

## The Crystal Structure of Jamesonite, $\text{FePb}_4\text{Sb}_6\text{S}_{14}$

By N. NIIZEKI<sup>1</sup> and M. J. BUERGER

With 19 figures

(Received February 25, 1957)

### Zusammenfassung

Die Kristallstruktur des Jamesonits gehört der Raumgruppe  $P2_1/a$  an; die Elementarzelle mit den Gitterkonstanten  $a = 15,07 \text{ \AA}$ ,  $b = 18,98 \text{ \AA}$ ,  $c = 4,03 \text{ \AA}$ ,  $\beta = 91^\circ 48'$  enthält 2  $\text{FePb}_4\text{Sb}_6\text{S}_{14}$ .

Drei  $\text{Sb}_3\text{S}_3$ -Gruppen sind parallel  $[120]$  angeordnet und können zusammen als  $\text{Sb}_3\text{S}_7$ -Gruppen aufgefaßt werden, die durch lose Bindung größere Gruppen  $\text{Sb}_6\text{S}_{14}$  ergeben. Fe- und zwei Lagen von Pb-Atomen nehmen die Räume zwischen S-Atomen der  $\text{Sb}_6\text{S}_{14}$ -Gruppen ein und verknüpfen die Sb-S-Gruppen miteinander. Jedes Fe-Atom wird von sechs S-Atomen in den Ecken eines verzerrten Oktaeders umgeben. Die Pb-Atome haben entweder 7 oder 8 S-Atome als nächste Nachbarn. Starke Bindung längs Ketten oder Schichten parallel der Längsrichtung der nadeligen Kristalle tritt beim Jamesonit nicht klar in Erscheinung. Die Spaltbarkeit des Minerals wird auf Grund der beobachteten interatomaren Abstände gedeutet.

### Abstract

The crystal structure of the mineral jamesonite has been determined. The space group is  $P2_1/a$ , and the unit cell dimensions are:  $a = 15.07 \text{ \AA}$ ,  $b = 18.98 \text{ \AA}$ ,  $c = 4.03 \text{ \AA}$ , and  $\beta = 91^\circ 48'$ . This unit cell contains 2  $\text{FePb}_4\text{Sb}_6\text{S}_{14}$ . The intensities were measured by the single-crystal GEIGER-counter method with  $\text{CuK}\alpha$  radiation. The structure projected along  $c$  axis was solved by the minimum function method. The  $z$  parameters of the atoms were determined by the implication method. The structure was refined by the successive FOURIER, and difference-FOURIER trials, and finally by the three-dimensional least-squares method.

In the structure three  $\text{Sb}_3\text{S}_3$  groups are arranged parallel to  $[120]$ , and can be described as forming  $\text{Sb}_3\text{S}_7$  groups. Two  $\text{Sb}_3\text{S}_7$  groups are loosely bonded together into a larger  $\text{Sb}_6\text{S}_{14}$  group. Fe and two kinds of Pb atoms are located in the interstices provided by the S atoms of the  $\text{Sb}_6\text{S}_{14}$  groups, and play the role of cementing these Sb-S groups. Fe has a distorted octahedral coordination of six S atoms. The Pb atoms have either 7 or 8 atoms of sulfur as closest neighbors.

<sup>1</sup> Present address: Mineralogical Institute, University of Tokyo, Tokyo, Japan.

The strongly bonded chains or layers running parallel to the acicular axis of the mineral is not well defined in jamesonite. The cleavage of the mineral has been accounted for in terms of the observed interatomic distances.

### Introduction

The crystallographic description of the mineral jamesonite,  $\text{FePb}_4\text{Sb}_6\text{S}_{14}$ , has been presented by BERRY<sup>2</sup>. Jamesonite is a member of the group of acicular sulfosalts, concerning which there has been a considerable increase in structural knowledge in recent years<sup>3-7</sup>. As in the case of livingstonite<sup>6</sup>,  $\text{HgSb}_4\text{S}_8$ , the crystal system of jamesonite is monoclinic. The needle axis of jamesonite is parallel to the  $c$  axis, while in livingstonite it is parallel to the unique 2-fold (or  $b$ ) axis.

The cleavages of the members of the group of acicular sulfosalts are known to occur in two ways. In one type, cleavage parallel to the acicular axis, or prismatic cleavage only, is observed. All the sulfosalts crystals of the acicular group with previously determined structures are of this type. In these crystal structures there are layers or chains composed of submetal atoms and sulfur atoms running parallel to the needle axis of the mineral. The prismatic cleavage of the mineral has been explained as due to the breaking of the weaker chemical bonds between the layers or chains in the structure, and, as a result, parallel to the acicular axis. A second type of cleavage occurs perpendicularly to the acicular axis. This basal cleavage is observed with or without accompanying prismatic cleavage. Among the minerals with this type of cleavage are jamesonite, owyheeite<sup>8</sup>, and falkmanite<sup>9</sup>. Accordingly, a somewhat different structural scheme than found in the previously determined structures can be expected for jamesonite.

<sup>2</sup> L. G. BERRY, Studies of mineral sulpho-salts: II. Jamesonite from Cornwall and Bolivia. *Miner. Mag.* **25** (1940) 597-608.

<sup>3</sup> F. E. WICKMAN, The crystal structure of galenobismutite. *Arkiv Chem. Geol.* **1** (1951) 219-225.

<sup>4</sup> F. E. WICKMAN, The crystal structure of aikinite,  $\text{CuPbBiS}_3$ . *Arkiv Chem. Geol.* **1** (1953) 501-507.

<sup>5</sup> M. J. BUERGER and THEODOR HAHN, The crystal structure of berthierite,  $\text{FeSb}_2\text{S}_4$ . *Am. Mineralogist* **40** (1955) 226-238.

<sup>6</sup> N. NIIZEKI and M. J. BUERGER, The crystal structure of livingstonite,  $\text{HgSb}_4\text{S}_8$ . *Z. Kristallogr.* **109** (1957) 129-157.

<sup>7</sup> N. NIIZEKI, The crystal chemistry of the mineral sulfosalts. To be published in *Geochemica Acta*.

<sup>8</sup> S. C. ROBINSON, Owyheeite. *Am. Mineralogist* **34** (1949) 398-402.

<sup>9</sup> J. E. HILLER, Über den Falkmanit und seine Unterscheidung von Boulangerit. *Neues Jb. Mineralog. Mh.* **1955**, 1-10.

### Unit cell and space group

The unit cell and space group of the mineral were determined from precession and DE JONG photographs using crystals from Cornwall, England, kindly furnished for our investigation by Professor CLIFFORD FRONDEL from the Harvard mineralogical collection. The results obtained for the unit cell dimensions are:

$$\begin{aligned} a &= 15.57 \text{ \AA} \\ b &= 18.98 \text{ \AA} \quad \beta = 91^\circ 48' \\ c &= 4.03 \text{ \AA} \end{aligned}$$

These values are in good agreement with those of BERRY. The space group  $P 2_1/a$  assigned by BERRY<sup>2</sup> was confirmed. The unit cell contains  $2\text{FePb}_4\text{Sb}_6\text{S}_{14}$ .

### Intensity determination

A single crystal of needle form having dimensions 0.03 mm.  $\times$  0.04 mm.  $\times$  1.5 mm. was selected for the intensity determination. The three-dimensional intensities were measured by the single-crystal

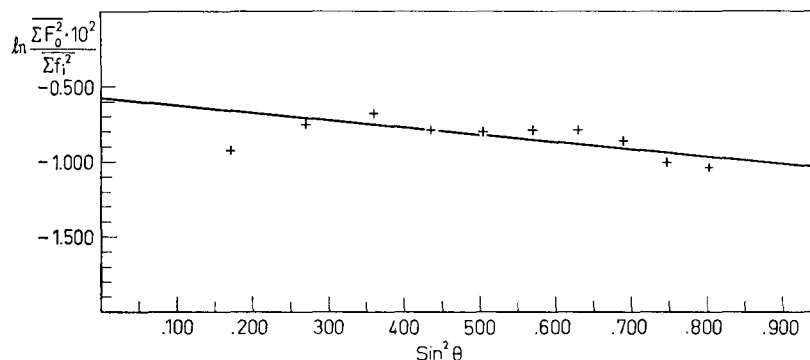


Fig. 1. Determination of scale factor and temperature coefficient by WILSON's statistical method applied to three-dimensional intensity data

GEIGER-counter goniometer method developed in the Crystallographic Laboratory, M.I.T., using  $\text{CuK}\alpha$  radiation. Intensities were corrected for LORENTZ and polarization factors, but no allowance was made for the absorption factor. The  $F^2(hkl)$  values were placed on an absolute basis using WILSON's method<sup>10</sup> applied three-dimensionally, Fig. 1. The temperature coefficient obtained by this method was  $B = 0.59$ .

<sup>10</sup> A. J. C. WILSON, Determination of absolute from relative intensity data. Nature 150 (1942) 151-152.

### General outline of the structure determination

Space-group equipoint considerations fix the position of the Fe atoms on one set of centers of symmetry. All the rest of the atoms presumably must occupy the general position  $4(e)$ . The existence of one short axis of length 4 Å suggests the possibility of solving the crystal structure as projected along this axis by means of minimum function method<sup>11</sup>.

As pointed out by BUERGER and HAHN elsewhere<sup>5</sup>, errors in solutions by the minimum-function method can arise if the PATTERSON peak chosen as the image point is not a single peak, but rather a coalescence of several peaks. During the present case of the structure determination of jamesonite, a false structure was obtained from an image point incorrectly selected. This false structure appeared very similar to the expected structure, at least in numbers of heavy peaks representing Pb and Sb atoms. The falseness of the structure could not be detected until a final electron-density map indicated certain abnormalities of the structure. Since this kind of confusion is apt to occur when the image-seeking method is applied to solve structures with large unit cells having many heavy atoms, such as those of many of the sulfosalt minerals, the discussion of the procedure will be given in some detail.

### Interpretation of PATTERSON peaks

The PATTERSON map  $P(xy)$ , Fig. 2, was obtained from the  $F^2(hk0)$ 's. The plane group of the projection along the  $c$  axis of space group  $P2_1/a$  is  $p2gg$ , and the corresponding PATTERSON plane group is  $p2mm$ . The relation between a rotation peak and its reflection satellites in this plane group is illustrated in Fig. 3. Since there are 2 Pb atoms and 3 Sb atoms in the asymmetric unit, then if no overlapping occurs, there must be 5 rotation peaks of single weight, and 10 reflection satellites of double weight in a quarter of PATTERSON space. Actually, as shown in Fig. 2, there are 6 peaks along the line  $x = 1/2$ , and 8 peaks along the line  $y = 1/2$ . These peaks have various heights, and the broadened shapes of some peaks at once suggest a considerable amount of overlapping at these locations. The excess number of peaks appearing along these lines is considered due either to interatomic vectors with accidental  $x$  or  $y$  component of  $1/2$ , or coalescence of reflection satellites of S atoms.

<sup>11</sup> M. J. BUERGER, A new approach to crystal-structure analysis. *Acta Crystallogr.* **4** (1951) 531–544.

Since it was impossible to choose definite satellite peaks, all the satellite-like peaks were used to find possible rotation peaks. Among the 48 possible positions for rotation peaks, Fig. 4, only three of them are associated with peaks which can be assumed reasonably as single-weight rotation peaks. The peak-height analysis was made assuming

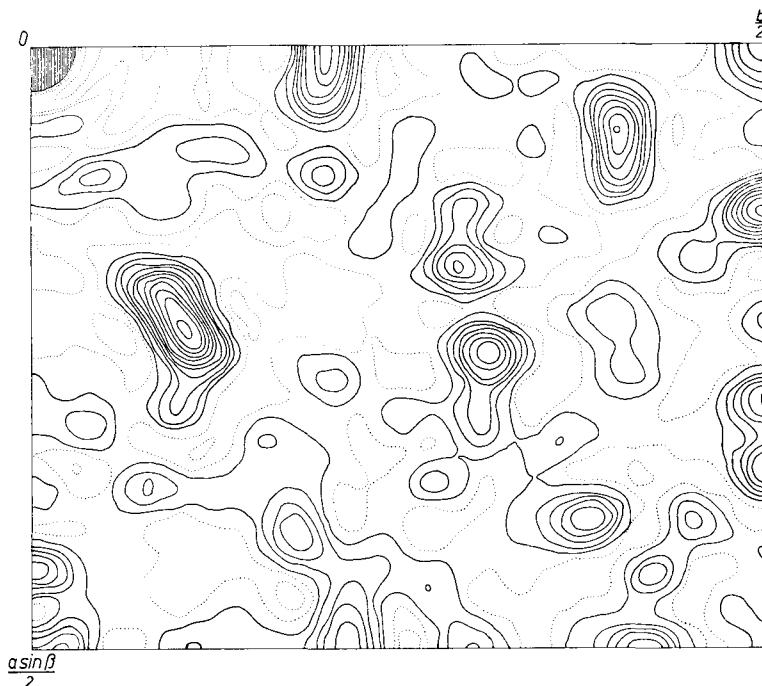


Fig. 2. PATTERSON diagram  $P(xy)$ . Contours are drawn at intervals of 50 units on an arbitrary scale. The dotted contours represent depressions. The details of the heavy peak at the origin are omitted.

a probably true zero contour, and it was found that all three of the peaks could be Pb—Pb rotation peaks. These peaks are numbered I, II, and III in Fig. 4.

#### Solutions by the image-seeking method

Assuming each of these three peaks as an image point in turn, three sets of  $M_2$  functions were obtained, and each of them was folded into an  $M_4$  function using a glide operation. These three  $M_4$  maps are shown in Figs. 5, 6 and 7. Among them the  $^{\text{III}}M_4$  map (an  $M_4$  map based upon the assumption that peak III is a Pb—Pb rotation peak)

gave a result completely unrelated to the expected number of heavy atoms in the structure, Fig. 7, and was accordingly discarded. Since both the  $^I M_4$  map and the  $^{II} M_4$  map gave 6 heavy peaks, no choice between them was considered at this stage. The structures based on peaks I and II will be identified as structures I and II, respectively. To resolve an extra peak in each map, another  $M_4$  map was tried for each structure. The peak with the heaviest contour in each  $M_4$  map was

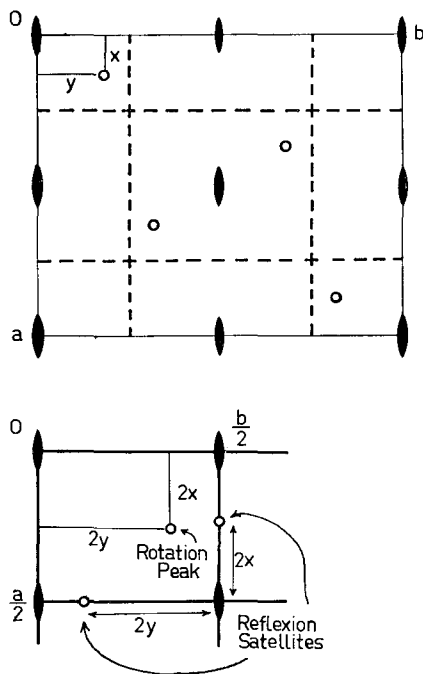


Fig. 3. Geometrical relation between a rotation peak and its reflection satellites in PATTERSON diagrams having plane symmetry  $p2mm$

assumed as the second probable atomic site for the *Pb* atom. In structure I, Fig. 5, it is designated as peak *a*, and in structure II, Fig. 6, as peak *A*. The  $^a M_4$  map and the  $^A M_4$  map were then prepared. Under the assumption that the atoms at I and *a* in one structure, and II and *A* in the other, are all of the same atomic specie (i. e., *Pb*) the  $^{I+a} M_8$  and  $^{II+A} M_8$  maps can be obtained by superposing the proper  $M_4$  maps. The  $^{I+a} M_8$  map, which was later found to represent the correct structure, is shown in Fig. 8. Also in Fig. 9, two  $M_8$  maps were compared, one map  $^{I+a} M_8$  in full lines, and the other  $^{II+A} M_8$  in dotted lines. From this comparison, however, nothing indicates which is the correct one.

### False structure

First the structure II was assumed to be correct, and since the

identification of heavy peaks in the  $M_8$  map with *Pb* and *Sb* was impossible, structure factors were computed using an average *f* curve:  $\frac{1}{2}(f_{Pb} + f_{Sb})$ . An electron-density map was prepared using signs determined in this way, and then refined by the usual procedures. The final electron-density map of structure II and its structural scheme, are shown respectively in Figs. 10 and 11. An examination of  $\rho(xy)$ , Fig. 10, however, reveals several peculiarities which are enough to

raise a question as to the validity of this structure. First, the relative weights of the five heavy peaks do not correspond to the chemical formula of jamesonite in a clear-cut way. Above all, there is one peak (peak *D* in Fig. 10) significantly too low to be assigned to an Sb atom. Furthermore, the shape of this particular peak is not well defined. The

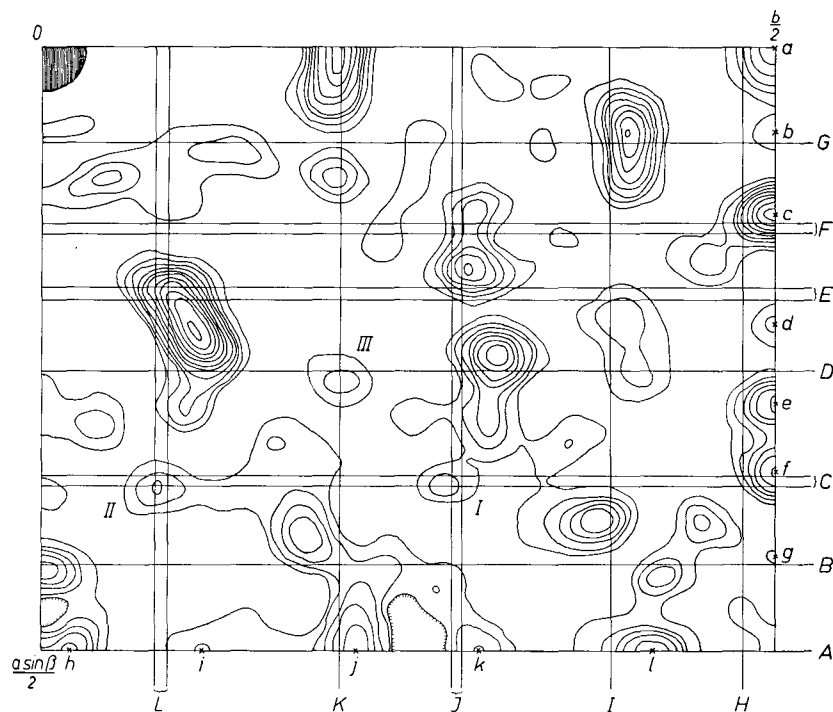


Fig. 4. Solution of rotation peaks from satellite-like peaks. Solutions are obtained at the intersections of horizontal and vertical lines drawn according to the relation illustrated in Fig. 3. Satellite-like peaks are designated by letters *a* to *l*, and the corresponding lines are designated by letters *A* to *L*. Three probable rotation peaks obtained by this method are indicated by I, II, and III.

above-mentioned aspects of the structure could not be improved by exchanging Pb with Sb in some of the atomic sites. Second, the peak shapes of the lighter atoms, especially of the Fe atom at the origin, are obscure. For these reasons structure II was considered incorrect. The significance of those features in the FOURIER diagrams which suggest an incorrect structure was recently pointed out by PINNOCK et al.<sup>12</sup>

<sup>12</sup> P. R. PINNOCK, C. A. TAYLOR and H. LIPSON, A re-determination of the structure of triphenylene. *Acta Crystallogr.* 9 (1956) 173–179.

Fig. 6. II  $M_4$  map

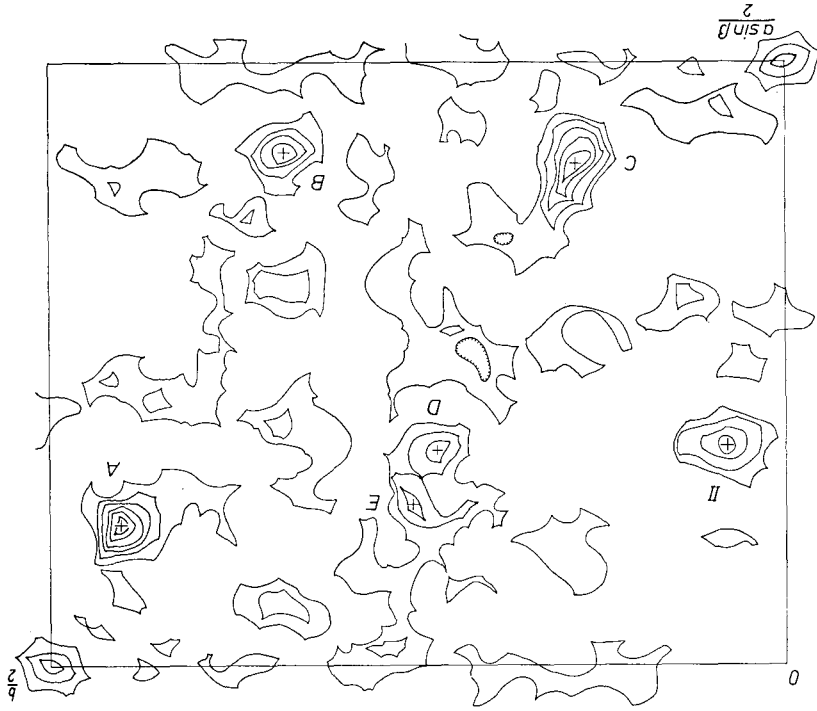
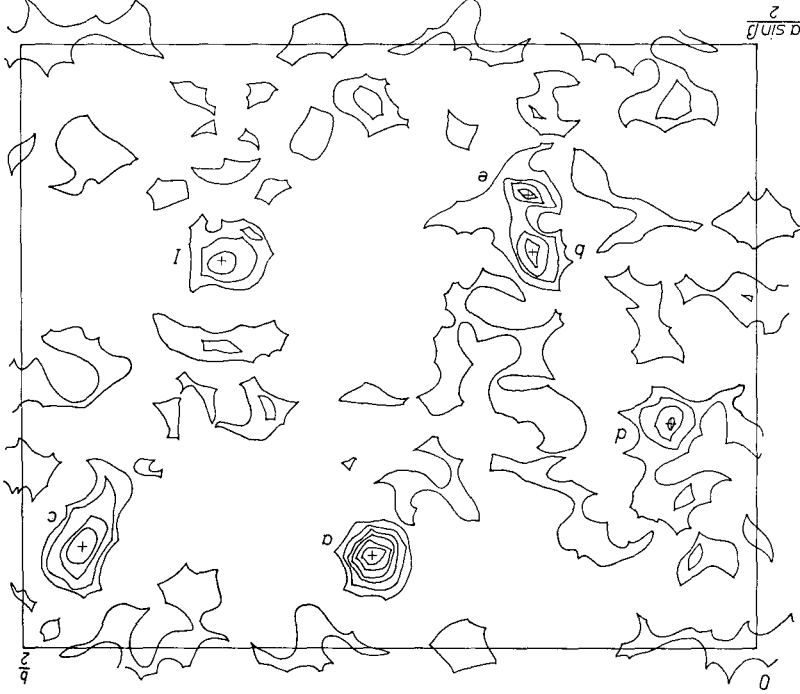


Fig. 5. I  $M_4$  map





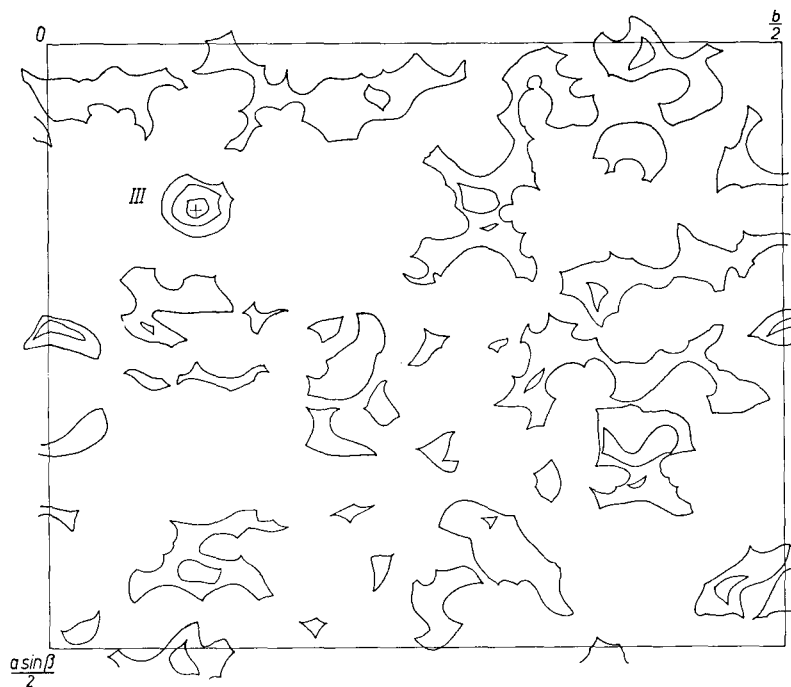


Fig. 7. III  $M_4$  map

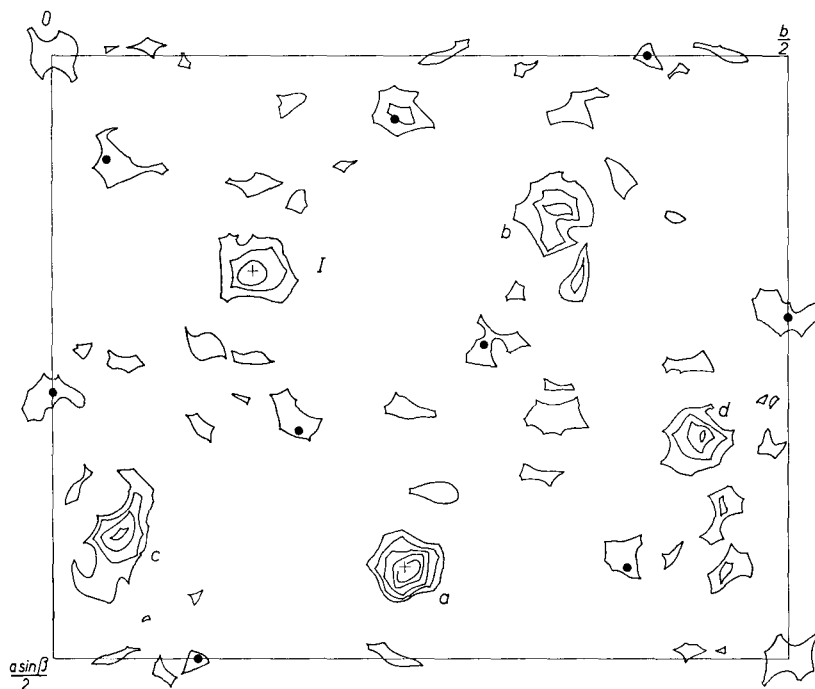


Fig. 8. I +  $aM_8$  map. Black dots indicate the final atomic sites for S atoms determined by FOURIER methods

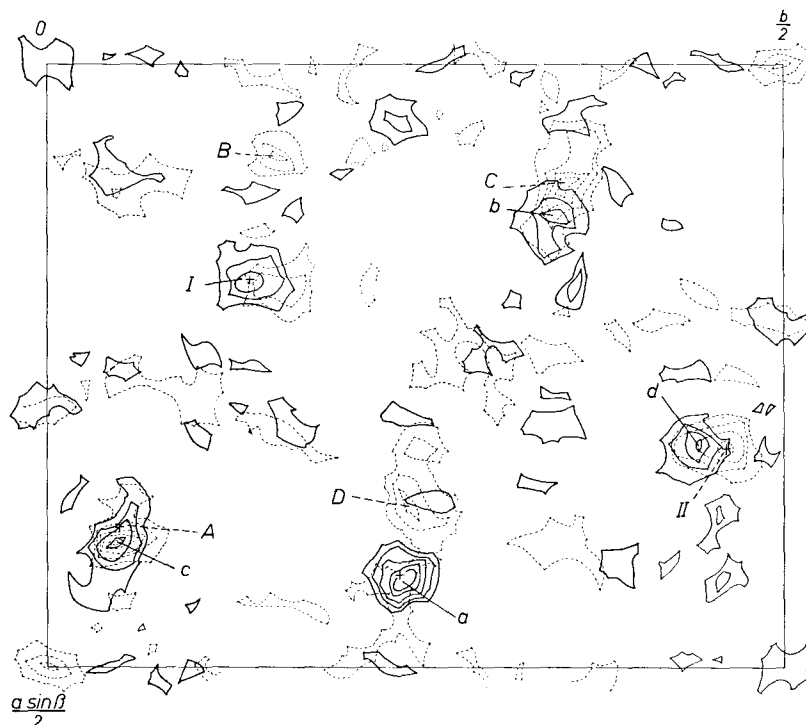


Fig. 9. Comparison of two  $M_8$  maps. The  $I+^a M_8$  map is drawn in full lines, and the  $II+^4 M_8$  map in broken lines

#### Correct structure

The alternative structure I based on the  $I+^a M_4$  map was then tried. Structure factors were computed as before with the averaged  $f$  curve. The electron-density map is shown in Fig. 12. In this map the shapes and the weight relations among the five heavy peaks are well defined. Peaks I and  $a$  are assigned to Pb atoms, and peaks  $b$ ,  $c$ , and  $d$  to the three Sb atoms.

Because of the identity of peaks I and  $a$ , the superposition of the  $I M_4$  map and the  $^a M_4$  map was justified, and this  $I+^a M_8$  map, Fig. 8, should contain enough information concerning the locations of S atoms. Although the refinement of the electron-density map, Fig. 12, should naturally indicate the sulfur peaks, it was considered useful to see how the image-seeking method would narrow the allowed region for the S atoms. This process was carried out by further constructing a  $b+c M_8$  map based on the rotation peaks  $b$  and  $c$ , both Sb—Sb rotation peaks. This map is shown in broken lines in Fig. 13 superposed on the

previously obtained  $I + {}^a M_8$  map, which is drawn in full lines. Since these two  $M_8$  maps are based on rotation peaks of different weights (different atomic species), the simple superposition to obtain an  $M_{16}$  map could not be made without proper weighting of contours. The final sulfur positions found by the FOURIER method are indicated in

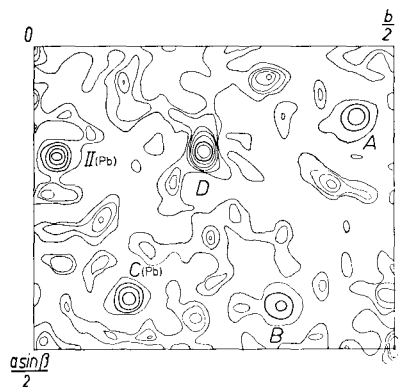


Fig. 10

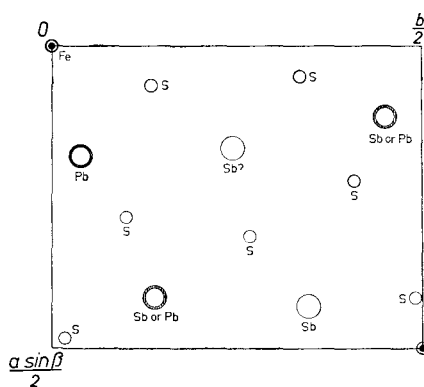


Fig. 11

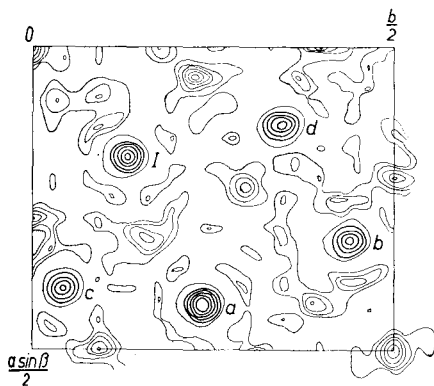


Fig. 12

Fig. 10. Electron density map  $\rho(xy)$  of false structure based on  $II + {}^A M_8$  map

Fig. 11. Structural scheme of false structure, Fig. 10

Fig. 12. Electron density map  $\rho(xy)$  of correct structure based on  $I + {}^a M_8$  map

Fig. 13 by black dots. They are all found at locations permitted by the minimum-function maps. Including these sulfur atoms in the structure-factor computation, the refinement of structure I was done by successive difference-FOURIER maps. The final atomic coordinates determined by this process are presented in Column III of Table 1. The reliability factor for this projection was computed as  $R = 0.19$ .

The final electron density map prepared with signs after the three-dimensional refinement is shown in Fig. 14 for the full unit cell.

Table 1. Atomic coordinates determined by several methods

Atom	I From minimum- function map		II From impli- cation-map	III From FOURIER maps		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
Pb <sub>I</sub>	0.183	0.136	0.060	0.184	0.139	0.066
Pb <sub>II</sub>	0.425	0.240	0.060	0.428	0.240	0.040
Sb <sub>I</sub>	0.320	0.436	0.480	0.320	0.436	0.488
Sb <sub>II</sub>	0.400	0.050	0.570	0.398	0.049	0.592
Sb <sub>III</sub>	0.128	0.346	0.620	0.132	0.340	0.628
S <sub>I</sub>				0.423	0.393	0.000
S <sub>II</sub>				0.102	0.043	0.460
S <sub>III</sub>				0.316	0.160	0.540
S <sub>IV</sub>				0.227	0.296	0.940
S <sub>V</sub>				0.045	0.230	0.560
S <sub>VI</sub>				0.010	0.397	0.920
S <sub>VII</sub>				0.282	0.009	0.060
Fe				0.000	0.000	0.000
				<i>R(hk0)</i> = 0.19		
				<i>R(h0l)</i> = 0.24		
				<i>R(hkl)</i> = 0.28		

### Determination of *z* coordinates of atoms

The *z* parameters of the heavy atoms were determined by the implication method<sup>13</sup>. A HARKER synthesis  $P(x \frac{1}{2} z)$  was performed and the result is shown in Fig. 15. The relations between crystal space, PATTERSON space, and implication space are illustrated in Fig. 16 for the general equipoints  $2(e)$  of plane group  $p2$ . There are sub-multiple translations of  $a/2$  in these projections. In Fig. 17, therefore, the implication map corresponding to this sub-multiple cell is shown. Underneath the  $I(x \frac{1}{2} z)$  map is placed the heavy atoms with the *x* coordinates determined from  $\rho(xy)$ . The 4-fold ambiguities were resolved first by assuming as zero the *z* coordinate of the center of symmetry where the Fe atom is located, then by measuring the projected interatomic distances in  $\rho(xy)$ . Approximate *z* coordinates for the Pb atom were found to be zero, and those for Sb atoms were found to be  $c/2$ . The *z* parameters determined in this way are tabulated in Column II of Table 1. A few extra peaks of medium weights are observed in the

<sup>13</sup> M. J. BUEGER, The interpretation of HARKER syntheses. J. Appl. Physics 17 (1946) 579–595.

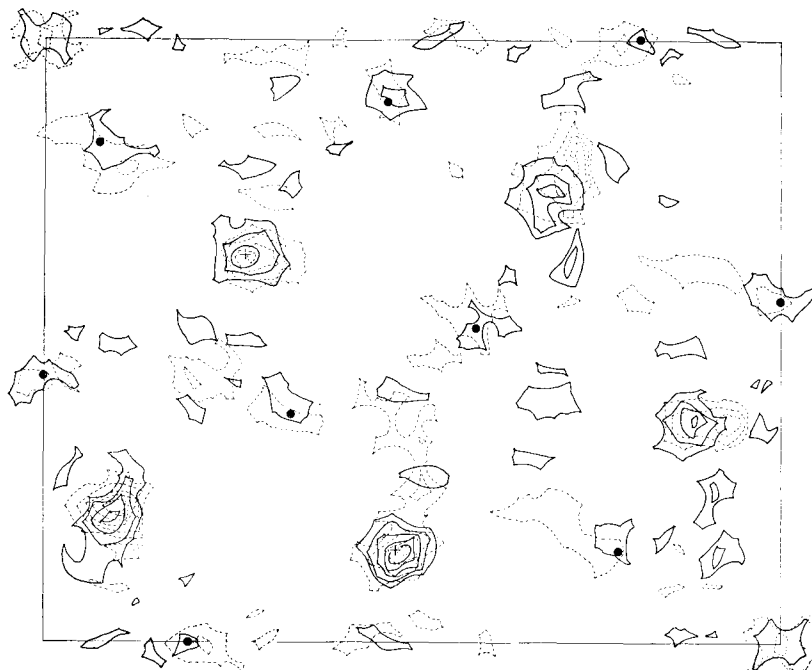


Fig. 13. Two  $M_s$  maps superposed. The  $1+aM_s$  map is drawn in full lines, and the  $b+cM_s$  map in dotted lines. Black dots indicate the final locations of S atoms determined by FOURIER methods.

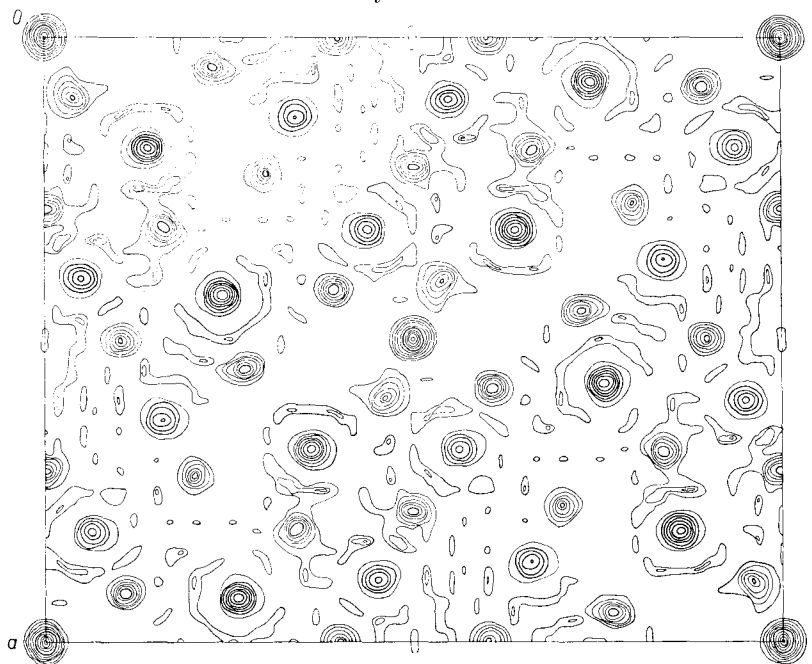


Fig. 14. Final electron density map  $\rho(xy)$

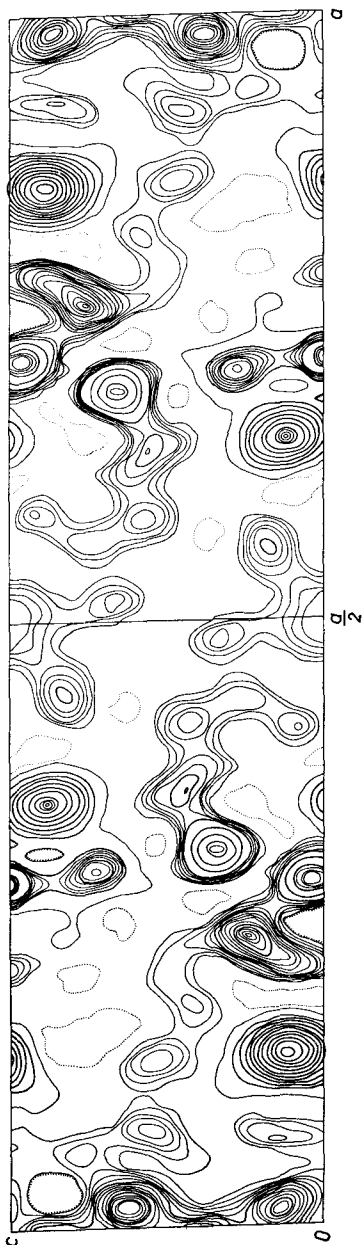


Fig. 15. HARKER section  $P(x, \frac{1}{2}, z)$ . Heavy contours represent the intervals of five light contours. The details between the heavy contours are omitted

implication map, Fig. 17. These are explained as due to interatomic vectors between atoms not related by a screw operation, but with  $y$  components of nearly  $\frac{1}{2}$ . Such a vector gives part of a PATTERSON peak in a HARKER section.

With an initial set of signs of structure factors determined by the heavy atoms, an electron-density map  $\rho(xz)$  was obtained, and then refined in the usual way. The final  $z$  coordinates determined by the FOURIER method are tabulated in Column III of Table 1, along with  $x$  and  $y$  coordinates. The reliability factor of this projection was computed as  $R = 0.24$ . This value was considered as low enough to proceed to three-dimensional refinement. The electron-density map  $\rho(xz)$  of the final structure is shown in Fig. 18.

### Three-dimensional refinements

The three-dimensional refinement of the structure was performed by the least-squares method developed by SAYRE<sup>14</sup> at the International Business Machine Corp., New York. The initial reliability factor of 1100  $F(hkl)$ 's was  $R = 0.28$ . After six cycles of the refinement process it went down to  $R = 0.166$ . Since no allowance was made for the

<sup>14</sup> P. H. FRIEDLANDER, W. LOVE and D. SAYRE, Least-squares refinement at high speed. *Acta Crystallogr.* 8 (1955) 732.

absorption effect, this value was regarded as sufficiently low to assure the accuracy of the structure.

The final atomic coordinates are tabulated in Table 2. The comparison between observed and computed structure factors is given in Table 4.

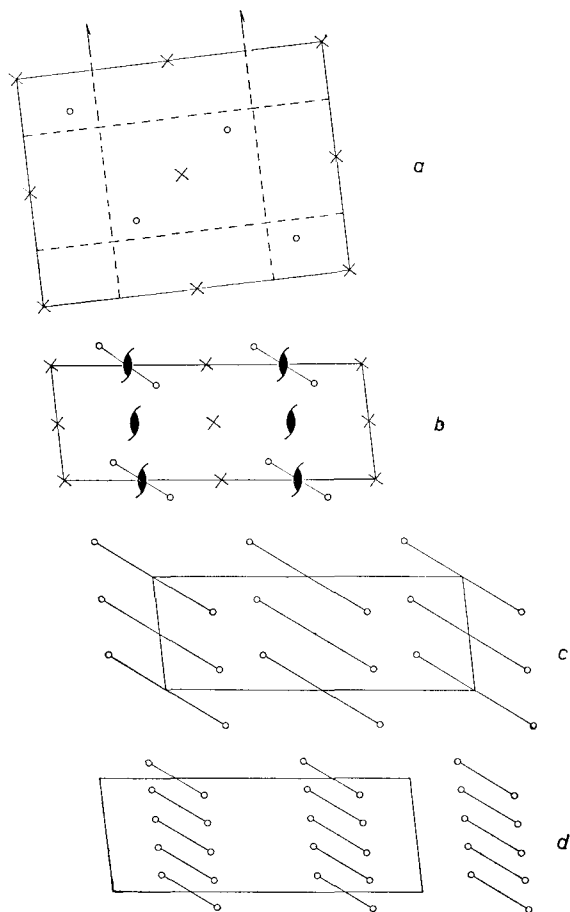


Fig. 16. Relations between crystal space, PATERSON space, and implication space. In drawings (a) and (b), space group  $P2_1/a$  is shown in two projections. In crystal space the general equipoints  $4(e)$  are indicated by small circles. Drawing (c) represents the HARKER section derived from (b). The origin is shifted from a center of symmetry to a  $2_1$  axis. The submultiple translation  $a/2$  is evident. In drawing (d) is shown the corresponding implication space,  $I(x_1/2z)$ . The origin is again shifted to a center of symmetry to compare with the crystal space. The 4-fold ambiguity is evident.

### Discussion of the structure

The interatomic distances between neighboring atoms are tabulated in Table 3. These distances are also indicated in a diagrammatic representation of the structure, Fig. 19.

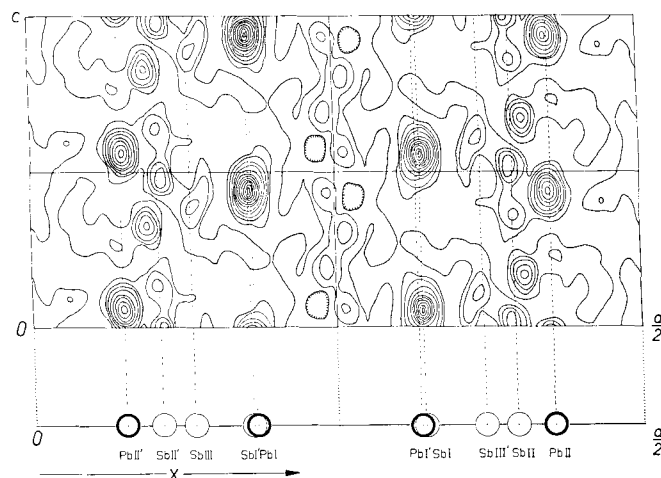


Fig. 17. Implication map  $I(x, \frac{1}{2}z)$ , and its interpretation. In the upper drawing the implication map is shown. In the lower drawing the  $x$  coordinates of the heavy atoms are indicated by circles on the straight line. The atoms related to each other by screw operations are indicated by primes. The  $z$  coordinate of each atom can be determined by tracing up the broken line into the implication map. Two-fold ambiguity of the solution is solved if interatomic distances in the projection  $\rho(xy)$ , Fig. 14, are taken into consideration.

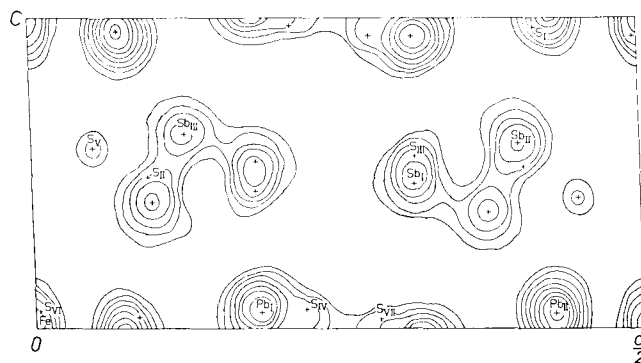


Fig. 18. Final electron density map  $\rho(xz)$



Table 2. *Final coordinates and temperature coefficients of atoms in jamesonite*

Atom	$x$	$y$	$z$	$B$
Pb <sub>I</sub>	0.182	0.141	0.036	1.21
Pb <sub>II</sub>	0.425	0.240	0.062	1.08
Sb <sub>I</sub>	0.319	0.437	0.408	0.75
Sb <sub>II</sub>	0.396	0.049	0.623	0.74
Sb <sub>III</sub>	0.130	0.340	0.620	1.05
S <sub>I</sub>	0.419	0.395	0.968	0.21
S <sub>II</sub>	0.095	0.042	0.524	0.59
S <sub>III</sub>	0.316	0.158	0.555	0.73
S <sub>IV</sub>	0.226	0.297	0.076	0.73
S <sub>V</sub>	0.050	0.230	0.573	0.17
S <sub>VI</sub>	0.002	0.398	0.052	0.71
S <sub>VII</sub>	0.285	0.004	0.027	0.41
Fe	0.000	0.000	0.000	1.08

Note:  $R = 0.166$  for 1100  $F(hkl)$ 's with this structure.  $B$  values were determined in the processes of three-dimensional least-squares refinement.

Table 3. *Interatomic distances in jamesonite*

	S <sub>I</sub>	S <sub>II</sub>	S <sub>III</sub>	S <sub>IV</sub>	S <sub>V</sub>	S <sub>VI</sub>	S <sub>VII</sub>
Pb <sub>I</sub>		3.01 Å 3.13	2.91 Å 2.92	3.04 Å	3.29 Å		3.04 Å
Pb <sub>II</sub>	2.97 Å		3.04 3.08	3.28	2.85 2.87	2.88 Å	
Sb <sub>I</sub>	2.52 2.82	2.41				3.29 4.08	2.67 2.90
Sb <sub>II</sub>			2.43			2.56 3.04 3.51 4.29	2.56 3.07
Sb <sub>III</sub>				2.56 2.81	2.44	3.18 2.94	3.67 4.40
Fe	2.36 (2)	2.57 (2) 2.66 (2)					

If account is taken of the nearest neighbors only, each of the three kinds of Sb atoms has three S atoms at distances of about 2.5 Å. The Sb and S atoms thus form an  $\text{SbS}_3$  group of trigonal-pyramidal shape. But this  $\text{SbS}_3$  group, described in terms of the three shortest distances, is different in its orientation from the corresponding groups found in

previously determined structures. In the structures of other sulfosalts, one edge of the pyramid is found to be parallel to the  $4\text{ \AA}$  axis. In jamesonite none of the edges is oriented in this way, but one edge is found as approximately parallel to the (001) plane.

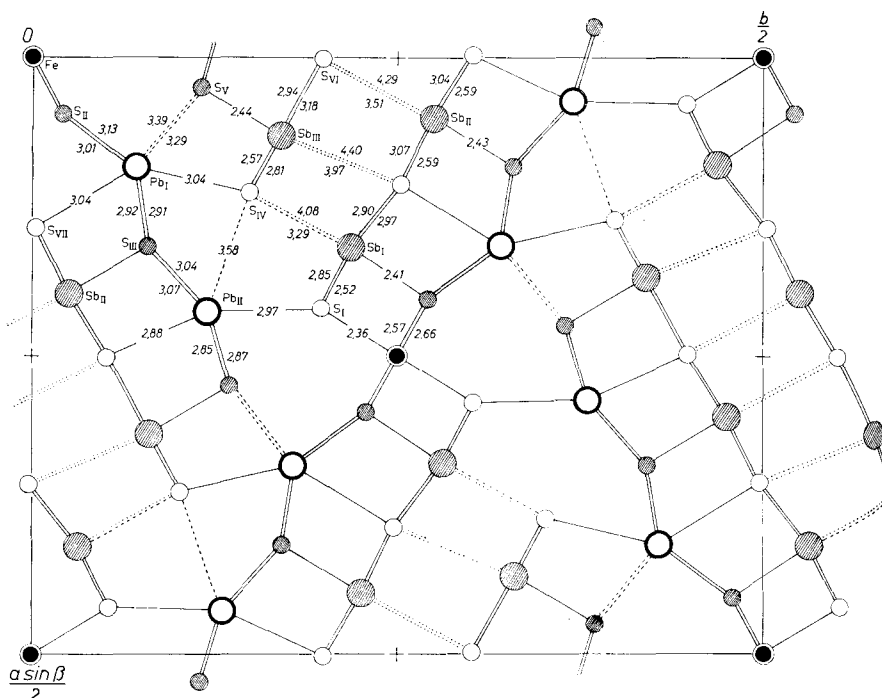


Fig. 19. Schematic representation of the structure. Open circles represent atoms with  $z$  coordinates close to zero, and shaded circles represent atoms with  $z$  coordinates close to  $\frac{1}{2}$ . The chemical bonds between neighboring atoms are indicated by lines. Broken lines are used to show the additional bonds from Pb to S beside the distorted octahedral bonds. Dotted lines indicate the weak bonds between Sb and S. All figures showing interatomic distances are in  $\text{\AA}$  units.

Three such groups,  $\text{Sb}_{(I)}\text{S}_3$ ,  $\text{Sb}_{(II)}\text{S}_3$ , and  $\text{Sb}_{(III)}\text{S}_3$  are arranged in an almost straight line parallel to  $[120]$ . Each trigonal pyramid shares corners with neighboring pyramids and forms an  $\text{Sb}_3\text{S}_7$  group. The distance between Sb atoms in the group and S atoms in their translation-equivalent group along the  $c$  axis is about  $3.0\text{ \AA}$ , and there is no strongly bonded Sb—S layer running parallel to the  $4\text{ \AA}$  axis in jamesonite.

Table 4. Observed and calculated structure factors

hkl	F <sub>obs</sub>	F <sub>calc</sub>	hkl	F <sub>obs</sub>	F <sub>calc</sub>	hkl	F <sub>obs</sub>	F <sub>calc</sub>	hkl	F <sub>obs</sub>	F <sub>calc</sub>	hkl	F <sub>obs</sub>	F <sub>calc</sub>
020	97	-101	470	259	-270	880	240	-228	13.10.0	51	-31	26T	259	-248
040	63	+20	480	142	+113	890	249	-220	13.11.0	179	+163	27T	340	-316
060	151	-70	490	369	+406	8.10.0	287	+268	13.12.0	101	+102	28T	71	-60
080	206	+182	4.10.0	414	+433	8.11.0	133	+116	14.0.0	115	-93	29T	95	+58
100	585	-630	4.11.0	50	-62	8.12.0	39	-19	14.1.0	187	+159	2.10.T	79	+56
120	158	+107	4.13.0	53	+12	8.13.0	82	-50	14.2.0	268	-210	2.11.T	28	-21
140	118	+116	4.14.0	94	+86	8.14.0	136	-136	14.3.0	46	-30	2.13.T	458	+506
160	105	+71	4.15.0	55	-23	8.15.0	94	+75	14.4.0	278	+238	2.14.T	194	-173
180	127	+80	4.16.0	79	+60	8.16.0	217	-167	14.5.0	74	-52	2.15.T	63	-56
200	292	+305	4.17.0	94	+91	910	314	-335	14.6.0	97	-89	2.16.T	79	+66
220	52	-12	4.18.0	73	-60	920	254	+264	14.7.0	73	-51	2.17.T	92	-81
240	173	-126	4.19.0	268	-280	930	123	+107	14.8.0	269	+222	2.18.T	85	+81
260	120	+83	510	213	+356	940	261	-253	14.9.0	153	+132	31T	135	-158
280	136	+78	520	114	-126	950	92	+69	14.10.0	277	+234	32T	121	-149
300	86	-119	540	26	-1	960	77	-56	15.1.0	36	-6	33T	263	+288
320	149	+133	550	31	+4	970	46	-11	15.2.0	142	+120	34T	263	+310
340	137	+122	560	215	-212	980	241	+219	15.3.0	187	+150	35T	124	+108
360	196	-162	570	33	+17	990	201	+168	15.4.0	140	-95	37T	308	-294
380	88	+63	580	74	+71	9.10.0	172	+162	15.5.0	22	+4	39T	117	+104
400	328	-325	590	265	-250	9.11.0	183	+161	15.6.0	208	-179	3.10.T	53	+32
420	112	+77	5.10.0	60	+44	9.12.0	255	-239	15.7.0	68	-66	3.11.T	274	+286
440	169	+173	5.11.0	400	-419	9.13.0	22	-17	15.8.0	105	+93	3.12.T	235	+208
460	85	-66	5.12.0	178	+143	9.14.0	200	+169	16.0.0	304	+244	3.13.T	51	+18
480	27	-22	5.13.0	247	+231	9.15.0	155	-129	16.1.0	190	+162	3.14.T	265	-241
500	288	+264	5.14.0	209	-193	10.0.0	313	+328	16.2.0	126	-104	3.15.T	117	+55
520	113	-117	5.15.0	106	+91	10.1.0	267	-262	16.3.0	278	-211	3.16.T	74	+71
540	32	+1	5.16.0	218	+210	10.2.0	247	+234	16.4.0	205	-170	3.17.T	182	+183
560	18	-27	5.17.0	151	+119	10.3.0	181	+182				3.18.T	109	-94
580	274	+293	5.18.0	181	+156	10.4.0	36	-28	00T	222	+245	40T	200	+235
600	113	-51	600	47	-5	10.5.0	287	-278	01T	5	+41	41T	402	+684
620	120	-125	610	54	+51	10.7.0	96	+85	02T	370	-374	42T	322	+455
640	31	-47	620	178	+210	10.8.0	51	-33	03T	85	-94	43T	97	+98
660	347	+346	630	54	-52	10.9.0	65	+57	04T	53	+38	44T	56	-57
680	552	+768	640	414	-512	10.10.0	144	-123	05T	147	+97	45T	26	+25
700	319	-309	650	47	-15	10.11.0	265	+224	06T	67	-50	46T	155	+154
720	164	-145	660	333	+345	10.12.0	140	-91	07T	242	-214	47T	64	-60
740	186	+144	670	36	+30	10.13.0	223	-206	08T	604	+656	48T	349	-368
760	96	-96	680	86	-57	10.14.0	36	+26	09T	47	-6	49T	317	+339
780	79	+69	690	41	-39	11.1.0	270	+260	0.10.T	131	+132	4.10.T	31	+4
800	105	-88	6.10.0	41	+15	11.3.0	187	-167	0.11.T	33	+1	4.11.T	314	-310
820	119	+104	6.11.0	223	-180	11.4.0	222	-186	0.12.T	129	+96	4.12.T	91	-70
840	67	+69	6.12.0	28	-11	11.5.0	94	-38	0.13.T	22	-24	4.13.T	130	-110
860	311	-317	6.13.0	205	+204	11.6.0	51	-30	0.14.T	45	+53	4.14.T	59	+42
880	351	-340	6.14.0	361	+363	11.7.0	245	+232	0.16.T	120	+104	4.15.T	18	+12
900	46	-18	6.15.0	46	+28	11.8.0	115	-90	0.17.T	206	+205	4.17.T	18	+5
920	50	+12	6.16.0	36	-28	11.9.0	170	-133	0.18.T	273	-298	4.18.T	258	+251
940	59	+69	6.17.0	59	-40	11.10.0	83	+55	0.19.T	38	-3	51T	115	-111
960	78	+79	710	65	-63	11.11.0	56	-31	11T	12	+68	52T	219	+259
980	119	-143	720	153	-167	11.12.0	126	-95	12T	150	-157	53T	73	-85
1000	101	+26	730	181	+179	11.13.0	123	+105	13T	294	-288	54T	69	-55
1020	112	+107	740	432	+498	11.14.0	228	+194	14T	185	+154	55T	33	+42
1040	205	-207	750	217	+208	12.0.0	245	+244	15T	38	-25	56T	162	-165
1060	310	+319	760	367	+454	12.1.0	81	-67	16T	246	+217	57T	149	+136
1080	411	-499	770	141	-124	12.2.0	38	-37	17T	532	+535	58T	59	+56
1100	64	+33	780	131	-124	12.3.0	168	+140	18T	92	+61	59T	208	+193
1120	190	+180	790	228	+203	12.4.0	77	+64	19T	146	-125	5.10.T	65	-22
1140	183	-166	7.10.0	146	-126	12.5.0	206	+187	1.10.T	156	-145	5.11.T	210	-209
1160	235	+226	7.11.0	73	-56	12.6.0	270	-233	1.11.T	82	+72	5.12.T	165	-146
1180	214	+194	7.12.0	26	+36	12.7.0	288	+238	1.12.T	250	+236	5.13.T	160	+145
1200	19	-7	7.13.0	104	+88	12.8.0	149	+133	1.13.T	62	+36	5.14.T	50	-34
1220	64	+71	7.14.0	246	-210	12.9.0	247	-211	1.14.T	186	-161	5.16.T	187	+193
1240	231	-214	7.15.0	65	+38	12.10.0	112	-83	1.15.T	54	+61	5.17.T	26	-4
1260	274	+253	7.16.0	249	-238	12.11.0	63	-39	1.16.T	120	-124	60T	79	-62
1280	32	+54	7.17.0	163	+159	12.13.0	108	-78	1.17.T	224	-226	61T	149	-154
1300	141	-132	800	295	-351	13.1.0	58	-34	1.18.T	240	-224	62T	122	+133
1320	176	+173	810	213	-235	13.2.0	241	-209	1.19.T	153	+141	63T	33	+64
1340	273	-373	820	205	+195	13.3.0	129	+120	20T	72	-53	64T	372	-440
1360	379	+426	830	39	+34	13.4.0	136	+103	21T	63	-82	65T	335	-357
1380	273	+34	840	40	-17	13.6.0	94	+86	22T	127	+147	66T	405	+493
1400	173	-184	850	106	-108	13.7.0	109	+75	23T	405	-551	68T	83	+68
1420	117	+71	860	258	+230	13.8.0	322	-273	24T	123	+113	69T	58	-54
1440	149	-122	870	115	+106	13.9.0	141	-129	25T	129	+122	6.10.T	33	+18

12\*

h k l	$F_{\text{obs}}$	$F_{\text{calc}}$	h k l	$F_{\text{obs}}$	$F_{\text{calc}}$	h k l	$F_{\text{obs}}$	$F_{\text{calc}}$	h k l	$F_{\text{obs}}$	$F_{\text{calc}}$	h k l	$F_{\text{obs}}$	$F_{\text{calc}}$
6.11.T	105	+103	11.12.T	213	-187	2.15.T	54	+42	7.7.T	51	-62	12.11.T	390	-338
6.12.T	179	+157	11.13.T	28	+28	2.16.T	79	+56	7.8.T	191	+158	12.12.T	158	+123
6.13.T	73	-44	12.0.T	377	+406	2.17.T	73	+65	7.9.T	50	+64	12.1.T	68	+28
6.14.T	190	+176	12.1.T	195	-159	2.18.T	140	+126	7.10.T	73	+74	12.2.T	123	-90
6.15.T	178	-177	12.2.T	268	-247	2.19.T	46	-51	7.11.T	33	-3	12.3.T	237	+200
6.16.T	232	-197	12.3.T	161	-150	3.1.T	53	-61	7.12.T	153	-243	12.4.T	53	-43
7.1.T	99	+104	12.4.T	26	-9	3.2.T	267	-358	7.13.T	206	+332	12.5.T	53	-44
7.2.T	224	-239	12.5.T	50	-24	3.3.T	424	+615	7.14.T	183	-154	12.6.T	170	-135
7.3.T	47	+39	12.6.T	26	-28	3.4.T	300	-342	7.15.T	112	-104	12.7.T	117	-99
7.4.T	335	-333	12.8.T	308	+261	3.5.T	38	+39	7.16.T	53	+64	12.8.T	138	-89
7.5.T	272	+256	12.9.T	181	-161	3.6.T	18	-16	8.0.T	222	-227	12.9.T	205	-139
7.6.T	32	+1	12.10.T	245	-235	3.7.T	324	-341	8.1.T	59	-49	12.10.T	47	+35
7.8.T	165	-145	12.11.T	129	+119	3.8.T	260	-254	8.2.T	308	+345	12.11.T	182	+151
7.9.T	81	+67	12.12.T	147	+105	3.9.T	33	-6	8.3.T	109	-109	12.12.T	188	+160
7.10.T	18	-32	13.1.T	228	-200	3.10.T	79	+61	8.4.T	78	-79	12.1.T	41	+9
7.11.T	181	-169	13.2.T	195	-162	3.11.T	190	+176	8.6.T	88	+74	12.2.T	77	+52
7.12.T	145	+127	13.3.T	178	+158	3.12.T	138	+111	8.7.T	251	-225	12.3.T	112	-87
7.13.T	124	+111	13.4.T	26	-2	3.13.T	238	-222	8.8.T	423	-396	12.4.T	376	+323
7.14.T	378	+370	13.5.T	64	-69	3.14.T	236	+211	8.9.T	50	+18	12.5.T	91	+77
7.15.T	83	+41	13.6.T	53	+39	3.15.T	210	+178	8.10.T	277	+251	12.6.T	354	-279
7.16.T	147	-169	13.7.T	26	-30	3.17.T	174	+169	8.11.T	131	+103	12.7.T	63	+41
8.0.T	314	-378	13.8.T	41	+25	3.18.T	153	+137	8.12.T	118	-96	12.8.T	54	-50
8.1.T	295	-310	13.9.T	154	+131	4.0.T	259	+298	8.13.T	150	+134	12.9.T	227	-186
8.2.T	156	+150	13.10.T	73	-51	4.1.T	328	-477	8.14.T	50	+15	12.10.T	135	-102
8.3.T	62	-28	13.11.T	244	+214	4.2.T	46	-29	8.15.T	26	+19	12.11.T	186	-140
8.4.T	118	+112	14.0.T	367	+313	4.3.T	137	+147	9.1.T	76	-61	12.12.T	47	+31
8.5.T	92	-74	14.1.T	67	+38	4.4.T	51	+12	9.2.T	65	-69	12.1.T	85	+64
8.6.T	104	-86	14.2.T	87	+60	4.5.T	129	-97	9.3.T	170	+141	12.2.T	227	+176
8.7.T	118	+98	14.3.T	59	-29	4.6.T	167	+182	9.4.T	28	+37	0.0.Z	602	+700
8.8.T	154	-145	14.4.T	305	+270	4.7.T	345	+370	9.5.T	83	+62	0.1.Z	212	+442
8.9.T	247	-237	14.5.T	191	+165	4.8.T	76	+47	9.6.T	88	+73	0.2.Z	58	-114
8.10.T	327	+331	14.6.T	251	-211	4.9.T	270	-289	9.7.T	246	-215	0.3.Z	109	-115
8.11.T	267	+245	14.7.T	110	-92	4.10.T	51	-44	9.8.T	186	+135	0.4.Z	13	+8
8.12.T	69	+51	14.8.T	115	-98	4.11.T	227	+214	9.9.T	109	+75	0.5.Z	58	-37
8.13.T	30	-32	14.9.T	126	+97	4.12.T	47	+38	9.10.T	142	-136	0.6.Z	40	-38
8.14.T	50	+12	15.1.T	60	+37	4.13.T	74	+73	9.11.T	109	-77	0.7.Z	26	+23
8.15.T	31	+24	15.2.T	141	+182	4.14.T	96	-79	9.12.T	226	+192	0.8.Z	273	+263
9.1.T	144	+113	15.3.T	65	+25	4.15.T	270	-259	9.13.T	87	+52	0.9.Z	350	+339
9.2.T	42	+85	15.4.T	65	-63	4.16.T	64	+40	9.14.T	42	+25	0.10.Z	236	-217
9.3.T	185	+168	15.5.T	60	+37	5.1.T	94	+103	10.0.T	26	+29	0.11.Z	159	-127
9.4.T	28	-22	15.6.T	229	-204	5.2.T	231	-277	10.1.T	146	-123	0.12.Z	46	+70
9.5.T	58	+54	15.7.T	53	-29	5.3.T	288	-348	10.2.T	370	-358	0.13.Z	92	+41
9.6.T	62	+73	1.1.T	146	+204	5.4.T	67	+9	10.3.T	285	-242	0.14.Z	41	+97
9.7.T	264	-229	1.2.T	361	+443	5.5.T	109	+104	10.4.T	327	+283	1.1.Z	214	+345
9.8.T	62	-49	1.3.T	126	+86	5.6.T	68	+47	10.5.T	350	+281	1.2.Z	355	-356
9.9.T	292	-270	1.4.T	79	-79	5.7.T	358	+380	10.6.T	349	-294	1.3.Z	141	+117
9.10.T	203	+170	1.5.T	193	-157	5.8.T	228	-223	10.7.T	303	+263	1.4.Z	72	+46
9.11.T	73	-43	1.6.T	147	+118	5.9.T	146	+124	10.8.T	88	-58	1.5.Z	147	-128
9.12.T	274	-258	1.7.T	360	+347	5.10.T	104	+87	10.9.T	167	+114	1.6.Z	223	-194
9.13.T	79	+50	1.8.T	308	-283	5.11.T	178	-180	10.10.T	150	+101	1.7.Z	155	-123
9.14.T	42	+26	1.9.T	86	-62	5.12.T	212	+193	10.11.T	177	+136	1.8.Z	123	-115
10.0.T	100	+83	1.10.T	33	+24	5.13.T	108	+104	10.12.T	288	+243	1.9.Z	244	-223
10.1.T	62	+50	1.11.T	374	-372	5.14.T	72	-35	10.13.T	117	+121	1.10.Z	297	+272
10.2.T	118	-99	1.12.T	209	-165	5.15.T	83	-67	11.1.T	31	+39	1.11.Z	122	-101
10.3.T	286	-278	1.13.T	18	-6	5.16.T	168	-168	11.2.T	64	-57	1.12.Z	64	-65
10.4.T	112	+98	1.14.T	223	+202	6.0.T	38	-42	11.3.T	78	+58	1.13.Z	141	-152
10.5.T	432	-449	1.15.T	145	+149	6.1.T	122	+126	11.4.T	47	+27	1.14.Z	101	-108
10.6.T	142	-119	1.16.T	114	-106	6.2.T	301	+353	11.5.T	73	-52	1.15.Z	473	+544
10.7.T	199	+163	1.17.T	47	+37	6.3.T	345	+402	11.6.T	182	+149	1.16.Z	219	-187
10.8.T	206	+191	1.18.T	198	+237	6.4.T	117	-122	11.7.T	46	+48	1.17.Z	49	-64
10.9.T	33	+42	1.19.T	150	+146	6.5.T	265	-278	11.8.T	131	+92	1.18.Z	73	+77
10.10.T	144	+97	2.0.T	96	-123	6.6.T	113	+123	11.9.T	79	-67	1.19.Z	208	-174
10.11.T	176	-142	2.1.T	144	-184	6.7.T	242	+226	11.10.T	186	-156	1.20.Z	47	+143
10.12.T	106	+76	2.2.T	173	+199	6.8.T	45	-30	11.11.T	65	+34	1.21.Z	190	+136
10.13.T	210	-177	2.3.T	172	-162	6.9.T	113	-96	11.12.T	69	-36	1.22.Z	71	-76
11.1.T	42	+32	2.4.T	172	-162	6.10.T	337	-301	11.13.T	158	+144	1.23.Z	137	+154
11.2.T	104	+64	2.5.T	296	-289	6.11.T	258	-240	12.1.T	437	+425	1.24.Z	249	+293
11.3.T	181	-163	2.6.T	173	+147	6.12.T	100	+104	12.2.T	213	-191	1.25.Z	91	+97
11.4.T	196	+155	2.7.T	42	+25	6.13.T	100	+113	12.3.T	123	+93	1.26.Z	236	+227
11.5.T	41	+27	2.8.T	31	-18	7.1.T	53	+48	12.4.T	58	-23	1.27.Z	296	-296
11.6.T	244	+204	2.9.T	51	-33	7.2.T	322	+363	12.5.T	38	+25	1.28.Z	177	+180
11.7.T	344	+305	2.10.T	36	+22	7.3.T	67	-67	12.6.T	95	-79	1.29.Z	156	+163
11.8.T	32	-22	2.11.T	388	+386	7.4.T	113	+110	12.7.T	205	+161	1.30.Z	246	-230
11.9.T	137	+95	2.12.T	274	-264	7.5.T	264	+257	12.8.T	348	+291			
11.10.T	82	+82	2.13.T	164	-163	7.6.T	71	+41	12.9.T	36	+5			

$h\ k\ l$	$ F_{\text{obs}} $	$F_{\text{calc}}$	$h\ k\ l$	$ F_{\text{obs}} $	$F_{\text{calc}}$	$h\ k\ l$	$ F_{\text{obs}} $	$F_{\text{calc}}$	$h\ k\ l$	$ F_{\text{obs}} $	$F_{\text{calc}}$	$h\ k\ l$	$ F_{\text{obs}} $	$F_{\text{calc}}$
3.11.2	33	+ 19	11.4.2	295	- 267	7 8 2	38	- 32	4 1 3	205	+ 280	5 4 3	59	- 46
3.12.2	31	- 3	11.5.2	65	- 52	7 9 2	156	+ 136	4 2 3	290	+ 379	5 5 3	59	+ 53
3.13.2	96	- 91	11.6.2	168	- 141	7.10.2	200	+ 177	4 3 3	138	+ 156	5 7 3	214	+ 210
4 0 2	320	- 420	12.0.2	279	+ 235	8 0 2	465	- 557	4 4 3	62	+ 5	5 9 3	168	- 170
4 1 2	90	+ 107	12.1.2	118	- 97	8 2 2	91	+ 128	4 7 3	88	+ 95	6 0 3	50	+ 25
4 2 2	74	+ 92	12.2.2	106	- 99	8 3 2	187	+ 174	4 8 3	245	- 241	6 1 3	47	- 28
4 3 2	198	- 147	12.3.2	108	- 96	8 6 2	146	+ 128	4 9 3	165	+ 164	6 2 3	120	+ 126
4 4 2	38	- 28	1 1 2	91	- 119	8 7 2	113	+ 75	5 1 3	162	+ 176	6 3 3	345	+ 417
4 5 2	95	- 113	1 3 2	119	- 86	8 8 2	195	- 144	5 2 3	109	+ 122	6 4 3	50	+ 56
4 6 2	218	+ 214	1 4 2	218	- 207	8 9 2	67	- 52	5 3 3	54	+ 60	6 5 3	42	- 37
4 7 2	327	- 352	1 6 2	311	- 290	8.10.2	460	+ 452	5 6 3	96	- 99	6 6 3	74	- 65
4 9 2	85	+ 77	1 7 2	258	+ 212	9 1 2	132	+ 130	5 7 3	79	- 72	6 7 3	163	+ 149
4.10.2	376	+ 420	1 8 2	104	+ 102	9 2 2	250	- 244	5 9 3	123	- 117	7 2 3	195	+ 156
4.11.2	133	+ 123	1.10.2	214	+ 195	9 3 2	26	- 29	6 0 3	46	+ 6	7 3 3	132	+ 125
4.12.2	31	+ 29	1.11.2	206	+ 190	9 4 2	176	+ 152	6 1 3	41	- 37	7 4 3	233	- 226
4.13.2	22	- 6	1.12.2	47	- 44	9 5 2	103	+ 68	6 3 3	227	+ 257	7 5 3	118	+ 105
5 2 2	177	+ 226	1.13.2	101	- 81	9 6 2	53	+ 36	6 4 3	224	- 341	7 6 3	85	- 90
5 3 2	172	- 208	2 0 2	88	- 116	9 7 2	67	- 52	6 5 3	58	- 65	7 7 3	169	- 155
5 4 2	113	- 120	2 2 2	60	- 64	9 8 2	213	- 195	6 6 3	370	+ 347	8 0 3	73	- 37
5 5 2	104	+ 85	2 3 2	118	+ 125	10.0.2	101	+ 119	6 7 3	117	+ 93	8 1 3	118	- 111
5 6 2	182	- 164	2 4 2	415	+ 505	10.1.2	105	+ 100	6 8 3	60	+ 80	8 2 3	158	+ 171
5 7 2	118	+ 110	2 4 2	88	+ 39	10.2.2	341	+ 328	7 2 3	69	- 50	8 6 3	96	+ 65
5 8 2	249	+ 238	2 6 2	387	- 402	10.3.2	41	- 38	7 3 3	99	+ 110	9 1 3	217	+ 210
5 9 2	62	+ 52	2 7 2	63	+ 59	10.4.2	169	- 153	7 4 3	36	+ 1	9 2 3	192	- 171
5.10.2	133	+ 108	2 8 2	144	+ 113	10.5.2	316	+ 283	7 5 3	108	+ 95			
5.11.2	199	- 194	2 9 2	63	+ 70	10.6.2	28	+ 28	7 6 3	227	+ 234	0 1 4	179	+ 285
5.12.2	88	- 90	2.10.2	85	+ 53	10.7.2	59	- 30	7 7 3	256	+ 60	0 2 4	26	- 38
6 0 2	108	+ 97	2.11.2	41	- 31	10.8.2	79	- 44	8 0 3	87	- 63	0 3 4	128	- 163
6 1 2	137	- 147	2.12.2	31	+ 28	11.1.2	140	+ 132	8 1 3	288	- 325	0 4 4	45	- 24
6 2 2	250	+ 298	2.13.2	142	- 140	11.2.2	46	+ 21	8 2 3	46	- 32	0 6 4	42	+ 48
6 4 2	236	- 250	3 1 2	150	- 182	11.3.2	191	- 156	8 3 3	115	- 116	0 7 4	109	- 118
6 5 2	285	- 291	3 2 2	73	+ 74	11.4.2	201	- 173	8 4 3	92	+ 89	1 1 4	135	+ 290
6 6 2	97	+ 78	3 3 2	49	+ 44	11.6.2	249	- 219	8 5 3	164	- 128	1 2 4	138	- 161
6 8 2	155	- 127	3 4 2	67	+ 69	12.0.2	212	+ 175	8 6 3	50	+ 51	1 3 4	91	- 90
6 9 2	76	- 57	3 5 2	86	+ 106	12.2.2	22	- 12	8 7 3	26	- 46	1 4 4	54	+ 55
6.10.2	41	- 56	3 6 2	349	+ 386	12.3.2	96	- 88	9 1 3	63	- 102	2 2 4	104	+ 140
6.11.2	99	+ 85	3 7 2	173	+ 174				9 3 3	126	+ 121	2 3 4	165	- 200
7 1 2	81	+ 69	3.10.2	105	- 91	0 0 3	181	+ 432	9 4 3	122	- 96	2 4 4	112	- 152
7 2 2	195	- 229	3.11.2	347	+ 359	0 1 3	100	+ 177	1 2 3	145	+ 171	2 5 4	69	+ 64
7 3 2	146	- 163	3.12.2	228	- 193	0 3 3	76	- 79	1 3 3	141	+ 148	2 6 4	22	+ 24
7 4 2	210	+ 217	3.13.2	59	+ 54	0 4 3	85	- 56	1 4 3	64	+ 75	3 1 4	41	- 57
7 5 2	133	+ 141	4 0 2	273	+ 345	0 5 3	142	+ 127	1 5 3	79	- 62	3 3 4	101	+ 127
7 6 2	315	+ 307	4 1 2	320	- 420	0 6 3	38	+ 50	1 6 3	88	- 71	3 4 4	106	+ 171
7 7 2	87	+ 86	4 2 2	50	+ 40	0 7 3	245	- 220	1 7 3	146	- 136	3 5 4	47	+ 70
7 8 2	223	- 237	4 4 2	71	+ 78	0 8 3	169	+ 136	1 8 3	262	+ 289	4 0 4	46	- 67
7 9 2	33	+ 40	4 5 2	100	+ 100	0 9 3	96	+ 82	1 9 3	64	- 46	4 1 4	31	+ 50
7.11.2	31	- 17	4 6 2	97	- 87	1 1 3	87	- 78	1.10.3	39	- 34	4 2 4	124	+ 169
8 0 2	73	- 74	4 7 2	68	+ 59	1 2 3	64	+ 41	2 0 3	96	+ 96	4 3 4	77	+ 80
8 1 2	154	- 154	4 9 2	374	- 389	1 3 3	224	- 210	2 1 3	13	+ 14	5 1 4	131	- 189
8 2 2	176	+ 163	4.10.2	137	- 125	1 4 3	22	+ 38	2 2 3	122	- 151	5 2 4	106	+ 158
8 3 2	301	+ 309	4.11.2	238	+ 227	1 5 3	99	- 41	2 3 3	112	- 140	5 3 4	47	- 48
8 4 2	149	+ 149	5 1 2	59	+ 106	1 6 3	36	- 16	2 4 3	222	+ 266	1 2 4	71	+ 97
8 5 2	53	+ 20	5 4 2	33	- 23	1 7 3	332	+ 352	2 5 3	261	- 297	1 3 4	28	+ 39
8 7 2	347	+ 353	5 5 2	99	- 94	1 8 3	201	+ 192	2 6 3	228	- 236	1 4 4	64	- 96
8 8 2	162	- 141	5 6 2	163	+ 148	1 9 3	153	+ 190	2 7 3	44	- 80	1 5 4	41	+ 55
8 9 2	274	- 265	5 7 2	42	+ 45	1.10.3	245	- 249	2 8 3	36	+ 17	1 6 4	88	- 125
8.10.2	63	+ 52	5 8 2	41	+ 35	2 0 3	119	- 143	2 9 3	76	+ 63	2 1 4	31	+ 30
9 1 2	299	- 340	5 9 2	81	- 82	2 1 3	46	- 59	2.10.3	28	- 39	2 2 4	54	- 96
9 3 2	200	+ 228	5.10.2	133	+ 122	2 2 3	117	+ 140	3 2 3	247	- 347	2 3 4	38	+ 58
9 4 2	92	- 93	5.11.2	197	- 199	2 3 3	186	- 173	3 3 3	164	+ 265	2 4 4	146	+ 211
9 5 2	50	+ 41	5.12.2	185	- 166	2 4 3	236	- 93	3 4 3	45	+ 61	2 5 4	196	+ 358
9 7 2	41	- 64	6 1 2	79	- 75	2 6 3	73	+ 38	3 5 3	136	+ 157	2 6 4	99	- 132
9 8 2	41	- 20	6 3 2	83	+ 78	2 7 3	162	- 143	3 6 3	169	- 178	3 2 4	53	- 92
9 9 2	158	+ 120	6 4 2	314	- 325	2 8 3	42	- 39	3 7 3	79	- 88	3 3 4	96	+ 174
10.0.2	217	+ 217	6 5 2	483	- 544	2.10.3	132	+ 114	4 0 3	67	+ 56	3 4 4	28	- 60
10.1.2	73	- 71	6 6 2	364	+ 361	3 1 3	64	- 38	4 1 3	144	- 172	3 5 4	33	- 42
10.2.2	185	- 178	6 8 2	95	+ 69	3 2 3	190	- 247	4 2 3	210	- 277	4 0 4	227	+ 385
10.3.2	236	+ 238	6.11.2	183	+ 164	3 3 3	36	+ 9	4 3 3	74	+ 83	4 1 4	68	- 94
10.4.2	69	+ 52	7 1 2	88	- 83	3 4 3	110	- 76	4 4 3	145	+ 111	4 2 4	45	- 47
10.5.2	213	- 195	7 2 2	90	+ 105	3 5 3	82	+ 142	4 7 3	181	+ 174	5 1 4	46	- 87
10.6.2	96	+ 83	7 3 2	240	+ 256	3 6 3	115	- 103	4 8 3	296	+ 333	5 2 4	63	- 82
10.7.2	181	+ 156	7 4 2	131	- 111	3 7 3	106	- 110	4 9 3	212	- 206	5 3 4	87	- 112
10.8.2	205	+ 157	7 5 2	196	+ 183	3 8 3	73	- 73	5 1 3	146	+ 166			
11.1.2	241	+ 228	7 6 2	88	- 81	3 9 3	53	+ 56	5 2 3	41	+ 58			
11.3.2	101	+ 79	7 7 2	126	- 117	4 0 3	213	- 273	5 3 3	199	- 207			

