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The Determination of the Crystal Structure of Pectolite, $Ca_2NaHSi_3O_9$

By **M. J. Buerger**

With 15 figures

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Zusammenfassung

Die Kristallstruktur des triklinen, zur Raumgruppe $P\bar{1}$ gehörenden Pektoliths wurde mit Hilfe von drei Patterson-Projektionen bestimmt.

Die Patterson-Projektion $P(xz)$ konnte gelöst werden nach Auffinden zweier konjugierter Spitzen im Diagramm. Diese legen zwei Paare von Spitzen, die durch Inversion einander zugeordnet sind, fest. Beide Paare wurden der Berechnung je einer Minimumfunktion zugrunde gelegt. Diese Funktionen vom Rang 2 ergaben kombiniert eine verstärkte Minimum-Funktion vom Rang 4, aus der die Struktur abgelesen werden konnte.

Die Patterson-Projektionen $P(xy)$ und $P(yz)$ und deren Lösungen durch die Minimum-Funktionen (sowie auch andere Fakten) zeigten, daß der Pektolith eine Unterstruktur besitzt, so daß es möglich war, die Unterstrukturtheorie anzuwenden. Dementsprechend wurden die partiellen Patterson-Projektionen gebildet. Die drei Projektionen des Pektoliths wurden dann durch Fourier-Synthesen verfeinert.

Die Struktur des Pektoliths wurde bereits früher beschrieben.[1] Es ist eine vom Pyroxentyp verschiedene Kettenstruktur. Die Na-Atome haben eine ungewöhnliche Umgebung und zeigen eine beträchtliche anisotrope Wärmebewegung. Die H-Atome verbinden O-Atome von zwei verschiedenen Tetraedern.

Abstract

Pectolite is triclinic, space group $P\,\bar{1}$, with 15 nonhydrogen atoms in the asymmetric unit. Its crystal structure has been determined by solving the three Patterson projections by the use of image-seeking functions.

The Patterson projection $P(xz)$ was solved after finding two conjugate peaks on the map. These located two sets of inversion peaks upon each of which a scaled minimum function was based. These two functions of rank 2 were combined to give the more powerful minimum function of rank 4. This was such a good approximation to the electron density that the general nature of the structure could be deduced from it.

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[1] M. J. Buerger, The arrangement of atoms in crystals of the wollastonite group of metasilicates. Proc. Nat. Acad. Sci. **42** (1956) 113—116.

The PATTERSON projections $P(xy)$ and $P(yz)$, and their solution by minimum functions (as well as other evidence) suggested that pectolite has a substructure, so that it became possible to apply substructure theory[2, 3]. Accordingly, the partial PATTERSON projections $\partial P(xy)$ and $\partial P(yz)$ were computed and solved for the locations of the atoms of the complement structure. The three projections of pectolite were refined by successive FOURIER syntheses and by difference maps.

The structure of pectolite has already been described[1]. It is based upon single silica chains differing from the pyroxene-type chains. The Na atoms have an unorthodox environment, and show considerable anisotropic thermal motion. The hydrogen atoms bond together oxygen atoms of two different tetrahedra.

Introduction

Pectolite was formerly regarded as monoclinic[4]. WARREN and BISCOE[5], examining it by the oscillating-crystal method, noted that the spectra required triclinic, rather than monoclinic, symmetry. PEACOCK[6] later confirmed the triclinic symmetry from a morphological study.

A brief note of the crystal structure of pectolite has already been published by the author[1] but the analysis was treated only in outline. A fuller account, describing the application of a new crystal-structure analysis method[3] suitable to crystals like pectolite, is given here.

Material and cell data

Professor CLIFFORD FRONDEL of the Mineralogical Department of Harvard University kindly made avaible to the writer some of the pectolite from Paterson, New Jersey, studied by PEACOCK. The cell, and later the intensities, were studied by means of c axis and a axis precession photographs (dial axis b^*), and by means of b axis DE JONG-BOUMAN photographs. Table 1 shows the cell characteristics as determined in the study, compared with the older results of WARREN and BISCOE[5] and of PEACOCK[6]. The new results are in good agreement with the older data.

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[2] M. J. BUERGER, Some relations for crystals with substructures. Proc. Nat. Acad. Sci. **40** (1954) 125—128.

[3] M. J. BUERGER, Partial FOURIER syntheses and their application to the solution of certain crystal structures. Proc. Nat. Acad. Sci. **42** (1956) 776—781.

[4] EDWARD SALISBURY DANA and WILLIAM E. FORD, A Textbook of Mineralogy. (John Wiley & Sons, 1932) 567.

[5] B. E. WARREN and J. BISCOE, The crystal structure of the monoclinic pyroxenes. Z. Kristallogr. **80** (1931) 391—401, especially 400—401.

[6] M. A. PEACOCK, On pectolite. Z. Kristallogr. **90** (1935) 97—111.