

MINERALOGICAL NOTES

X-RAY STUDY OF CHALCOSIDERITE,  $\text{CuFe}_6(\text{PO}_4)_4(\text{OH})_8 \cdot 4\text{H}_2\text{O}$

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INTRODUCTION

Chalcosiderite (Maskelyne, 1875; Schaller, 1912) is related to turquoise by isomorphous substitution of Al by Fe. The structure of turquoise was recently determined by the author (Cid-Dresdner, 1965), and a determination of the structure of chalcosiderite was considered desirable. Chalcosiderite crystals from West Phoenix, England, were kindly provided by Professor Clifford Frondel of Harvard University for this investigation.

PRECESSION WORK

Several single crystals of chalcosiderite were examined optically before one satisfactory for x-ray study was found. The crystals tend to form groups in which they maintain nearly parallel orientations, building a sort of sheaf. The smaller crystals presented rounded faces which were mostly striated, but the striations disappeared when the crystal was immersed in a liquid with a refractive index similar to its own.

A small crystal which gave good extinction under the polarizing microscope was chosen for the determination of the lattice constants. The crystal was oriented on the optical goniometer so that a normal to one of the best-developed faces was parallel to the spindle axis. The crystal was then transferred to the precession camera and the orientation was corrected by the method of Evans *et al.* (1949).

Two precession photographs were taken using as precessing axes the crystallographic directions analogous to the *a* and *b* axes of turquoise (Cid-Dresdner, 1965). As expected, the reduced cell (Buerger, 1957; Balashov, 1956) of chalcosiderite retained the orientation of the turquoise cell. The relations of the reduced cell of chalcosiderite with respect to the previous cells reported by Maskelyne (1875) and Graham (1948) are given on Table 1. The transformation matrices for chalcosiderite are identical to the transformation formulas used for turquoise (Cid-Dresdner, 1965) to obtain Schaller's (1912) and Graham's (1948) settings. This is due to the fact that both authors based their choice of the turquoise cell on the values reported for chalcosiderite.

Table 2 gives the lattice constants for chalcosiderite obtained from precession photographs. Graham's values for chalcosiderite and the

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TABLE 1. DIRECT AND INVERSE TRANSFORMATIONS FOR THE THREE REPORTED UNIT CELLS OF CHALCOSIDERITE

	Direct transformation	Inverse transformation
Maskelyne to Graham	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 1 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$
Graham to Cid-Dresdner	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$
Maskelyne to Cid-Dresdner	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & -1 \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix}$

turquoise parameters are also included for the similarity of the lattice constants.

#### CYLINDRICAL-FILM MEASUREMENTS

In order to transfer the chalcosiderite crystal to the single-crystal counter diffractometer, a reorientation of the crystal was necessary. The orientation was made by the use of the double-oscillation techniques of Weiss and Cole (1948). A rotation photograph of the chalcosiderite crystal showed the existence of two parallel lattice translations of similar dimensions. One of them corresponded to the value of the *b* axis determined by precession photographs. The other was a slightly smaller translation and included the weaker diffraction spots. A zero-level Weissenberg photograph (Fig. 1) of the same crystal also showed the existence of the slightly smaller lattice.

In order to understand the relationship between the two lattices, the

TABLE 2. COMPARISON OF CHALCOSIDERITE AND TURQUOIS UNIT CELLS

	Chalcosiderite		Turquoise	
	Graham	Cid-Dresdner	Graham	Cid-Dresdner
<i>a</i>	7.68 Å	7.68 Å	7.46 Å	7.424 Å
<i>b</i>	7.90 Å	7.82 Å	7.65 Å	7.629 Å
<i>c</i>	10.20 Å	10.21 Å	9.01 Å	9.910 Å
$\alpha$	67.5°	67.5°	68.35°	68.61°
$\beta$	69.0°	69.1°	69.43°	69.71°
$\gamma$	64.7°	64.8°	64.62°	65.08°

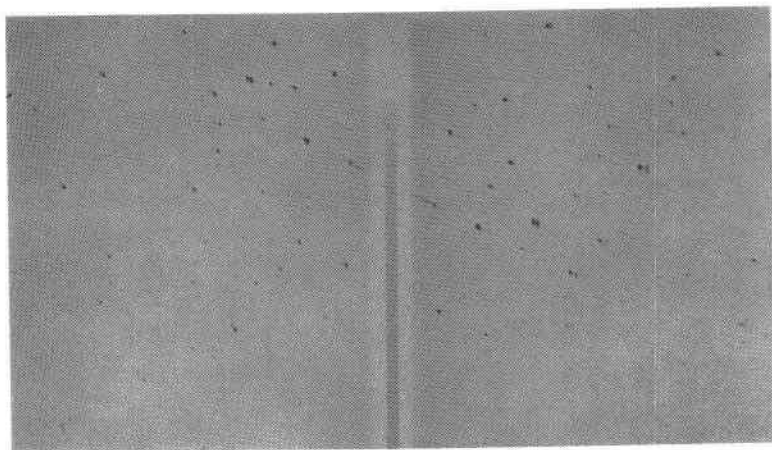


FIG. 1. Zero-level Weissenberg photograph of chalcosiderite.

Weissenberg photograph of Fig. 1 was plotted in reciprocal space, as shown in Fig. 2. When the data from the rotation and the Weissenberg photographs were combined, it turned out that the parameters corresponding to the smaller translations were very close to the turquoise lattice constants. Table 3 compares the results of the cylindrical-film method with the previous known data for chalcosiderite and turquoise. The comparison is made in terms of reciprocal-lattice constants since no information about the other two angles was included in these photographs.

The results from Table 3 pointed out that the "single" crystals of chalcosiderite also include turquoise crystals. A well-known relation that could explain this fact is epitaxial growth of turquoise on chalcosiderite. Attempts were made to see the two minerals under the polarizing microscope. It was thought that it should be possible to differentiate between the refractive indices of chalcosiderite and turquoise. The lowest refractive index of chalcosiderite is 1.775 and the highest index of refraction of

TABLE 3. IDENTIFICATION OF THE TWO LATTICES FOUND IN ROTATING-CRYSTAL PHOTOGRAPHS OF CHALCOSIDERITE

	Lattice 1	Lattice 2	Chalcosiderite <sup>1</sup>	Turquoise <sup>2</sup>
$a^*$	0.230 r.l.u.	0.238 r.l.u.	0.228	0.2353
$c^*$	0.168 r.l.u.	0.173 r.l.u.	0.169	0.1721
$\beta^*$	102° 0'	102° 30'	103° 15'	103°
$b$	7.856 Å	7.620 Å	7.82 Å	7.629 Å

<sup>1</sup> From precession photographs.

<sup>2</sup> From back-reflection Weissenberg least-squares method.

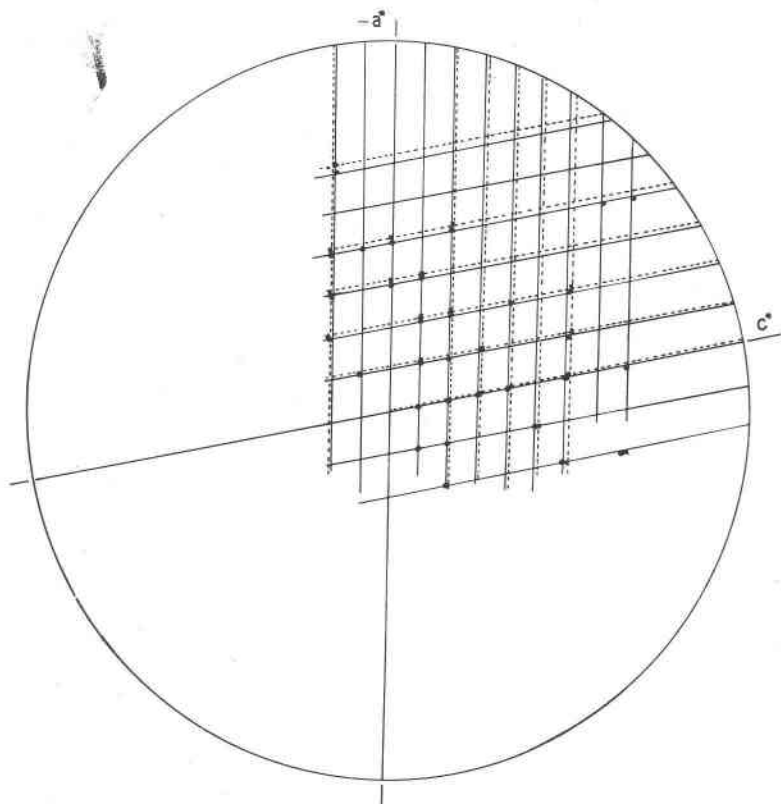


FIG. 2. Weissenberg photograph of Fig. 1 plotted in reciprocal space.

turquoise is 1.65. Chalcosiderite crystals were immersed in a liquid of refractive index 1.75 to look for an edge that would possibly show a lower index. Even if this was actually observed in some cases, the evidence was not considered conclusive due to the limitations of the method used by Wahlstrom (1943).

Four other crystals were examined by  $x$ -ray methods. All of them presented evidence of the existence of the two structures. Two of these crystals were broken but in both cases the usable fragments still showed the two characteristic translations corresponding to turquoise and chalcosiderite.

Under these conditions the structural study of chalcosiderite was postponed. It is, however, certain that chalcosiderite and turquoise have the same structure. Both of the replaceable elements accept octahedral coordination. The reported Fe-O distance for Fe in octahedral coordination

(Ito and Mori, 1951; Mori and Ito, 1950) is 2.02 Å, whereas the average Al-O in octahedral coordination is 1.9 Å. This difference could very well account for the larger cell presented by chalcosiderite.

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RHABDOPHANE FROM THE CHAMPION PEGMATITE,  
AMELIA COUNTY, VIRGINIA

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Rhabdophane has been identified by x-ray diffraction in a rock specimen from the abandoned Champion pegmatite, Amelia County, Virginia. The mineral, hexagonal  $(\text{RE})\text{PO}_4 \cdot \text{H}_2\text{O}$ , also occurs at Cornwall, England, and Salisbury, Connecticut (Hildebrand *et al.*, 1957). Although rhabdophane is apparently rare, there has been much interest in it recently because of the discovery of several related minerals. Brockite,  $(\text{Ca}, \text{Th})\text{PO}_4 \cdot \text{H}_2\text{O}$ , recently described by Fisher and Meyrowitz (1962) is probably isostructural with rhabdophane. Impure thorium phosphates, probably related to brockite, have been reported by Dooley and Hathaway (1961).