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THE COMPOSITION AND SPACE GROUP OF LEGRANDITE

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ABSTRACT

Legrandite from the Ojuela Mine, Mapimi, Mexico has the cell dimensions, $a=12.70$, $b=7.87$, $c=10.23$ Å, $\beta=104°24'$. The space group is $P2_1/c$. A new analysis indicates the formula is $4ZnO\cdot As_2O_5\cdot 3H_2O$. $Z=3.88$. The calculated density is 4.08, the measured density 3.98.

The mineral legrandite was described by Drugman and Hey (1932). On the basis of their chemical analysis the composition $Zn_{14}(AsO_4)_9(OH)\cdot 12H_2O$ was given. A density of 4.01 was measured, and the unit cell dimensions were determined. According to their chemical analysis, a composition of $Zn_3(AsO_4)_2\cdot 3H_2O$ could be assigned, but this formula was discarded as a possibility because, for this composition $Z=4.5$. The formula $Zn_{14}(AsO_4)_9(OH)\cdot 12H_2O$ is essentially $Zn_3(AsO_4)_2\cdot 3H_2O$ multiplied by 4.5. Legrandite is monoclinic but no information as to the point or space group was given in the original paper.

The specimen of legrandite used in this investigation is from the Ojuela Mine, Mapimi, Mexico. The unit cell dimensions have been determined from (*h*0*l*) and (*hk*0) Weissenberg photographs and the values $a=12.70$, $b=7.87$, $c=10.23$ Å, $\beta=104°24'$ confirm the values of Drugman and Hey.

TABLE 1. CHEMICAL ANALYSES OF LEGRANDITE

	1	2	3	4
ZnO	53.42	51.02	52.10	46.70
As_2O_5	37.71	37.73	38.53	42.02
H_2O	8.87	9.18	9.37	9.36
Fe_2O_3		.75		2.14
MnO		.21		.05
Al[1]		.20		
Ca[1]		.05		
Cd[1]		.20		
Mg[1]		.50		
Si[1]		.20		
Total	100.00	99.94	100.00	100.27

All analyses given in weight per cent.

1. $Zn_2(AsO_4)(OH)\cdot H_2O$. 2. Present analysis (Ochs). 3. Recalculation of major constituents to 100%. 4. Drugman and Hey (1932).

[1] Elements determined by emission spectrograph.

TABLE 2. *X*-RAY POWDER DATA FOR LEGRANDITE, $Zn_2(AsO_4)(OH)\cdot H_2O$ AND ADAMITE, $Zn_2(AsO_4)(OH)$

Legrandite		Adamite	
d	I	d	I
12.33 Å	wm		
6.70	m		
5.90	s	5.92 Å	s
5.04	w		
4.88	w	4.90	s
4.19	s	4.24	m
4.05	vs		
3.77	wm	3.78	m
3.63	m		
3.43	w		
3.29	w		
3.09	vs		
3.02	s	3.04	w
2.96	ms	2.97	vs
2.86	w		
2.77	m		
2.67	wm	2.70	ms
2.61	ms	2.64	wm
		2.58	wm
2.51	m	2.52	wm
2.47	vw	2.45	vs
2.43	w	2.42	m
2.36	wm	2.36	m
2.31	vw		
2.22	wm		
2.18	wm		
2.09	vvw	2.07	vw
2.05	vvw		
2.01	vw	2.02	vvw
1.97	vvw	1.96	wm
		1.91	w
1.87	wm	1.89	vw
1.83	vvw	1.85	vvw
1.80	w		
1.76	vw		
1.73	vvw	1.74	vvw
1.72	vvw	1.71	wm
1.69	vw		
1.65	wm	1.66	wm
		1.62	vw
1.61	vvw	1.61	m

vs = very strong; s = strong; ms = moderate-strong; m = moderate; wm = weak-moderate; w = weak; vw = very weak; vvw = very very weak.

The following conditions for reflection were observed:

hkl: None
$h0l$: $l = 2n$
$0k0$: $k = 2n$

These restrictions uniquely determine the space group as $P2_1/c$. On the basis of one formula weight of the composition $Zn_{14}(AsO_4)_9(OH)\cdot 12H_2O$ per unit cell (Drugman and Hey, 1932), a fundamental difficulty arises. It is impossible to place nine arsenate tetrahedra in the unit cell. That is, there are no unique positions in the space group $P2_1/c$, *i.e.* nor in any other centric monoclinic space group except $P2/m$ (for which there are no systematic absences). Furthermore, the noncentric arsenate tetrahedron cannot be placed at a center of symmetry.

The density was redetermined with a Berman balance as 3.98 which confirms the value, 4.01, determined by Drugman and Hey. Because the unit cell dimensions also agree, the discrepancy must be the chemical analysis.

A complete chemical analysis was undertaken by Mr. H. Ochs of Denver, Colorado on 190 mg of pure legrandite from Mina Ojuela, Mapimi, Mexico. The results are listed in Table 1, together with the chemical analysis of Drugman and Hey (1932).

On the basis of the new analysis, the formula can be written:

$$4ZnO\cdot As_2O_5\cdot 3H_2O$$

For this formula $Z=3.88$. The cell formula is $Zn_{16}(AsO_4)_8(OH)_8\cdot 8H_2O$ and the cell volume is 990 Å^3. The calculated density of 4.08 compares well with the 3.98 that was measured.

The powder patterns of legrandite and adamite show some similarities and it is possible that there are gross features of the structures that are similar notwithstanding the different unit cell dimensions and symmetries. Table 2 lists the d-values to 1.60 Å for legrandite and adamite. A determination of the structure of legrandite is being undertaken to ascertain the degree of similarity to adamite.

The author wishes to thank Mr. H. Ochs for the chemical analysis.

Reference

Drugman, J. and M. H. Hey (1932) Legrandite, a new zinc arsenate. *Mineral. Mag.* **32**, 175–178.

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