) | O(9)* | 2.50(2) | | |
| O(2) | 1.78(1) | O(10) | 2.28(2) | | |
| O(3) | 1.72(2) | O(14) | 2.80(2) | | |
| O(11) | 1.75(2) | O(15) | 2.55(2) | | |
| mean | 1.74 | mean | 2.48 | | |

*Estimated standard deviations in parentheses.

**This value corresponds to the distance of the center from the vertices of the triangle formed by O(12), O(14) and O(15).

Final atomic parameters are given in Table 3. The observed and calculated structure factors are compared in Table 4.¹ Bond distances and angles are listed in Tables 5 and 6.

Description and Discussion of the Structure

Latiumite is a sheet silicate, as Tilley and Henry had supposed. Corrugated double layers of tetrahedra connected by Ca atoms represent the main structural feature of this mineral. The SO_4^{2-} groups act as 'bridges' between calcium atoms linked to different double layers.

The aluminosilicate layer. Each single layer (Fig. 1) is formed by rings of six and eight tetrahedra; the adjacent layer is superposed on the first by screw rotation in such a way that the eight-membered ring of one sheet is connected with a six-membered ring of the other. In this way four of the five independent tetrahedra share all their oxygen atoms, while the remaining tetrahedron, $T(4)$, has only two shared oxygens. Note that if the $T(4)$ tetrahedra were elimi-

¹ To obtain a copy of Table 4, order NAPS Document 02058 from Microfiche Publications, 305 East 46th Street, New York, N.Y. 10017. Please remit in advance \$1.50 for microfiche or \$5.00 for photocopies, payable to Microfiche Publications. Please check the most recent issue of this journal for the current address and prices.

TABLE 6. Tetrahedral Bond Angles of Latiumite*

| | | | |
|------------------|------------|-----------------|------------|
| O(1)-T(1)-O(2) | 112.8 (8)° | O(1)-T(5)-O(2) | 111.8(10)° |
| O(3) | 107.9 (9) | O(3) | 108.4 (8) |
| O(4) | 108.7 (9) | O(11) | 114.2 (8) |
| O(2)-T(1)-O(3) | 109.9(10) | O(2)-T(5)-O(3) | 110.0 (8) |
| O(4) | 108.2 (7) | O(11) | 107.5 (7) |
| O(3)-T(1)-O(4) | 109.3 (8) | O(3)-T(5)-O(11) | 104.6 (8) |
| O(4)-T(2)-O(5) | 106.9 (8) | T(1)-O(1)-T(5) | 122.5(10) |
| O(6) | 109.4 (7) | T(1)-O(2)-T(5) | 159.5(10) |
| O(7) | 106.3 (8) | T(1)-O(3)-T(5) | 125.3 (9) |
| O(5)-T(2)-O(6) | 110.2(11) | T(1)-O(4)-T(2) | 126.6(10) |
| O(7) | 111.2 (8) | T(2)-O(5)-T(3) | 120.7(10) |
| O(6)-T(2)-O(7) | 112.5 (9) | T(2)-O(6)-T(3) | 154.3(10) |
| O(5)-T(3)-O(6) | 112.3 (9) | T(2)-O(7)-T(3) | 120.8 (9) |
| O(7) | 107.8 (8) | T(3)-O(8)-T(4) | 132.9(12) |
| O(8) | 104.9 (9) | T(4)-O(11)-T(5) | 132.5(12) |
| O(6)-T(3)-O(7) | 114.2(11) | | |
| O(8) | 107.4 (8) | O(12)-S-O(13) | 113.0(11) |
| O(7)-T(3)-O(8) | 109.7 (8) | O(14) | 113.2(13) |
| | | O(15) | 106.3(12) |
| O(8)-T(4)-O(9) | 103.0 (9) | O(13)-S-O(14) | 110.2(13) |
| O(10) | 110.9 (9) | O(15) | 106.3(12) |
| O(11) | 106.9 (8) | O(14)-S-O(15) | 107.3(11) |
| O(9)-T(4)-O(10) | 116.2 (9) | | |
| O(11) | 108.2 (9) | | |
| O(10)-T(4)-O(11) | 110.9 (9) | | |

*Estimated standard deviations in parentheses.

nated and if $T(3)$ and $T(5)$ were joined together, the sheet becomes identical to the aluminosilicate layer in hexagonal $\text{CaAl}_2\text{Si}_2\text{O}_8$ (Takeuchi and Donnay, 1959).

The double layer can also be visualized as rings of five tetrahedra repeated by the screw axis (Fig. 2). These rings are nearly parallel to (010), and the resulting double layer is parallel to (100), which is a plane of perfect cleavage.

On the basis of the relationship between T -O distances and Al contents given by Smith and Bailey (1963), it has been possible to determine the distribution of Si and Al in the five independent tetrahedra (Table 3).

The calcium-sulfate layer. Three independent

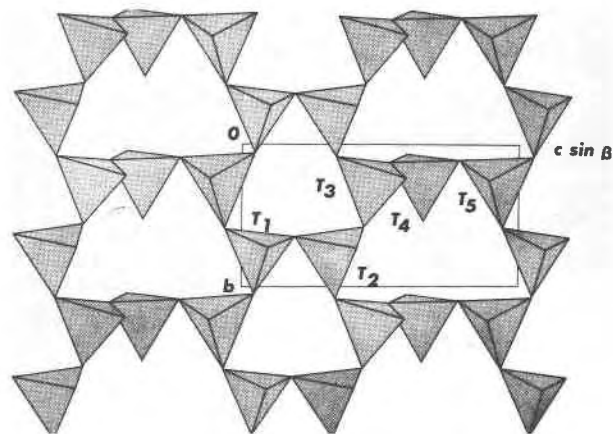


FIG. 1. Single tetrahedral layer projected along [100].

calcium atoms occur in the asymmetric unit. Ca(1) is surrounded by eight oxygen atoms, while Ca(2) and Ca(3) have sevenfold coordination. Some of the oxygen atoms linked to Ca belong to the aluminosilicate layer, others belong to the SO_4^{2-} groups. Ca(3) connects two silicate double layers directly, while Ca(1) and Ca(2) perform the same function indirectly with the SO_4^{2-} groups acting as bridges between Ca atoms linked to different double layers (Fig. 2). The Ca atoms and the sulfate ions form a positively-charged intermediate layer which is sandwiched between the negatively-charged silicate layers.

The multipliers of the Ca atoms were allowed to vary during the least-squares refinement but did not show any deviation from full occupancy greater than one standard deviation.

The mean S-O bond length in the SO_4 tetrahedron (1.47 Å) is in good agreement with the values reported recently for several sulphate structures. The multipliers of S and O(13) are smaller than the theoretical values by several standard deviations (Table 3), while the remaining oxygen atoms of the SO_4 tetrahedron have a full occupancy. This observation suggests a partial substitution of CO_3^{2-} for SO_4^{2-} , which agrees with the chemical analysis. The three oxygen atoms showing full occupancy should belong to both the SO_4^{2-} and CO_3^{2-} groups. An attempt to find the carbon atom on the electron density map, near the center of the triangle formed by O(12), O(14) and O(15), proved unsuccessful, probably because of its low atomic number and overlapping of the sulfur peak. The partial occupancy of O(13) only slightly disturbs the coordination of Ca(1) and Ca(2).

Potassium atoms occur in cavities between two superposed five-membered rings of tetrahedra in the silicate double layer. The K-O distances range from 2.91 to 3.24 Å and the potassium occupancy is about 85 percent.

The chemical formula. The chemical formula resulting from the crystal structure analysis can be written as follows:

$\text{K}_{0.85}\text{Ca}_3(\text{Si}_{2.15}\text{Al}_{2.85}\text{O}_{11})(\text{SO}_4)_{0.7}(\text{CO}_3)_{0.3}$, $Z = 2$.
The chemical analysis, computed on the basis of this formula (Table 1, column 4 and 5) differs from that given by Tilley and Henry (Table 1, column 2 and 3) mainly in regard to its lower SiO_2 content, and its higher SO_3 content. Unfortunately the available material was insufficient to carry out a new chemical analysis.

A fairly satisfactory balance of electrostatic

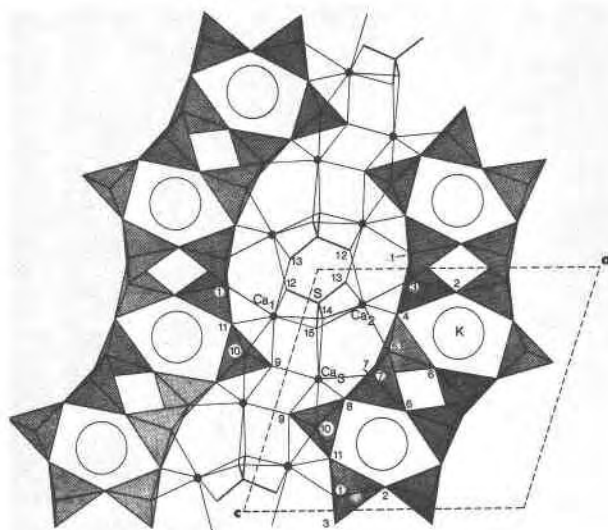


FIG. 2. The crystal structure of latiumite projected on (010).

valences (Table 7) can be computed using the method of Donnay and Allman (1970) and the chemical formula obtained from the structure analysis. Only O(10), O(14) and O(15) have deviations greater than 10 percent from the formal value of two positive charges reaching each oxygen atom. The unbalanced oxygens are involved in Ca-O distances which are well below, for O(10), or above, for O(14) and O(15), the Ca-O average distances of their respective coordination polyhedra. There are several cases, for example, buergerite and omphacite (Martin and Donnay, 1972), where similar effects occur. The unbalancing of some oxygen atoms seems to be due to the fact that with the Donnay and Allman approach the bond strengths of the shorter bonds are underestimated and those of the longer ones are overestimated.

Tilley and Henry supposed that latiumite was a solid solution series. If so, its general formula can be written, on the basis of this structure determination, as $\text{K}(\text{Ca},\text{Na})_3(\text{Al},\text{Si})_5\text{O}_{11}(\text{SO}_4,\text{CO}_3)$. The mineral analyzed in this work is hence an Al-rich member of the series. An amount greater than three Al atoms per formula unit would imply the replacement of Ca by some trivalent cation or of K by Ba. On the other hand a complete replacement of Al by Si and of Ca by Na would not be possible without changes in the structure because some oxygen atoms would be heavily unbalanced. Some such substitutions could possibly take place, but only additional occurrences of latiumite will establish the limits of the solid solution series.

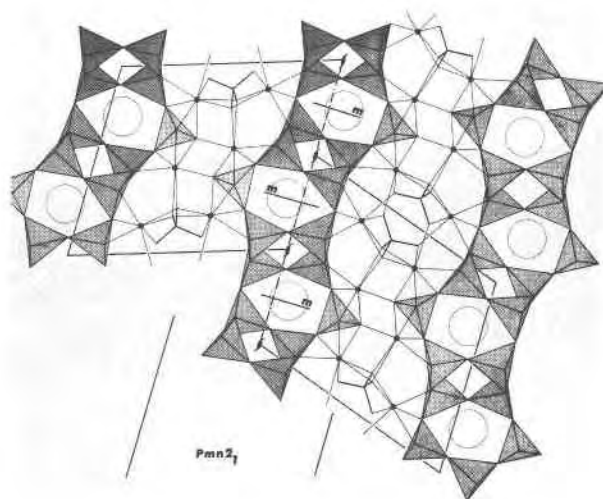


FIG. 3. Structural interpretation of twinning in latiumite. The two individuals of the twin are related by the pseudo-glide plane n .

Twinning of latiumite. Latiumite often shows single or repeated twinning with twin plane (100). Twinning can be explained from a structural point of view in the following way: a pseudo-mirror plane (103) is present in each five-membered ring (Fig. 3) and also governs the Ca atoms directly bonded to the ring; the combination of this pseudo-mirror plane with the 2_1 screw axis results in a pseudo- n glide-plane (100) which becomes the twin glide-plane. Morphologically it appears as a twin mirror plane. The portion of the structure common to the two individuals of the twin has $Pmn2_1$ pseudo-symmetry. The formation of the twin produces only small distortions in the calcium-sulphate substructure.

Acknowledgments

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TABLE 7. Bond Lengths (Å) and Estimated Bond Valences (V.U.)

| | T(1) | T(2) | T(3) | T(4) | T(5) | Ca(1) | Ca(2) | Ca(3) | K | S | C | ΣCv | |
|-------------|-------------------|------|------|------|------|-------|-------|-------|------|------|-------|-------------|--------|
| 0(1) | 1.65 | | | | 1.78 | 2.57 | | | | 3.16 | | | |
| | 0.93 | | | | 0.70 | 0.24 | | | | 0.06 | | | 1.93 |
| 0(2) | 1.62 | | | | 1.72 | | | | | 2.98 | | | |
| | 0.98 ^a | | | | 0.78 | | | | | 0.14 | | | |
| | | | | | | | | | | 3.24 | | | 1.93 |
| | | | | | | | | | | 0.03 | | | |
| 0(3) | 1.66 | | | | 1.72 | | 2.40 | | | | | | |
| | 0.91 | | | | 0.78 | | 0.33 | | | | | | 2.02 |
| 0(4) | 1.62 | 1.73 | | | | | 2.51 | | | | | | |
| | 0.98 | 0.76 | | | | | 0.28 | | | | | | 2.02 |
| 0(5) | | 1.76 | 1.69 | | | | 2.46 | | 3.21 | | | | |
| | | 0.73 | 0.86 | | | | 0.30 | | 0.04 | | | | 1.93 |
| 0(6) | | 1.73 | 1.66 | | | | | | 2.93 | | | | |
| | | 0.76 | 0.92 | | | | | | 0.18 | | | | |
| | | | | | | | | | 3.18 | | | | |
| | | | | | | | | | 0.05 | | | | 1.91 |
| 0(7) | | 1.74 | 1.68 | | | | | 2.49 | 3.19 | | | | |
| | | 0.75 | 0.86 | | | | | 0.28 | 0.05 | | | | 1.94 |
| 0(8) | | | 1.69 | 1.65 | | | | 2.47 | 3.15 | | | | |
| | | | 0.86 | 0.92 | | | | 0.28 | 0.06 | | | | 2.12 |
| 0(9) | | | | 1.58 | | 2.62 | | 2.25 | | | | | |
| | | | | 1.05 | | 0.23 | | 0.38 | | | | | |
| | | | | | | | | 2.50 | | | | | |
| | | | | | | | | 0.27 | | | | | 1.93 |
| 0(10) | | | 1.63 | | 2.33 | | 2.28 | 3.23 | | | | | |
| | | | 0.96 | | 0.35 | | 0.37 | 0.04 | | | | | 1.72 |
| 0(11) | | | 1.65 | 1.75 | 2.47 | | | | 2.91 | | | | |
| | | | 0.92 | 0.74 | 0.28 | | | | 0.20 | | | | 2.14 |
| 0(12) | | | | | | 2.60 | 2.48 | | | 1.46 | | | |
| | | | | | | 0.23 | 0.29 | | | 1.08 | 0.044 | | 2.00 |
| 0(13)* | | | | | | 2.62 | 2.55 | | | 1.50 | | | |
| | | | | | | 0.16 | 0.19 | | | 0.98 | | | 1.33 |
| | | | | | | | | | | | | | (1.90) |
| 0(14) | | | | | | 2.54 | 2.38 | 2.80 | | 1.45 | | | |
| | | | | | | 0.25 | 0.32 | 0.17 | | 1.11 | 0.4 | 2.25 | |
| 0(15) | | | | | | 2.53 | 2.50 | 2.55 | | 1.48 | | | |
| | | | | | | 0.26 | 0.29 | 0.25 | | 1.03 | 0.4 | 2.23 | |
| ΣAv | 3.80 | 3.00 | 3.50 | 3.85 | 3.00 | 2.00 | 2.00 | 2.00 | 0.85 | 4.20 | 1.2 | 29.40 | |

ΣCv = valence of bonds reaching anion.

ΣAv = valences of bonds emanating from cation summed over the bonded anions.

* This atom has an occupancy of 0.7; the value in parentheses is the ΣCv extrapolated to full occupancy.

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