UNIT CELL OF HYDROMAGNESITE

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ABSTRACT

X-ray study of hydromagnesite crystals confirms the monoclinic character of the mineral, but shows that it is pseudo-orthorhombic in structure. Equator, first and second layer line Weissenberg photographs show that the presently accepted a axis should be doubled. Systematic extinctions show the symmetry to be a near match for $D_2^5(C222_1)$, with a few faint spots unaccounted for. *X*-ray powder photographs can be satisfactorily indexed using the formula for an orthorhombic structure. The unit cell dimensions determined by Weissenberg photographs are in reasonably close agreement with previously determined values, if a_0 is taken as twice the earlier value. These measurements are as follows:

$$a_0 = 18.58 \text{ Å}, \qquad b_0 = 9.06 \text{ Å}, \qquad c_0 = 8.42 \text{ Å}.$$

Typical crystals are pseudo-orthorhombic, due to multiple twinning on {100}, and goniometric measurements are consistent with previous determinations.

INTRODUCTION

Previous work on hydromagnesite has shown certain inconsistencies, some writers considering the mineral to be monoclinic, others orthorhombic. An early investigation by J. D. Dana (1) gave a probably monoclinic symmetry with β about 107°. Weinschenk (2) in studying crystals optically, observed multiple twinning and oblique extinction in the sections showing this twinning. He considered the mineral to be monoclinic. Brugnatelli (3) was unable to find any but parallel extinction, and concluded from the morphology and optics that hydromagnesite must be orthorhombic. E. S. Dana (4), p. 304, however, confirmed the monoclinic character of the crystals, but stated that β must be very close to 90°. Goldschmidt (5) in the Winkeltabellen lists it as orthorhombic. Rogers (6) measured some crystal angles under the microscope and calculated others, using minute crystals from Alameda County, California. He observed multiple twinning on {100} with oblique extinction on {010} ($\beta \wedge c = 42° 51'$). From these observations, he concluded that the mineral is definitely monoclinic, owing its orthorhombic aspect to twinning. Assuming Dana's pyramid to be {011}, and taking a small {$h0l$} face as {001}, he calculated β to be 114° 33′ 20″.

Fenoglio (7, 8) made the first *x*-ray study of hydromagnesite, taking powder photographs, Laue photographs, and rotation photographs about c. From these he derived a rectangular lattice, which he called orthorhombic, space group D_{2h}^1. He recognized the presence of oblique extinction in some sections, but attempted to explain it by twinning on {021}, which would produce the proper obliquity. His diagram to demon-

strate this theory is shown in Fig. 1, together with the optical orientation and twinning plan according to Rogers.

Crystallography

Recently the author received specimens of well crystallized hydromagnesite from Crestmore, California, and it seemed desirable, in view of discrepancies among earlier observations, to attempt a more complete *x*-ray and morphological study of the mineral. The available material included small but well developed crystals, and measurements on the

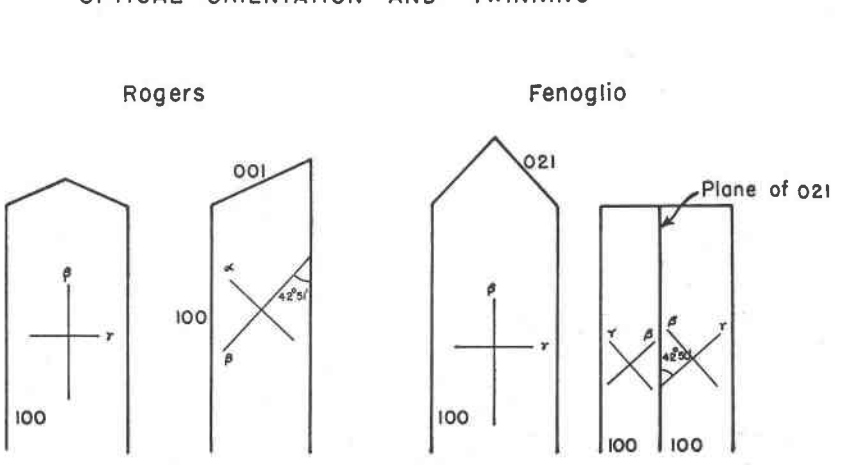

Fig. 1

goniometer gave results which are in reasonable agreement with earlier morphological work. Crystals are of typical lath-like habit, with {100} dominant, {210} usually present, with striations indicating other prisms which were unmeasurable, {111} always present and usually excellent. A few crystals showed {121}, {101} and {201} as well. The following Table 1 shows the angles for these forms as calculated from the *x*-ray pictures, and as measured on the goniometer.

Multiple twinning on {100} as observed by Rogers, is universally present. The twin lamellae are sometimes almost submicroscopic in thickness, so that a true extinction angle is sometimes difficult to measure. However, apparently simple lamellae give an average extinction angle of about 35° on *c* as compared with Rogers' value of 42° 51′. It may be that submicroscopic twinning is responsible for this apparent variation.

TABLE 1

Form	*Calculated*		*Measured* (average)	
	ϕ	ρ	ϕ	ρ
a 100	90°00′	90°00′	90°00′	90°00′
l 210	44°17′	90°00′	44°28′	90°00′
k 101	90°00′	24°23′	88°12′	24°12′ (poor)
d 201	90°00′	42°11′	90°00′	45°12′ (poor)
p 111	26°00′	45°57′	25°43′	45°55′
t 121	13°42′	62°24½′	14°47′	63°30′ (poor)

EQUIVALENT FORMS

Dana	*Rogers*	*Murdoch*
100	100	100
110	110	210
101	001	101
201	101	201
121	011	111
141	021	121
181	041	141

X-RAY STUDY

X-ray powder photographs were taken of selected pure material using copper radiation and nickel filter. The resulting spacings and intensities are shown in the accompanying Table 2, and agree well with Fenoglio's, although showing many more lines than he reported.

"Single" crystal photographs were then taken with the Weissenberg camera, also using copper radiation and nickel filter. These consisted of rotation photographs about [001] of three crystals (for one of these about [010] as well), and equator, first and second layer line pictures, also about [001] and [010]. From these, the translations on *a*, *b* and *c* were measured and calculated from the rotation photographs, and values for a^*, b^* and c^* of the reciprocal lattice averaged from many spacings of the layer line pictures, using direct measurements on the films and graphic determinations on the Schneider constructions of the reciprocal lattice. From these average determinations, the values of a_0, b_0, c_0, and the linear axes, were derived. These values agree reasonably well with Fenoglio's *x*-ray work, and Rogers' morphology. The following Table 3 shows these comparative values.

The pattern in the Schneider constructions from the layer line pictures is orthorhombic, at least within the limits of observation, showing bi-

TABLE 2. HYDROMAGNESITE

X-ray powder photograph data, using Cu radiation, Ni filter

$\frac{d}{n}$	I	hkl	$\frac{d}{n}$	I	hkl
9.18 Å	4	200	1.84 Å	½	830
6.44	4	210	1.82	½	10.1.0
5.79	10	111	1.756	½	624
4.58	½	400	1.74	1	604
4.47	2	020	1.67	½	10.1.2
4.21	2	002	1.65	½	115
4.05	½	220	1.62	3	840
3.81	1	012	1.58	½	10.3.0
3.50	1	212	1.564	1	044
3.31	3	321	1.53	½	505
3.21	½	420	1.50	½	060
3.15	½	511	1.477	½	824, 761
3.09	½	600, 022 (?)	1.448	½	525
2.90	9	222, 610	1.420	½	062
2.84	½	230	1.407	½	006, 715
2.78	½	131 (?) 003 (?)	1.396	½	13.1.1
2.69	3	521	1.385	½	016
2.63	½	113	1.367	½	216
2.50	3	430 (?) 602, 313 (?)	1.330	½	416
2.42	½	612, 711 (?)	1.278	½	606
2.35	½	123	1.257	½	616
2.30	3	800	1.237	½	470
2.20	1	240	1.205	½	117
2.15	5	630	1.176	½	317
2.09	½	004	1.159	½	16.1.0
2.03	½	802, 440	1.113	½	280
1.99	2	042, 812	1.051	½	008
1.966	½	333 (?)	1.021	½	—
1.93	1	242, 632	0.9060	½	—
1.90	½	024, 404	0.8975	½	—
1.86	½	224, 10.0.0			

lateral symmetry, both of distribution and intensities, in all three axial planes. However, distribution of points in the first layer line picture shows that the value of a^* in the reciprocal lattice must be halved, as compared with the value from the equator picture. Furthermore, there are systematic extinctions, which throw the symmetry very nearly into space group D_2^5 ($C222_1$), as contrasted with Fenoglio's determination of D_{2h}^1. The presence of occasional faint spots $\{0k0\}$, $\{h0l\}$, $\{00l\}$, with h, k, and l odd, interfere with perfect matching of the pattern with this space group, and

TABLE 3. CELL DIMENSIONS FROM *X*-RAY MEASUREMENTS

	a	*b*	*c*	
Fenoglio	9.32 Å	8.98 Å	8.42 Å	(orthorhombic)
Murdoch	18.58 Å =9.29×2	9.06 Å	8.42 Å	90°

Axial Elements

	a	*b*	*c*	
Rogers (morphological)	1.1374	1	0.9034	114°0′8″
Fenoglio (*x*-ray)	1.0378	1	0.9376	[90°]
Murdoch (*x*-ray)	2.0508 =1.0254×2	1	0.9293	90°

may well be due to the truly monoclinic structure of the mineral. There are in addition faint superstructure spots which the author has not attempted to interpret.

In view of the apparent monoclinic symmetry of hydromagnesite, as shown by its optical behavior, it is desirable to attempt an explanation of the distinctly orthorhombic aspect of the lattice. The possibility that the mineral might be truly orthorhombic, as suggested by Fenoglio, was first considered. In this case, twinning on a macrodome is required, to produce the observed oblique extinction on {010}. However, it was found by trial that no orthorhombic lattice, tilted to the appropriate angle, could be found which would produce coincidence of points to form a rectangular pattern of the twinned lattices. Accordingly, this possibility may be ruled out.

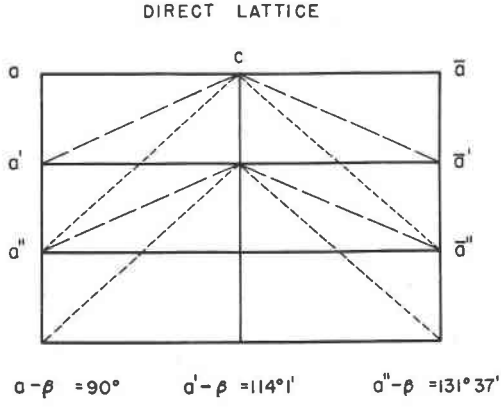

FIG. 2

The other possibility is that the mineral is truly monoclinic, with any value for β which would produce exact, or nearly exact, coincidence of patterns when twinned on {100}. There are of course a number of such values, and three of the more likely are shown in the following Fig. 2. Here a and c are drawn in the proportions of the observed direct lattice, and possible values for β are 90°, 114° 1′ and 131° 37′. Other angles are conceivable, but less and less probable because of the increasing obliquity of the resulting cell. Rogers on morphological grounds selected 114°+, but 90° is equally possible, and in the author's opinion should be chosen, as the simplest way of accounting for both morphological and x-ray characteristics of the mineral.

The writer wishes to acknowledge the assistance of his colleague, Professor George Tunell, in making available x-ray facilities, and in giving valuable counsel in the preparation of this paper. A spectroscopic analysis to determine purity of the material was made possible by research funds from the University of California.

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Manuscript received Sept. 15, 1952