AN *X*-RAY STUDY OF THE MINERAL LIVINGSTONITE

D. H. GORMAN,* *University of Toronto, Toronto, Canada*

ABSTRACT

Livingstonite from Guerrero, Mexico is triclinic, with probable space group $P\bar{1}$. The unit cell with $a=7.65$, $b=10.82$, $c=3.99$ kX, $\alpha=99°12\frac{1}{2}'$, $\beta=102°01'$, $\gamma=73°48'$, contains $HgSb_4S_7$. Specific gravity 4.88 calculated, 5.00 measured. Cleavage (010), (100) perfect, (001) poor. The monoclinic cell of Richmond (1936) has four times the volume, with $a'=2a$, $b'=c$, $c'=2b$, $\beta=104°$.

A modern presentation of the crystallography of livingstonite—$HgSb_4S_7$—was published in the *American Mineralogist* (Richmond, 1936). Data from this paper were used in the description of livingstonite in Dana's *System of Mineralogy*, Volume 1 (1944), where it is described as monoclinic $2/m$, with unit cell dimensions a 15.14 A, b 3.98 A, c 21.60 A, β 104° and a Z factor of 4.

Some time ago Professor Peacock of the University of Toronto discovered from a study of *x*-ray Weissenberg photographs that livingstonite possesses triclinic symmetry. Later, S. Kaiman, one of Professor Peacock's graduate students, proved conclusively, in an unpublished work, that the mineral is triclinic. In the fall of 1949 the professor suggested that I make a formal *x*-ray study of this mineral, which would serve as a research problem, and fulfil partially the requirements of his *x*-ray crystallography course.

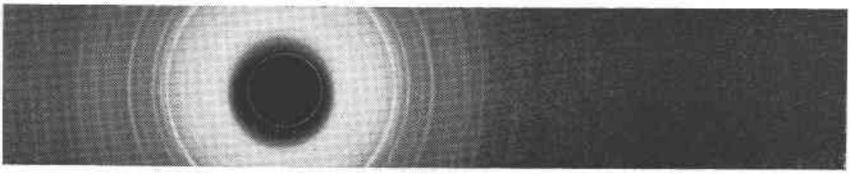

FIG. 1. *X*-ray powder photograph; nickel filtered copper radiation ($\lambda=1.5374$ kX) Camera radius 57.3 mm; actual size print.

A few grams of livingstonite from Guerrero, Mexico, were obtained from Mr. Frank Ebbutt, Geologist, of Toronto. No individual crystals of the material were observed, but several fine cleavage fragments were isolated. A few of these were powdered, and an *x*-ray powder photograph made. Figure 1 is a contact print of this photograph, taken with a Philips type camera of 57.3 mm radius, using nickel filtered copper radiation.

The spacings represented by the three most intense lines were measured, and when compared with Harcourt's values (1942), as shown in Table 1, served to identify my material with Harcourt's. The remaining spacings were measured and are recorded in Table 2.

---

* Holding a National Research Council of Canada studentship.

TABLE 1. COMPARISON OF HARCOURT AND GORMAN SPACING VALUES FOR LIVINGSTONITE

Intensity	*d* Harcourt (1942)	*d* Gorman
2	3.75 kX*	3.73 kX
3	3.45	3.47
1	2.99	2.99

* Called Angstrom units in Harcourt (1942), probably kX.

TABLE 2. LIVINGSTONITE *X*-RAY POWDER DATA IN kX UNITS; Cu/Ni radiation
Triclinic; $P\bar{1}$; *a* 7.65, *b* 10.82, *c* 3.99; α 99°12′; β 102°01′; γ 73°48′

I (Cu)	*d* (meas.)	(*hkl*)	*d* (calc.)	*I* (Cu)	*d* (meas.)	(*hkl*)	*d* (calc.)	*I* (Cu)	*d* (meas.)	(*hkl*)	*d* (calc.)
4	5.14	020	5.16	½	2.49	310	2.49	3	1.875	321	1.880
1	4.86	120	4.82	3	2.42	320	2.44			$2\bar{4}0$	1.879
7	3.73	210	3.72			211	2.44			012	1.870
7	3.47	130	3.47			240	2.41	3	1.840	$\bar{4}21$	1.841
1	3.27	$0\bar{2}1$	3.28			300	2.41	5	1.729	$\bar{1}22$	1.733
10	2.99	021	2.95	6	2.27	$0\bar{4}1$	2.27	½	1.643	—	—
		$\bar{2}\bar{1}1$	3.03			330	2.27	2	1.501	—	—
		$1\bar{1}1$	3.03	2	2.03	340	2.04	1	1.423	—	—
1	2.86	$1\bar{3}0$	2.84			141	2.03	½	1.193	—	—
3	2.66	140	2.66	2	1.984	$1\bar{4}1$	1.976	½	1.097	—	—
		$2\bar{2}0$	2.66								

A cleavage fragment ½ mm in length was isolated, and mounted on an *x*-ray goniometer so that the cleavage edge between two good cleavage faces was parallel to the axis of rotation of the goniometer head. Rotation, zero layer and first layer Weissenberg photographs were then taken.

The cleavage edge was arbitrarily chosen as the direction of the *c* axis, hence the rotation photograph gave *c*. The zero layer Weissenberg gave *d*(100) and *d*(010), and γ^*. The first layer Weissenberg gave the horizontal offset of the reciprocal lattice, measured by the rectangular co-ordinates *x* and *y*, which are functions of α^* and β^*. The lengths *x* and *y* were measured in millimeters. From these six measurements the reciprocal lattice elements were calculated. Standard formulae were then used to convert these reciprocal lattice values to those of the direct lattice.

Thus from one setting of the cleavage fragment, the direct lattice elements were obtained. The elements *a*, *b*, α and β are dependent on the measurement of *x* and *y* and are less accurate than *c* and γ which are independent of graphical measurement. In Table 3 the lattice constants used in the calculations are given. Table 2 shows the lattice constants modified to conform with the accuracy of measurements.

TABLE 3. LIVINGSTONE LATTICE CONSTANTS USED IN CALCULATION

Measured		Reciprocal Lattice		Direct Lattice	
c	3.990 kX	a*	0.13819	a	7.650 kX
$d(100)$	7.236 kX	b*	0.09685	b	10.817 kX
$d(010)$	10.326 kX	c*	0.25776	c	3.990 kX
γ^*	104°44½′	α^*	83°46′	α	99°12½′
x	8.2 mm.	β^*	80°04′	β	102°01′
y	4.3 mm.	γ^*	104°44½′	γ	73°48′

The unit cell was chosen with a less than b and α and β both obtuse. This is the modern setting for triclinic crystals, which restricts the slope of the base (001) to the front and the right of the front pinacoid. Fortuitously c is less than a or b.

The cell constants having been found, the next task included calculating the spacings of the planes whose spacings had been obtained from the powder photograph. This involved the use of the "Bravais Sphere," and a graphical method of determining the spacings of lattice planes as proposed by Peacock (1938). The measured spacings were used to find, on a gnomonic projection, planes with indices that might possibly be responsible for such spacings. Then these indices were used in a formula involving the lattice constants to calculate spacings. When the calculated spacings agreed with the observed spacings within 2/10 of θ angle, then the plane used in the calculation was recorded as a plane responsible for a diffraction line on the powder photograph. Table 2 gives the complete x-ray data for livingstonite, with observed intensities for copper radiation based on a 10-1 scale, and measured and calculated planar spacings with their corresponding indices.

A comparison of Richmond's cell to the present author's is given in Table 4.

TABLE 4. COMPARISON OF RICHMOND AND GORMAN CELLS FOR LIVINGSTONITE

Richmond		Gorman			
a	15.14 kX*	a	7.65 kX	α	99°12′
b	3.98	b	10.82	β	102°01′
c	21.60	c	3.99	γ	73°48′
β	104°				

* Given by Richmond as A; probably kX.

From Table 4 it may be seen that two of the linear elements of Richmond are halved by the present author, and that *b* and *c* are interchanged. Otherwise, the similarity of the cells is apparent. From his unit cell dimensions, Richmond has calculated that the *Z* factor must be 4, which means that the cell contents are 4 [$HgSb_4S_7$]. Since the new cell volume is approximately $\frac{1}{4}$ that of Richmond's, one would expect the structural formula to be 1 [$HgSb_4S_7$].

The new elements give a cell volume of 308.27kX^3. The calculated density using this value and the structural formula 1 [$HgSb_4S_7$] is 4.88 grams per cubic centimeter, which is in fair agreement with 5.00 as measured on the Berman balance. Richmond's calculated value was 4.79 as against 5.00 measured by Frondel (Dana, 1944). The agreement is sufficiently close to warrant the acceptance of the structural formula 1 [$HgSb_4S_7$].

The change in the orientation of the cell, apart from the modification of monoclinic to triclinic, necessitates a renaming of the cleavage directions. Nevertheless, there is little change in the calculated angle between the two best cleavages, recorded by Richmond as 104° and here as 104°21′. Table 5 shows the comparison between cleavages in the old and new setting.

TABLE 5. CLEAVAGES OF LIVINGSTONITE

Richmond		Gorman	
(001)	perfect	(010)	perfect
(100)	perfect	(100)	perfect
(010)	poor	(001)	poor

The space group $P\bar{1}$ was chosen in preference to $P1$, merely because the former is common, the latter rare.

I would like to express my appreciation to the National Research Council of Canada for their financial aid, and for their permission to publish this paper. I would like also to record my thanks to Dr. E. W. Nuffield of the University of Toronto for his critical reading of the manuscript.

REFERENCES

DANA, J. D. & E. S. (1944): *System of Mineralogy* **1,** by C. Palache, H. Berman & C. Frondel, New York.

HARCOURT, G. A. (1942): Tables for the identification of ore minerals by *x*-ray powder patterns, *Am. Mineral.*, **27,** 63.

PEACOCK, M. A. (1938): A general graphical method for determining the spacings of lattice planes, *Zeits. Krist.*, (A), **100,** 93–103.

RICHMOND, W. E. (1936): Crystallography of livingstonite, *Am. Mineral.*, **21,** 719.