Refinement of the Crystal Structure of Beryllonite, 
NaBePO₄

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With 2 Figures

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Summary

The refined lattice parameters of beryllonite are: 

- \( a = 8.178 (3) \) Å,
- \( b = 7.818 (2) \) Å,
- \( c = 14.114 (6) \) Å,

with \( \beta = 90.00° (2) \); space group \( P2_1/n \), 

\( Z = 12 \). Integrated Weissenberg photographs were taken by using CuK\( \alpha \) radiation and multiple film packs. The anisotropic refinement of the crystal structure by means of least-square methods gave a final R value of 0.063 for the 1388 observed reflections. In the crystal structure PO₄ and BeO₄ tetrahedra, linked by shared oxygen atoms in a three-dimensional network, form pseudo-ditrigonal rings perpendicular to the \( b \) axis. The independent Na atoms lying in the channels formed by the rings are coordinated as an irregular "nine-cornered" polyhedron and as distorted octahedra.

Zusammenfassung

Verfeinerung der Kristallstruktur des Beryllonits, NaBePO₄

Verfeinerte Gitterkonstanten des Beryllonits lauten: 

- \( a = 8.178 (3) \) Å,
- \( b = 7.818 (2) \) Å,
- \( c = 14.114 (6) \) Å,

mit \( \beta = 90.00° (2) \); Raumgruppe: \( P2_1/n \), 

\( Z = 12 \). Integrierte Weissenbergaufnahmen wurden mit CuK\( \alpha \)-Strahlung und multiplen Filmpaketen aufgenommen. Die anisotope Verfeinerung der Kristallstruktur nach der Methode der kleinsten Quadrate ergab für 1388 beob. Reflexe einen abschließenden R-Wert von 0.063. In der Kristallstruktur bilden PO₄- und BeO₄-Tetraeder, die über gemeinsame Sauerstoffe zu einem dreidimensionalen Gerüst verknüpft sind, pseudo-ditrigonale Ringe senkrecht zur \( b \)-Achse. Die kristallographisch unabhängigen Arten von Na-Atomen, welche in den aus Ringen gebildeten Kanälen liegen, sind in der Form eines unregelmäßigen neuneckigen Polyeders bzw. in der Form verzerrter Oktaeder koordiniert.

This work is part of a project of the authors on the crystal structure of trimerite which will be studied next. Trimerite shows clear analogies to beryllonite as to the chemical formula and the lattice con-
The present research is, therefore, in some respect an advance of the crystal structure of the mineral trimerite.

Several investigations on the crystal structure of beryllonite were made previously: Gossner and Besslein (1934) and Wehrenberg (1954) determined the unit cell parameters and the space-group. Golovastikov (1962) carried out an interesting study on the crystal structure of beryllonite and found the coordinates of all the atoms by 2-dimensional electron density projections. The \( R \) factors obtained from the [010] and [100] projections were 0.218 and 0.243 respectively.

Because of the inherent errors in the results from projection data and the growing need for more accurate interatomic distances for theoretical purposes, it was decided to reinvestigate this structure. The present paper describes the structure derived from a three-dimensional anisotropic refinement.

A new accurate determination of the lattice constants was carried out by means of the least-squares method, measuring the 2 \( \theta \) values of a powder diffraction pattern (CuK\( \lambda \) radiation). The results are as follows: \( a = 8.178 \) (3) \( \AA \), \( b = 7.819 \) (2) \( \AA \), \( c = 14.114 \) (6) \( \AA \); the angle \( \beta \) is 90.00 (2)\(^{\circ}\); \( Z = 12 \) and \( D_\alpha = 2.805; \) space group \( P2_1/n \).

A specimen of beryllonite from the Stoneham deposit (Maine, U.S.A.), with spherical shape (\( \mu = 82.67 \) cm\(^{-1}\), \( \mu R = 1.438 \)), was used to collect the X-ray data. Integrated Weissenberg pictures of eight reciprocal lattice layers (\( k \) from 0 to 7) were obtained using the multiple films technique. A total of 1808 reflections in the CuK\( \lambda \) limiting sphere (about 87\%) were inspected; 1388 of them were measured photometrically, 420 were too faint to be suitably measured or did not give any blackening on the films. The intensities were corrected for the Lorentz-polarization and absorption factors and for the \( z_1-z_2 \) spot doubling.

The positions of the atoms obtained from Golovastikov's investigation were confirmed on the basis of a 3-dimensional Patterson synthesis and of a 3-dimensional electron density map. The refinement of the crystal structure was carried out by several cycles of least-squares and by introducing first isotropic and then anisotropic thermal parameters. The refinement was stopped when the shifts in the parameters were less than the standard deviations. The final \( R \) index for the observed reflections was 0.063 (\( R = 0.083 \) for all the reflections).

The observed and calculated structure factors are listed in Table 1. The revised coordinates and thermal parameters are reported in Table 2; the analysis of the ellipsoid of the thermal vibration in Table 3. All the interatomic distances and angles with their standard deviations, calculated by using Busing, Martin, and Levy's (1964) ORFFE program are listed in Tables 4 and 5 respectively.