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THE CRYSTAL STRUCTURE OF PLATARSITE, Pt(As, S)$_2$, AND A COMPARISON WITH SPERRYLITE, PtAs$_2$

J. T. SZYMAŃSKI
Mineral Sciences Laboratories, CANMET, Department of Energy, Mines and Resources, 555 Booth Street, Ottawa, Ontario K1A 0G1

ABSTRACT

The crystal structure of platarsite, Pt(As,S)$_2$ (Cabri *et al.* 1977), has been determined, and that of sperrylite re-examined, to determine the crystallographic differences between the two minerals. They both crystallize in *Pa*3: platarsite with $a = 5.788(1)$Å, sperrylite PtAs$_2$ with $a = 5.9681(1)$ Å (precision value: least-squares refinement and extrapolation function). Both minerals have a pyrite-type structure. Platarsite shows no evidence of ordering of As and S atoms in position 8*c*. The parameter of (As,S) in platarsite, $x = 0.38580(8)$, gives bond lengths metal–(As,S) = 2.4208(3)Å and (As,S)–(As,S) = 2.2898(4)Å. Corresponding values in sperrylite are $x = 0.38345(4)$, Pt–As = 2.4909(1)Å, As–As = 2.4097(2)Å. The angular geometries in the two structures are nearly identical.

SOMMAIRE

La structure cristalline de la platarsite Pt(As,S)$_2$ a été affinée, et celle de la sperrylite ré-examinée, afin de déterminer leurs différences cristallographiques. Toutes deux cristallisent en *Pa*3: la platarsitee avec *a* 5.788(1)Å, la sperrylite avec *a* 5.9681(1)Å (mesure de précision: affinement par moindres carrés, avec fonction d'extrapolation). Les deux minéraux possèdent une structure du type pyrite. Nulle mise en ordre des atomes As et S en position 8*c* n'a été décelée dans la platarsite. Dans cette structure, le paramètre de (As,S), $x = 0.38580(8)$, donne les longueurs de liaison métal–(As,S) = 2.4208(3)Å, (As,S)–(As,S) = 2.2898(4)Å. Dans la sperrylite, les valeurs correspondantes sont $x = 0.38345(4)$, Pt–As = 2.4909(1)Å, As–As = 2.4097(2)Å. Les relations angulaires dans chacune des deux structures sont presque identiques.

(Traduit par la Rédaction)

INTRODUCTION

The mineral platarsite Pt(As,S)$_2$ was first described by Cabri *et al.* (1977), who discussed the crystallochemistry of the Pt–As–S system and gave full details of the analyses of platarsite grains examined. The composition of the specimen examined crystallographically and reported here is $(Pt_{0.34}Rh_{0.30}Ru_{0.28}Ir_{0.05}Os_{0.01})_{0.98}As_{1.03}S_{0.99}$ (Cabri *et al.* 1977, Table 1, anal. 1).

The space group of platarsite was unequivocally determined as *Pa*3, which requires that As and S be statistically distributed in one position in the structure. Thus, although the analyses show As≃S in all specimens examined, the mineral may be considered crystallographically as a disulfide or a diarsenide, ideally Pt(As,S)$_2$. If the mineral is to be considered a diarsenide, then the question arises: in what manner does it differ from sperrylite PtAs$_2$, which has the same space group? Cabri *et al.* (1977) have discussed the possibility of a miscibility gap in the system Pt–As–S.

From an examination of X-ray rotation photographs, Aminoff & Parsons (1928) determined that sperrylite has the pyrite structure. The single As positional parameter *x* and the cell edge *a* have been redetermined by a number of authors, most recently by Furuseth *et al.* (1965), though not with least-squares refinement. In an attempt to resolve the problem of the relationship of platarsite and sperrylite, the structure of platarsite was examined, and that of sperrylite was re-examined to provide an accurate comparison.

EXPERIMENTAL

Platarsite

An irregular tabular fragment of platarsite, approximately 0.08 x 0.05 x 0.025 mm, was extracted from a polished section after microprobe analysis, and mounted on a precession camera for preliminary photographic examination.

Much more attention than is usual in such simple structures was paid to the unique determination of the space group. Extensive investigation of the reciprocal lattice using Zr-filtered Mo*Kα* radiation with photographs of up to 220 hours failed to reveal any spots not conforming to the required systematic absences for space group *Pa*3. Nevertheless, when the crystal was mounted on a four-circle X-ray diffractometer in a general orientation, a detailed examination was carried out for any reflections not permitted by this space group.

Recently, Bayliss (1977) has refined the structure of anisotropic pyrite in the triclinic system, based on the occurrence of weak axial reflections with odd indices and of other reflections not permitted in space group $Pa3$. In the preliminary diffractometer examination of the crystal of platarsite, the six {100} and the twelve {110} reflections were all observed. These are not genuine reflections, because changing the voltage and current settings applied to the molybdenum X-ray tube from 50 kV, 16 mA to 35 kV, 20 mA totally eliminated them. To confirm this conclusion, a crystal of graphite was mounted on our diffractometer; the 001 reflection (which is systematically absent) was detected when the instrument was run at 50 kV, but it totally disappeared when the voltage was decreased to 35 kV. Bearing in mind that the excitation voltage for a wavelength equal to half that of Mo$K\alpha$ is about 35 kV, and that the diffraction geometry is exactly right for this forbidden reflection if it is a $\lambda/2$ satellite of an intense second-order reflection (*i.e.*, the $\lambda/2$ incident radiation will pass through the monochromator as the graphite 004 reflection rather than the 002, and will be diffracted to the 2θ position of the graphite 001 reflection for λ), the only possible explanation for this forbidden reflection could be a faulty pulse-height analyzer and discriminator circuit. The problem was indeed found here and repaired; when the discriminator levels were subsequently adjusted, all traces of the graphite 001 reflection and of the platarsite {100} and {110} were eliminated. This somewhat lengthy explanation is included to indicate that before any lowering of symmetry from a high-symmetry space group is claimed, both possible Renninger effects and the electronics of the instrument should be carefully examined.

Despite all indications that $Pa3$ was the correct space group, complete segments of data were collected without regard to systematic absences and chosen to be equivalent in the lower-symmetry space-group $P2_13$. Six equivalent segments were collected using graphite-monochromatized Mo$K\alpha$ radiation to $2\theta = 110°$, these segments being the hkl, $h\bar{k}\bar{l}$, $\bar{h}k\bar{l}$, $\bar{h}\bar{k}l$, klh and $k\bar{l}\bar{h}$ (for $|h|, |k| \geqslant |l|$). A θ–2θ scan was used at a 2θ rate of 2°/min, with the scan width adjusted for dispersion (2.0–3.0°). Background counts were made for 30 seconds on either side of the peak. Three linearly-independent standard reflections were recorded every 50 measurements to monitor crystal alignment and instrument stability. Absorption corrections were applied using a Gaussian integration procedure (Gabe & O'Byrne 1970). The data were averaged to provide 417 unique reflections permitted in space group $Pa3$, of which 274 can be considered observed on the criterion that $I_{obs} > 1.65 \times \sigma(I)$, together with additional 68 reflections that would be permitted in space group $P2_13$. Of this last group, none were observed on the criterion that $I_{obs} > \sigma(I)$. The overall disagreement factor between the absorption corrected segments ($\Sigma|I-\bar{I}|/\Sigma I$) was rather high (8.4%). This reflects the problems of calculating accurate absorption corrections where (1) the uncorrected intensity of equivalent reflections varies by a factor of two, and (2) the crystal shape is difficult to describe in terms of plane faces; the crystal in this case is small, with curved "faces", some of them concave.

The cell dimensions for platarsite were determined by a least-squares refinement of the 2θ, χ, ω values (Busing 1970) of 54 reflections in the range $74° > 2\theta > 52°$. The parameters were refined for a triclinic cell; the variation between a, b and c was 0.0004Å and the variation from orthogonality was 0.006°, both well within the standard deviations. The final value for a is 5.788(1)Å.

Sperrylite

A fragment of sperrylite from Sudbury, Ontario was ground using the Bond method (1951) in an attempt to make a sphere. The result, however, was an ellipsoid 0.19 x 0.14 x 0.13 mm. After preliminary photographic examination which showed it to be a single crystal, the specimen was mounted on a four-circle X-ray diffractometer in a general orientation. The cell dimension was determined from a least-squares fit of the observed 2θ, χ, ω values (Busing 1970). A systematic variation in the apparent cell-edge with 2θ was observed; this was interpreted to be due to severe absorption by the crystal ($\mu r = 9.3$ to 6.2). An extrapolation using the Taylor & Sinclair (1945) function was made, but in this case, single-crystal rather than powder data were plotted (Fig. 1, Table 1). The individual points represent the least-squares value and standard deviation of the apparent cell parameter a obtained from a refinement of the complete form of a given hkl. In all, 286 reflections were used in obtaining the 12 points shown in Figure 1. The intercept of the final weighted least-squares line through the points of Figure 1 gives the cell dimension of sperrylite as $a = 5.9681(1)$Å.

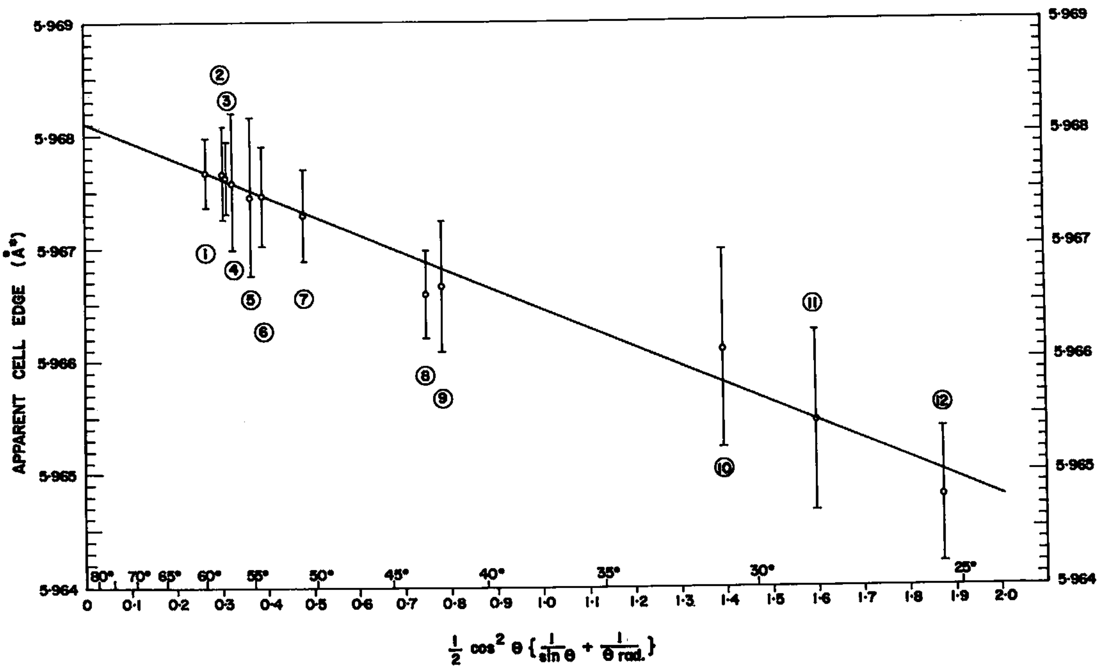

FIG. 1. Extrapolation of the apparent cell edge a of sperrylite using the function of Taylor & Sinclair (1945). Each point was obtained using a least-squares refinement (Busing 1970) of the 2θ, χ, ω values observed for a complete *hkl* form. The apparent cell edge, with its standard deviation, were then fitted by least-squares to give as the intercept $a = 5.9681(1)$Å. See also Table 1.

Five segments of intensity data were collected (hkl, klh, lhk, $h\bar{k}\bar{l}$ and $\bar{h}k\bar{l}$, for $|h|$, $|k| \geqq |l|$), to $2\theta = 120°$. The experimental procedure was the same as for platarsite. The intensities were corrected using the arbitrary crystal absorption correction program (ACACA) of Wuensch & Prewitt (1965) and reduced to a single set of structure factors with the application of Lorentz and polarization corrections. Of the 550 unique reflections measured, 417 were observed on the criterion that $I_{obs} > 1.65 \times \sigma(I)$, where $\sigma(I)$ was derived from counting statistics and the relative agreement of the individual measurements. The disagreement factor for the five segments of intensities is 4.7%; the improvement over the corresponding figure for platarsite reflects the more precise description of the larger and more regular crystal shape.

TABLE 1. SPERRYLITE CELL DIMENSION EXTRAPOLATION

Point no.	Index of form	Multiplicity of form	Apparent $a,\sigma(a)$ (Å*)	$\frac{\cos^2\theta}{2}(\frac{1}{\sin\theta}+\frac{1}{\theta})$
1	14 4 0 12 8 2	24 48	5.96766(32)	0.2652
2	10 10 2	24	5.96766(42)	0.3024
3	13 5 3	48	5.96762(32)	0.3071
4	10 10 0	12	5.96758(62)	0.3216
5	8 8 8	8	5.96745(72)	0.3616
6	9 9 5	24	5.96746(44)	0.3877
7	9 9 3	24	5.96729(41)	0.4771
8	10 4 4	24	5.96659(38)	0.7458
9	8 8 0	12	5.96666(58)	0.7788
10	5 5 5	8	5.96609(89)	1.0991
11	8 0 0	6	5.96545(81)	1.3938
12	6 4 0	24	5.96479(60)	1.8738

The apparent cell edge and its standard deviation, $a,\sigma(a)$(Å*) were obtained from least-squares refinement of all reflections in a given form.

The crystal was removed from the diffractometer for microprobe analysis of the composition. Minor replacement of As by Sb was found, and no elements other than Pt, As and Sb were detected. The results are quoted in Table 2.

STRUCTURE ANALYSIS AND REFINEMENT

Platarsite

As the apparent systematic absences point to $Pa3$, the structure was refined in this space

TABLE 2. CRYSTAL DATA

	Platarsite	Sperrylite
Source:	former Onverwacht mine, Transvaal (Cabri *et al.* 1977)	Frood mine, Sudbury, Ontario
Composition: (microprobe analysis)	$(Pt_{0.34}Rh_{0.30}Ru_{0.28}Ir_{0.05}Os_{0.01})_{0.98}As_{1.03}S_{0.99}$	$Pt_{1.00}(As_{1.99}Sb_{0.01})_{2.00}$
Cell dimension:	a = 5.788(1)Å	a = 5.9681(1)Å at 25°C
Systematic absences:	$0kl$, k=2n+1, $h0l$, l=2n+1, $hk0$, h=2n+1	as for platarsite
Space group:	$Pa3$ (#205)	$Pa3$ (#205)
Absorption:	$\mu(MoK\alpha)$ = 173.0 cm^{-1}	$\mu(MoK\alpha)$ = 970.2 cm^{-1}
Calculated density:	8.437 g.cm^{-3}	10.806 g.cm^{-3}
Intensity data:	6 segments to 2θ = 110° 417 unique reflections 273 with $I>1.65*\sigma(I)$	5 segments to 2θ = 120° 550 unique reflections 417 with $I>1.65*\sigma(I)$

group. This symmetry requires that As and S be disordered and statistically distributed in the $8c$ positions. Composite scattering curves were prepared for the metal and for (As,S) according to the stoichiometric composition found by microprobe analysis. The scattering curves were adjusted for both the real and imaginary parts of the anomalous dispersion using a weighted arithmetic mean of the components of the individual atoms. Anisotropic temperature factors and an extinction parameter g (Larson 1970) were used in the latter stages of refinement. The refinement converged to a final R value of 0.058 for all 417 data and 0.032 for the 274 observed reflections.

Finally, the 68 reflections that would be permitted in space group $P2_13$ were included at their actual observed values, and an attempt was made to refine the structure with As and S in distinct positions. The attempted refinement of both enantiomorphs was totally unsuccessful. The isotropic temperature factor for S remained strongly negative, and the agreement factor did not drop below $R = 0.100$.

At the suggestion of one of the referees of this paper, a refinement of a partly ordered structure was attempted in space group $P2_13$, using the 485 data permitted in this space group. The starting premise was to vary the site occupancy α of an average (As,S) atom at coordinates x_1, x_1, x_1, and to restrict the site occupancy of the second (As,S) atom at $-x_2$, $-x_2$, $-x_2$, (where $x_1 \simeq x_2$) to $2-\alpha$. From an arbitrary starting value of 1.2, α decreased rapidly, though the refinement was very ill-conditioned. In the final cycles, α oscillated between 1.03 and 0.99, with a standard deviation of 0.02. The final disagreement factor for all 485 data considered as observed was 0.060, an increase over the value of 0.058 obtained in space group $Pa3$ with 417 data. The only possible conclusion that can be drawn is that the space group is truly $Pa3$ and consequently, that there is a random distribution of As and S in the $8c$ positions. The final parameters are quoted in Table 3.

Sperrylite

The refinement of the structure of sperrylite proceeded from the value of the x coordinate published by Furuseth *et al.* (1965). The As scattering curve was adjusted for the minor replacement by Sb. The calculations were made using the X-RAY system of programs (Stewart *et al.* 1972). The scattering curves were taken from Cromer & Mann (1968) for the neutral atomic species, and the anomalous dispersion corrections from Cromer & Liberman (1970). In the least-squares refinement, the need for inclusion of an extinction parameter g (Larson 1970) soon became evident; with this, and with anisotropic temperature factors, the refinement converged to $R = 0.039$ for all data and 0.026 for the observed data only. The observed (10 x F_o) and calculated (10 x F_c) structure factors for platarsite and sperrylite are given

TABLE 3. STRUCTURAL PARAMETERS

	Platarsite	Sperrylite
Metal in position $4a$ (0,0,0)	(Pt,Rh,Ru,Os,Ir)	Pt
Metal thermal parameters (Å^2):	U_{11}=0.00389(10) U_{12}=-.00008(6)	U_{11}=0.00213(5) U_{12}=0.00005(2)
Position $8c$ (x,x,x)	(As,S) x=0.38580(8) U_{11}=0.00575(14)Å^2 U_{12}=0.00001(15)Å^2	As x=0.38345(4) U_{11}=0.00307(7)Å^2 U_{12}=0.00022(6)Å^2
Extinction (g):	2.81(6) x 10^{-5}	1.74(2) x 10^{-4}
Bond lengths, (Å):	Metal-(As,S) 2.4208(3) (As,S)-(As,S) 2.2898(4)	Pt-As 2.4909(1) As-As 2.4097(2)
Non-bonded distances, (Å):	(As,S)...(As,S) 3.5844(6), 3.2934(6)	As...As 3.6575(3) 3.3825(3)

in Tables 4a and 4b, available at a nominal charge from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2.

DISCUSSION

The possible analogy of platarsite and sperrylite with ordered and disordered cobaltite (Giese & Kerr 1965) was kindly pointed out to the author by one of the referees. Disordered cobaltite, obtained by heating cobaltite to 800–850°C for two days and then quenching, has the pyrite structure, space group *Pa*3, with As and S disordered in exactly the same way as found here in platarsite. Ordered cobaltite is orthorhombic, space group $Pca2_1$, with As and S occupying distinct and identifiable positions. In reflected light, ordered cobaltite is anisotropic.

In platarsite, there is no evidence to suggest a symmetry lower than cubic. Platarsite is isotropic under reflected light (Cabri *et al.* 1977), although this may not be a critical test. Ordered cobaltite has a powder pattern that includes weaker reflections not permitted in space groups *Pa*3 or even $P2_13$. No such reflections are observed in the platarsite pattern (Cabri *et al.* 1977). Again, it could be argued that such reflections could be weak and lost in a powder pattern, but the very long precession photographs taken failed to reveal any such reflections. Furthermore, the single-crystal diffractometer data did not show any such reflections to be present using the criterion $I_{obs} > \sigma(I)$. The systematic absences for space group $Pca2_1$ ($0kl$, $l=2n+1$; $h0l$, $h=2n+1$; $hk0$, no conditions) differentiate one projection from the other two. Even with the carefully collected single-crystal diffractometer data, there is no evidence to suggest that in platarsite, one projection is different from the other two; in fact, all three projections show the same absences, both systematic and non-systematic. In the absence of evidence to the contrary, it must be accepted that platarsite is cubic and that *Pa*3 is the correct space group.

Figure 2 illustrates the structure and the atomic coordination of platarsite and sperrylite. The structure refinements described in this paper result in the precise determinations of the following bond lengths: metal–(As,S) 2.4208(3)Å, (As,S)-(As,S) 2.2898(4)Å in platarsite; Pt-As 2.4909(1)Å, As–As 2.4097 (2)Å in sperrylite. The latter values compare with 2.490(4) and 2.41_8(0.04)Å given by Furuseth *et al.* (1965). The platarsite bond-lengths are significantly shorter than those of sperrylite, but this is not unexpected in view of the smaller atomic radius of the composite (Pt,Ru,Rh,Os,Ir) atom with respect to Pt, and with the smaller atomic radius of the composite (As,S) atom with respect to As.

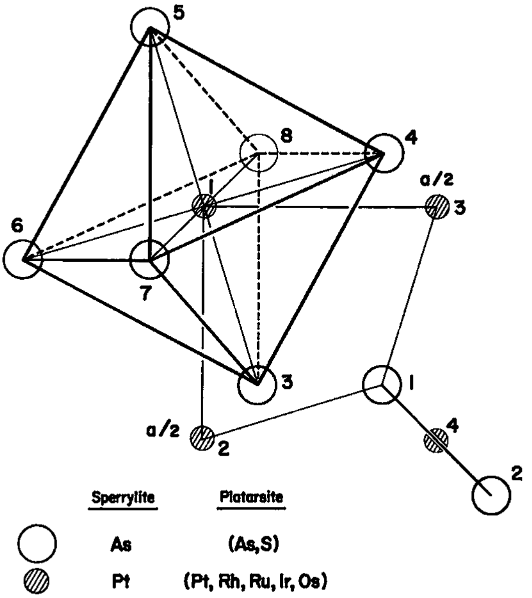

FIG. 2. Diagrammatic view of the platarsite and sperrylite structures, showing distorted octahedral coordination around the metal and distorted tetrahedral coordination around (As,S) in platarsite, As in sperrylite.

However, the angular geometry in the two species is remarkably similar. Within the As_2Pt_6 unit in sperrylite, the As–As–Pt and the Pt–As–Pt angles are 102.002(7)° and 115.794(6)°. The corresponding angles in platarsite are 102.55(1)° and 115.42(1)°. The distorted octahedron of As atoms around Pt in sperrylite has a As–Pt–As angle of 94.473(6)° between As atoms related by the 3-fold axis along [111] (labeled 3,4,7 and 5,6,8 in Fig. 2), and the supplement of this angle between the As atoms not related by the 3-fold axis and Pt (3–6, 3–8, 4–5, 4–8, 5–7, 6–7 in Fig. 2). The corresponding angle in platarsite is 94.28(1)°. The non-bonded As–As distances within this octahedron are larger in sperrylite (3.6575(3), 3.3825(3)Å) than the corresponding distances in platarsite (3.5488(6), 3.2934(6)Å), but this is a function of the longer Pt–As distances in sperrylite; the angular geometry, as previously discussed, is nearly identical.

The precise determination of these two structures leads to the conclusion that the minerals are isostructural to a remarkable degree. It is evident, from the present work, that platarsite should be formulated as $Pt(As,S)_2$ rather than as PtAsS. The reasons for the proposed miscibility gap (Cabri *et al.* 1977) in the Pt–As–S system between the platarsite and sperrylite phases are certainly not crystallographic. More mineralogical and chemical studies are necessary before this system is fully understood.

POWDER PATTERN OF SPERRYLITE

In the course of the structural redetermination of sperrylite, a Debye-Scherrer powder pattern was obtained using Ni-filtered Cu$K\alpha$ radiation. In addition, the powder-pattern-generating program POWGEN (Hall & Szymański 1975) was run using the parameters from the presently refined structure. Excellent agreement was found between the observed and calculated intensities, and with the published powder-pattern (PDF 9-452; Berry & Thompson 1962). The only serious disagreement with the latter pattern occurs at $d = 0.777$ (731,553, $I = 90/100$), which appears to have been severely underestimated. POWGEN calculates and a visual examination confirms that the α_1 component of this line is about 1.55 times stronger than Thompson's reference intensity of 100. As this line appears in the high back-reflection region for Cu$K\alpha_1$ ($2\theta = 164.9°$), the broad shape can easily result in underestimation of the intensity. This minor criticism should not reflect on the generally high quality of this pattern.

The more recent calculated pattern (PDF 25-403) of Smith *et al.* (1973), however, bears little resemblance to Thompson's pattern or to our measured and calculated values. The cell edge used by Smith *et al.* ($a = 5.957$Å) is unusually low with respect to Thompson's ($a = 5.967$Å) and to the present values ($a = 5.9681(1)$Å). There is also serious disagreement between the relative intensities obtained by Smith *et al.* and those given by Thompson and observed in the present work. The earlier pattern of Thompson should definitely be used as a reference in any identification or pattern searches, particularly if the convention of excluding lines with $d < 1.00$ is followed (even if these be the strongest lines). It is also suggested that the values given here be used to supersede the pattern of Smith *et al.* (1973).

Table 5 gives the calculated powder pattern for sperrylite obtained from POWGEN, with the intensities scaled to give I ($d = 1.7995$) $= 100$. Where the intensities of the *hkl* and *khl* reflections are different, only the index of the strongest reflection is given in Table 5.

TABLE 5. X-RAY POWDER PATTERN OF SPERRYLITE CALCULATED FOR Cu$K\alpha$ RADIATION FROM OBSERVED SINGLE-CRYSTAL DIFFRACTOMETER INTENSITIES

d(Å)	I_{calc}	*hkl*	*d*(Å)	I_{calc}	*hkl*
3.4457	54	111	1.0550	19	440
2.9840	67	200	1.0088	15	531
2.6690	33	210	0.9947	16	600,442
2.4365	28	211	0.9811	2	610
2.1100	50	220	0.9682	6	611,532
1.7995	100	311	0.9436	13	620
1.7228	18	222	0.9101	20	533
1.6553	12	230	0.8997	14	622
1.5950	17	321	0.8897	4	542,630
1.3692	18	331	0.8799	4	361
1.3345	22	420	0.8357	13 α_1	551,711
1.3023	7	421	0.8276	18 α_1	640
1.2724	3	332	0.8198	6 α_1	270,461
1.2182	21	511,333	0.8122	7 α_1	721,663,552
1.1486	37	250,342	0.7975	38 α_1	642
1.1082	7	521	0.7770	155 α_1	731,553
1.0896	4	440			

The powder pattern of platarsite given by Cabri *et al.* (1977) is based upon intensities measured from a Gandolfi photograph of the grain used in the present structure analysis. As relative intensities from Gandolfi photographs may not correspond to those obtained in a Debye-Scherrer powder pattern, the POWGEN calculated powder pattern for platarsite is given in Table 6. The relative intensities given here and those given by Cabri *et al.* (1977) differ somewhat, particularly in the mid-range of *d* spacings. The indexing convention described above for Table 5 is followed in Table 6.

TABLE 6. X-RAY POWDER PATTERN OF PLATARSITE CALCULATED FOR Cu$K\alpha$ RADIATION FROM OBSERVED SINGLE-CRYSTAL DIFFRACTOMETER INTENSITIES

d(Å)	I_{calc}	*hkl*	*d*(Å)	I_{calc}	*hkl*
3.342	62	111	1.075	6	342,250
2.894	88	200	1.057	4	521
2.588	36	210	1.023	16	440
2.363	31	211	0.9784	13	531
2.046	56	220	0.9647	16	442,600
1.745	100	311	0.9389	6	532,611
1.671	20	222	0.9152	11	620
1.605	11	302	0.8827	20	533
1.547	16	321	0.8726	14	622
1.328	18	331	0.8628	4	630,542
1.294	18	420	0.8534	4	631
1.263	6	421	0.8105	22	551,711
1.234	3	332	0.8027	34	640
1.182	20	422	0.7950	10	461,270
1.114	37	333,511	0.7877	13	552,633,721

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