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THE ATOMIC ARRANGEMENT AND CHEMICAL COMPOSITION OF KRENNERITE¹

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ABSTRACT

The crystal structure of krennerite has been analyzed by means of Weissenberg photographs and powder diffraction photographs. The dimensions of the unit cell, all determined röntgenographically, are $a_0=16.54 \text{ \AA}$, $b_0=8.82 \text{ \AA}$, $c_0=4.46 \text{ \AA}$, all $\pm 0.03 \text{ \AA}$. The density determined pycnometrically on five single crystals from Cripple Creek, Colorado, crushed into fragments is 8.63; the x -ray density is 8.86. The unit cell contains 8(Au, Ag) Te₂; the ratio of Au to Ag was found by analyses of crystals from Cripple Creek to be close to 4 to 1. The space-group is C_{2v}^4-Pma . The eighteen parameters defining the atomic positions were determined by calculation of the intensities of the diffraction lines of a powder photograph (which had been rigorously indexed from the single crystal data), and of the diffraction spots of Weissenberg equator photographs of crystals rotating about the c - and b -axes; the positions of the atoms were confirmed by a Fourier projection of the structure on the plane 001 made from a Weissenberg equator photograph taken with the crystal rotating about the c -axis. The gold (or silver) atoms are situated in (a) with $z=0$ (arbitrary), in (c) with $y_1=0.319$, $z_1=0.014$, and in (d) with $x_2=0.124$, $y_2=0.666$, $z_2=0.500$; the tellurium atoms are situated in (c) with $y_3=0.018$, $z_3=0.042$ and $y_4=0.617$, $z_4=0.042$ and in (d) with $x_5=0.003$, $y_5=0.699$, $z_5=0.042$, and $x_6=0.132$, $y_6=0.364$, $z_6=0.500$, and $x_7=0.119$, $y_7=0.964$, $z_7=0.500$. Each gold (or silver) atom is surrounded by six tellurium atoms, and each tellurium atom is surrounded by three gold (or silver) atoms and three tellurium atoms, or by five gold (or silver) atoms and one tellurium atom, or by one gold (or silver) atom and five tellurium atoms.

INTRODUCTION

The atomic arrangement of krennerite has been determined in the present investigation⁴ by x -ray analysis of euhedral crystals from Cripple Creek, Colorado. The crystals had a metallic luster and pale yellowish white color; their identity was confirmed by measurement on the two-

¹ A report on research carried out under the auspices of the Geophysical Laboratory of the Carnegie Institution of Washington, the U. S. Geological Survey, and the Office of Naval Research. Published by permission of the Director of the U. S. Geological Survey.

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⁴ The work of the senior author was carried out mainly at the Geophysical Laboratory of the Carnegie Institution of Washington while he was a member of the staff.

circle reflection goniometer. Euhedral crystals of krennerite have been measured previously with the reflection goniometer by Krenner,⁵ vom Rath,⁶ Schrauf,⁷ Miers,⁸ and Smith.⁹ They found the symmetry of the crystals to be that of the orthorhombic system. The values of the axial elements calculated by the various authors are given in Table 1. Krenner did not calculate axial elements, but his indices and angles imply the same choice of axes, unit forms, and orientation as that of vom Rath. Schrauf and Smith followed vom Rath's choice of axes and unit forms.

TABLE 1. AXIAL ELEMENTS OF KRENNERITE DETERMINED BY PREVIOUS INVESTIGATORS

	<i>a</i>	<i>b</i>	<i>c</i>
vom Rath	0.9407	1	0.5045
Schrauf	0.9396	1	0.5073
Miers*	0.9389	1	0.5059
Smith	0.9369	1	0.5068

* Miers' values are here recalculated to conform with the orientation of vom Rath, Schrauf, and Smith.

Miers followed vom Rath's choice of unit forms, but interchanged the *a*- and *b*-axes. The present *x*-ray analysis leads to unit cell dimensions from which the following axial elements have been calculated

$$a:b:c=1.875:1:0.506,$$

and these agree well with the morphological elements if the value of *a* in the morphological elements be multiplied by 2. Thus the following transformation is obtained:

vom Rath to Tunell and Murata 200/010/001.

Rotation and Weissenberg equator and equi-inclination layer-line photographs of krennerite were made with crystals rotating about the *a*- and *c*-axes and rotation and Weissenberg equator photographs with a crystal rotating about the *b*-axis. Copper K-radiation was used. Powder photographs were made with filtered cobalt K-radiation and with filtered and unfiltered copper K-radiation. A crystal¹⁰ from Cripple Creek measured previously on the two-circle reflection goniometer by Professor M. A. Peacock, was rotated about the *c*-axis and a rotation photograph was made. It was then oscillated 180° about the *c*-axis and equator and

⁵ Krenner, J. A.: *Ann. d. Phys. u. Chem.*, **1**, 636-640 (1877).

⁶ vom Rath, G.: *Z. Kryst. Mineral.*, **1**, 614-617 (1877).

⁷ Schrauf, A.: *Z. Kryst. Mineral.*, **2**, 235-239 (1878).

⁸ Miers, H. A.: *Mineralog. Mag.*, **9**, 184-186 (1890).

⁹ Smith, G. F. H.: *Mineralog. Mag.*, **13**, 264-267 (1903).

¹⁰ Kindly supplied by Professors Palache and Peacock.

equi-inclination layer-line Weissenberg photographs were made. The crystal was developed prismatically and terminated by a cleavage face 001; it was roughly rectangular in cross-section with dimensions 0.36 mm. and 0.60 mm. in the plane 001. A second crystal from Cripple Creek, also measured previously on the two-circle reflection goniometer by Professor Peacock, was rotated about the *c*-axis and an equator Weissenberg photograph was made. This crystal was then remounted and rotated about the *b*-axis and a rotation photograph and an equator Weissenberg photograph were made. It was remounted again and rotated about the *a*-axis and a rotation photograph and Weissenberg equator and equi-inclination layer-line photographs were made. This crystal was bounded by a large basal cleavage at one end of the *c*-axis and predominantly by large faces of the pyramid *u* at the other end of the *c*-axis; the prism *l* was dominant in the vertical zone. The approximate dimensions of the crystal in the *a*-, *b*-, and *c*-directions were 0.90 mm., 0.90 mm., and 0.50 mm. A crystal¹¹ from the Vindicator Mine, Cripple Creek, Colorado (U. S. National Museum No. 96647), measured on the two-circle reflection goniometer by Tunell was oscillated 180° around the *c*-axis and Weissenberg equator and equi-inclination layer-line photographs were made. This crystal was elongated parallel to the *c*-axis and the diameters of its cross-section were approximately 0.04 mm. and 0.08 mm. Powder photographs were made with unfiltered copper K-radiation of one of the crystals supplied by Professors Palache and Peacock. A powder photograph was made with filtered copper K-radiation of crystals from the Vindicator Mine (U. S. National Museum No. 96647). A powder photograph of euhedral crystals from the Moose Mine, Cripple Creek, Colorado, was made with filtered cobalt K-radiation.

CHEMICAL COMPOSITION AND DENSITY

No complete chemical analysis or determination of the density of crystallographically studied krennerite free from admixed impurities had been made previously. Five euhedral crystals of krennerite from the Moose Mine were therefore freed from adhering gangue in order to obtain these data. One of these crystals had been measured on the two-circle reflection goniometer; the other four had been observed to have exactly the same habit. A few very minute crystals of pyrite attached to these krennerite crystals could not be completely removed since they were partly embedded in the krennerite crystals; the pyrite left in the sample was believed to be insignificant in amount, however, and this was confirmed by the analysis which shows only 0.05 per cent of iron.

The density of the five crystals (total weight of crystals, 0.9476 g.)

¹¹ Kindly lent by Dr. W. F. Foshag of the U. S. National Museum.

was measured by means of the pycnometer described by Johnston and Adams.¹² Since krennerite characteristically shows minute voids under the binocular microscope on cleavage surfaces, the crystals were crushed and their density was measured with specially purified toluene as pycnometer fluid, the pycnometer being filled under reduced pressure to promote entrance of the fluid into the voids. All weights were reduced to a vacuum. The value of the density found, corrected for the 0.05 per cent of iron present as pyrite, is 8.63.

The crushed sample was analyzed by the following method. It was dissolved in a minimum amount of aqua regia; the resulting solution

TABLE 2. ANALYSIS OF KRENNERITE FROM MOOSE MINE,
CRIPPLE CREEK, COLORADO

	Per Cent	Atomic Ratios
Au	36.19	0.1835
Ag	4.87	0.0451
Te	58.50	0.4584
Fe*	.05	0.4584 or 2.005
Insoluble	.09	
	99.70	

* The iron was derived from a small amount of pyrite that was present as a contaminant.

was diluted until its acidity was about one normal and allowed to stand overnight. Throughout the analysis a record was kept of the amounts of acids used so that rough adjustments of the acidity could readily be made.

Silver chloride, together with any residue unattacked by aqua regia, was caught and weighed on a sintered glass filtering crucible. Its correct weight was obtained by dissolving it from the crucible with warm dilute ammonium hydroxide and reweighing, and the amount of insoluble residue was obtained by subtracting from this second weight the known weight of the crucible itself.

The filtrate containing gold, tellurium, and other constituents was digested on the steam bath with hydrochloric acid to free it from nitric acid. Gold and tellurium were precipitated together in a hot solution, which was about three-normal with respect to hydrochloric acid, by means of sulphurous acid and hydrazine, as described by Lenher and Homberger.¹³ The precipitate was washed as rapidly as possible with a

¹² Johnston, J., and Adams, L. H.: *Jour. Am. Chem. Soc.*, **34**, 566-568 (1912).

¹³ Lenher, Victor, and Homberger, A. W.: *Jour. Am. Chem. Soc.*, **30**, 387-391 (1908).

very dilute solution of sulphurous acid until free from chloride. It was treated in a beaker with a minimum amount of cold dilute nitric acid to dissolve tellurium, leaving gold to be filtered off, ignited, and weighed.

The nitric acid solution of tellurium was evaporated to dryness on the steam bath and then digested with dilute hydrochloric acid. The element was reprecipitated as before in three-normal hydrochloric acid solution, caught, and weighed on a sintered glass crucible. The filtrate from this precipitation was reduced in volume and treated further with sulphurous acid to recover any tellurium that passed through the filter. The final filtrate was added to that from the combined precipitate of gold and tellurium, treated with nitric acid, and placed on the steam bath to evaporate. The difficulty arising from the tendency of precipitated tellurium to oxidize and pass through the filter might perhaps be overcome by determining the small amounts found in the filtrate by a colorimetric method like that described by Pierson.¹⁴

The filtrate from the combined precipitate of gold and tellurium was evaporated to dryness on the steam bath. The small amounts of silver chloride and tellurous acid, which were apparent in the evaporated residue, were determined after separation by means of dilute nitric acid. The filtrate from the final recovery of tellurium was reduced to a small volume, boiled with a few drops of nitric acid, and iron precipitated with ammonium hydroxide, to be subsequently estimated as the thiocyanate. The ammoniacal filtrate from the separation of iron gave no precipitate upon being treated with hydrogen sulphide.

A partial analysis of krennerite crystals from a different specimen from Cripple Creek (U. S. National Museum No. 96647) was also made (weight of sample 0.1678 g.). One crystal from this specimen had been measured on the two-circle reflection goniometer. The crystals analyzed were hand-picked under the binocular microscope and identified by the perfect cleavage perpendicular to the striated zone. The sample was believed to be very pure and this was confirmed by the analysis, no iron or insoluble impurity being found.

The values of the atomic ratio of gold to silver determined by us, namely, 4.07:1 and 3.56:1, are rather close to that obtained by Sipöcz¹⁵ for krennerite from Săcărâmbu (Nagy-Ág), namely, 3.26:1. Sipöcz also determined the densities of two samples of krennerite from Săcărâmbu (Nagy-Ág) to be 8.63 and 8.18. The analysis of Sipöcz shows that his material contained the following percentages of impurities: quartz 2.29, copper 0.33, iron 0.58, antimony 0.64; hence it is not surprising that while one of his density values agrees with ours the other is considerably too

¹⁴ Pierson, G. G.: *Ind. Eng. Chem., Anal. Ed.*, **6**, 437-439 (1934).

¹⁵ Sipöcz, L.: *Math. és Term. Tud. Köz.*, **20**, 174-176 (1885).

low. The incomplete analysis of krennerite from Cripple Creek made by Myers¹⁶ yielded only 0.45 per cent of silver. Since our two analyses of krennerite from different mines in the Cripple Creek district and the analysis of Sipöcz of krennerite from Săcărâmbu (Nagy-Ág) all yielded a silver content of approximately 5 per cent, the existence of krennerite at Cripple Creek of such low silver content seems doubtful.

TABLE 3. ANALYSIS OF KRENNERITE FROM VINDICATOR MINE,
CRIPPLE CREEK, COLORADO
(U. S. National Museum No. 96647)

	Per Cent
Au	35.1
Ag	5.4
Te	Not determined
Fe	None
Insoluble	None

DETERMINATION OF THE UNIT CELL AND SPACE-GROUP

The dimensions of the structural unit cell, all determined by purely röntgenographic measurements, are $a_0 = 16.54 \text{ \AA}$, $b_0 = 8.82 \text{ \AA}$, $c_0 = 4.46 \text{ \AA}$, all $\pm 0.03 \text{ \AA}$.¹⁷ The volume of the unit cell is accordingly 650.6 \AA^3 . The density computed from the x -ray measurements with use of the average of our two chemical analyses of krennerite from Cripple Creek is 8.86 .¹⁸ This is in reasonable agreement with the density determined by us with the pycnometer, namely, 8.63 , and establishes the content of the unit cell as $8(\text{Au,Ag})\text{Te}_2$.

Diffraction effects were obtained on the Weissenberg photographs from the following planes: $g00$, $0u0$, $0g0$, $00u$, $00g$, $0uu$, $0ug$, $0gu$, $0gg$, $g0u$, $g0g$, $uu0$, $ug0$, $gu0$, $gg0$, uuu , uug , ugu , ugg , guu , gug , ggu , ggg , where u denotes any odd number and g denotes any even number. No diffraction effects were obtained from the following: $u00$, $u0u$, $u0g$, although representatives of each were in a position to diffract. Thus krennerite belongs to one of

¹⁶ Myers, W. S., (in) Chester, A. H.: *Am. Jour. Sci.*, (4) 5, 376 (1898).

¹⁷ Based on the wave-lengths: copper $K\alpha_1$, $\lambda = 1.5405 \text{ \AA}$, copper $K\alpha_2$, $\lambda = 1.5443 \text{ \AA}$; copper $K\beta_1$, $\lambda = 1.3922 \text{ \AA}$. (In a preliminary report on the crystal structure of krennerite by Tunell and Ksanda (*Jour. Wash. Acad. Sci.*, 26, 507-509 (1936)), the dimensions of the unit cell were given in kX units.)

¹⁸ The density ρ was calculated by the use of the equation

$$\rho = 1.660 \Sigma A / V,$$

where ΣA is the sum of the atomic weights of the atoms in the unit cell and V is the volume of the unit cell in \AA^3 .

the following space-groups: C_{2v}^2 - $P2am$, C_{2v}^4 - Pma , D_{2h}^5 - $Pmam$; which are characterized by the absence of diffraction effects from $u00$, $u0u$, $u0g$, owing to the presence of a glide plane parallel to 010 with a glide component of $a/2$.

DETERMINATION OF THE ATOMIC ARRANGEMENT

In his morphologic study of sylvanite and krennerite Schrauf¹⁹ noted that the angles in one zone of sylvanite including its cleavage are closely similar to the angles in one zone of krennerite including its cleavage. The angles²⁰ in these zones are as follows according to Schrauf:

Sylvanite $mt=31^\circ 38'$, $mr=42^\circ 44'$, $ms=61^\circ 35'$, m : cleavage= 90° ,
 Krennerite $ar=31^\circ 41'$, $ap=42^\circ 48'$, $ah=61^\circ 38'$, a : cleavage= 90° ;

the forms in Schrauf's table have the following indices referred to the sylvanite axes of Tunell²¹ and the krennerite axes of Tunell and Murata:

Sylvanite m -{001}, t -{013}, r -{012}, s -{011}, and
 Krennerite a -{100}, r -{601}, ρ -{401}, h -{201}.

X-ray measurements by the authors have confirmed this analogy and shown that it is even closer than Schrauf supposed. Thus the spacing of the cleavage plane of sylvanite is $d_{010}=4.49 \text{ \AA}$ ²² and that of the cleavage plane of krennerite is $d_{001}=4.46 \text{ \AA}$. The plane 001 of sylvanite has the spacing $d_{001}=8.30 \text{ \AA}$; Schrauf showed that the analogous plane of krennerite is 100, and we have found that the spacing $d_{100}=16.54 \text{ \AA}$, very nearly twice the spacing of the plane 001 of sylvanite. The a -axis of sylvanite has an identity period $a_0=8.96 \text{ \AA}$, and the analogous direction of krennerite, the b -axis, has an identity period $b_0=8.82 \text{ \AA}$. Moreover, the intensities of the diffraction effects from the analogous pairs of planes 001 of sylvanite and 100 of krennerite, and 010 of sylvanite and 001 of krennerite are similar, as shown in Table 4. These facts strongly suggest a basic similarity in the structures of the two minerals. The structure of sylvanite can be described as consisting of lines of atoms parallel to the a -axis lying alternately in or near the plane $y=0$ and near the plane $y=\frac{1}{2}$. Along these lines the gold (or silver) atoms are separated by pairs of tellurium atoms. Similar lines of atoms should therefore exist in krennerite parallel to the b -axis and should lie alternately in or near the plane

¹⁹ Schrauf, A.: *Z. Kryst. Mineral.*, **2**, 209-252 (1878).

²⁰ G. F. H. Smith found for these angles of krennerite $ar=31^\circ 38\frac{1}{2}'$, $ap=42^\circ 45'$, $ah=61^\circ 35\frac{1}{2}'$, thus confirming the close similarity with the angles mt , mr , and ms of sylvanite. *Mineralog. Mag.* **13**, 267 (1903).

²¹ Tunell, George: *Am. Mineral.*, **26**, 457-477 (1941).

²² The dimensions of the unit cell of sylvanite reported by Tunell (op. cit.) were in kX units, although they were given in \AA units in accordance with custom at that time.

$z=0$ and in or near the plane $z=\frac{1}{2}$. Such a structure for krennerite would be possible in the space-groups C_{2v}^2-P2am and D_{2h}^5-Pmam only if the atoms lay exactly in the planes $z=0$ and $z=\frac{1}{2}$. The planes $z=0$ and $z=\frac{1}{2}$

TABLE 4. COMPARISON OF INTENSITIES OF ANALOGOUS PLANES IN SYLVANITE AND KRENNERITE

Sylvanite				Krennerite			
<i>hkl</i>	Spacing	Intensity	Cu K-Radiation	<i>hkl</i>	Spacing	Intensity	Cu K-Radiation
001	8.30 Å	0	$\alpha_1+\alpha_2$	100	16.54 Å	0	$\alpha_1+\alpha_2$
				200	8.27	0	$\alpha_1+\alpha_2$
002	4.15	0	$\alpha_1+\alpha_2$	300	5.51	0	$\alpha_1+\alpha_2$
				400	4.14	0	$\alpha_1+\alpha_2$
003	2.77	0	$\alpha_1+\alpha_2$	500	3.31	0	$\alpha_1+\alpha_2$
				600	2.76	0	$\alpha_1+\alpha_2$
004	2.08	s	$\alpha_1+\alpha_2$	700	2.36	0	$\alpha_1+\alpha_2$
				800	2.07	s	$\alpha_1+\alpha_2$
005	1.66	0	$\alpha_1+\alpha_2$	900	1.84	0	$\alpha_1+\alpha_2$
				10.0.0	1.65	0	$\alpha_1+\alpha_2$
006	1.38	0	$\alpha_1+\alpha_2$	11.0.0	1.50	0	$\alpha_1+\alpha_2$
				12.0.0	1.38	0	$\alpha_1+\alpha_2$
007	1.19	0	$\alpha_1+\alpha_2$	13.0.0	1.27	0	$\alpha_1+\alpha_2$
				14.0.0	1.18	0	$\alpha_1+\alpha_2$
008	1.04	m	α_1	15.0.0	1.10	0	$\alpha_1+\alpha_2$
				16.0.0	1.03	m	$\alpha_1+\alpha_2$
009	0.92	0	α_1	17.0.0	0.97	0	$\alpha_1+\alpha_2$
				18.0.0	0.92	0	α_1
0.0.10	0.83	w	α_1	19.0.0	0.87	0	α_1
				20.0.0	0.83	w	α_1
010	4.49	w	$\alpha_1+\alpha_2$	001	4.46	w	$\alpha_1+\alpha_2$
020	2.25	s	$\alpha_1+\alpha_2$	002	2.23	s	$\alpha_1+\alpha_2$
030	1.49	m	$\alpha_1+\alpha_2$	003	1.49	m	$\alpha_1+\alpha_2$
040	1.12	w	$\alpha_1+\alpha_2$	004	1.11	m	$\alpha_1+\alpha_2$
050	0.90	m	α_1	005	0.89	w	α_1

are reflection planes in these space-groups and a slight displacement of any atom from one of the planes $z=0$ or $z=\frac{1}{2}$ would require the presence of an additional atom on the other side of the reflection plane. If the atoms were situated in the planes $z=0$ and $z=\frac{1}{2}$ in a structure of this type no odd order reflections should be present from the plane 001. Such reflections are present, however, and therefore the space-groups C_{2v}^2-P2am and D_{2h}^5-Pmam may be left out of consideration.

Such a structure differs from that of sylvanite in one respect: in sylvanite the gold (or silver) atoms lie in a single series of parallel planes that are perpendicular to 010 and parallel to the c -axis; in krennerite the gold (or silver) atoms do not lie in a series of parallel planes but instead lie in or near a series of corrugated sheets. These corrugated sheets are made up of two sets of parallel planes, both sets perpendicular to 001

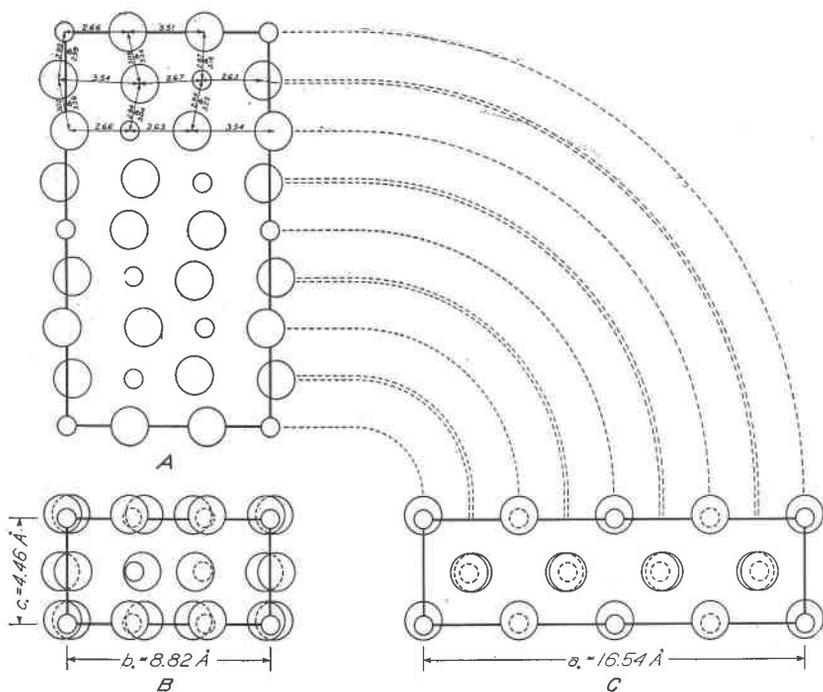


FIG. 1. Orthographic projections of the unit cell of krennerite. *A*. Top view. *B*. Front view. *C*. Side view. Small circles—gold (or silver) atoms. Large circles—tellurium atoms.

and inclined at an angle of 35° to the b -axis, one set lying in the angle between the positive end of the b -axis and the positive end of the a -axis and the other set lying in the angle between the positive end of the b -axis and the negative end of the a -axis. The corrugation of the sheets of gold (or silver) atoms is caused by the presence of the reflection planes $x = \frac{1}{4}$ and $x = \frac{3}{4}$. The zigzag pattern of the corrugated sheets is clearly evident in projection in Fig. 1*A* and Fig. 3.

There are eight gold (or silver) and sixteen tellurium atoms to be located in the unit cell. The space-group C_{2v}^4-Pma furnishes the following sets of equivalent positions:

(a) $00z$; $\frac{1}{2}0z$, (b) $0\frac{1}{2}z$; $\frac{1}{2}\frac{1}{2}z$, (c) $\frac{1}{2}yz$; $\frac{3}{4}yz$, (d) xyz ; $\bar{x}yz$; $\frac{1}{2}-x, y, z$; $\frac{1}{2}+x, y, z$,²³

of which (a) and (b) have the symmetry C_2-2 , (c) the symmetry C_s-m , and (d) the symmetry C_1-1 . In krennerite gold (or silver) atoms are situated in (a) with $z=0$ (arbitrary), in (c) with $y_1=0.319$, $z_1=0.014$, and

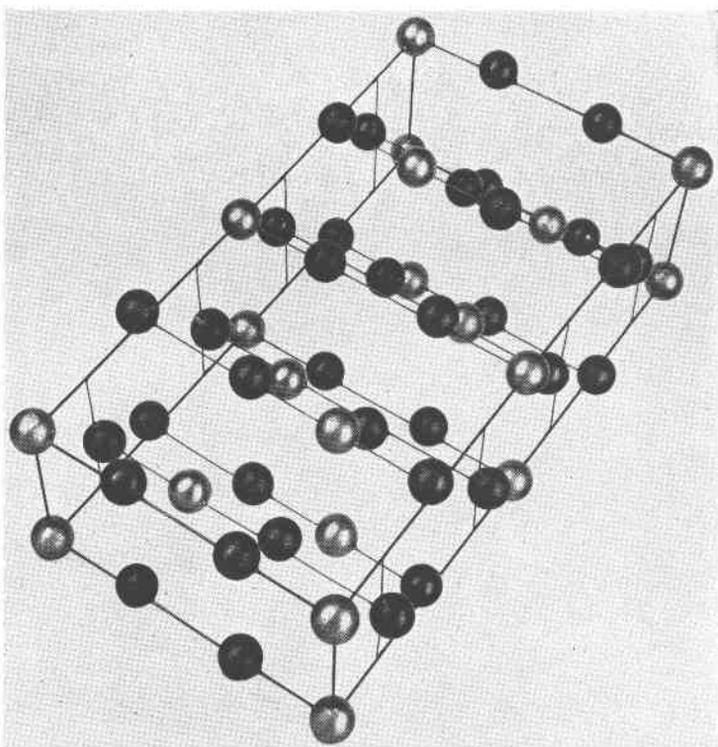


FIG. 2. Model showing the arrangement of the atoms in krennerite. The parallelepiped represented by the outside wires is the unit cell. The longest edge represents the a -axis, the edge intermediate in length represents the b -axis, the shortest edge represents the c -axis. The grey spheres represent gold (or silver) atoms; the black spheres represent tellurium atoms.

in (d) with $x_2=0.124$, $y_2=0.666$, $z_2=0.500$; tellurium atoms are situated in (c) with $y_3=0.018$, $z_3=0.042$, and $y_4=0.617$, $z_4=0.042$ and in (d) with $x_5=0.003$, $y_5=0.699$, $z_5=0.042$, and $x_6=0.132$, $y_6=0.364$, $z_6=0.500$, and $x_7=0.119$, $y_7=0.964$, $z_7=0.500$. Orthographic projections of this struc-

²³ As is customary, x denotes an atomic coordinate along the a -axis expressed as a fraction of a_0 ; y denotes an atomic coordinate along the b -axis expressed as a fraction of b_0 ; z denotes an atomic coordinate along the c -axis expressed as a fraction of c_0 .

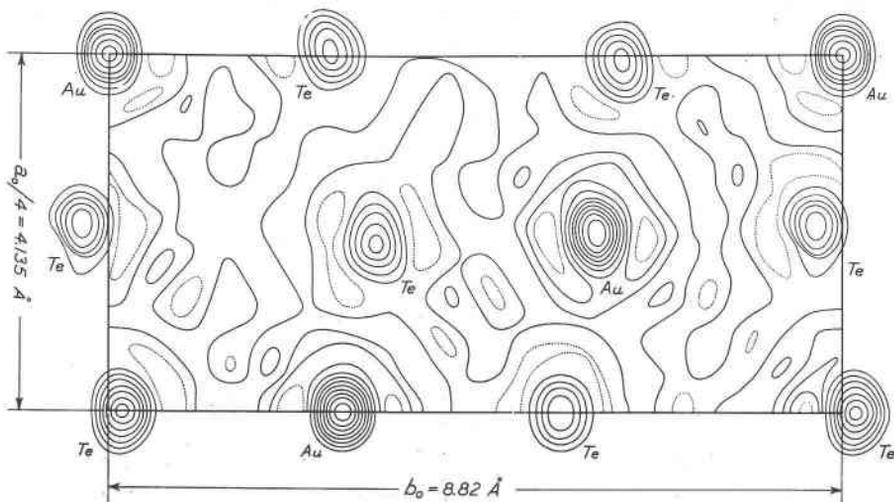


FIG. 3. Fourier projection along the c -axis of the structure of krennerite. The contour map within the rectangle represents the projection on the plane 001 of one-fourth of the unit cell. The peaks lettered Au represent gold (or silver) atoms; those lettered Te represent tellurium atoms. Dotted lines are depression contours. The origin is in the upper left-hand corner of the rectangle. The positive direction of the a -axis is from top to bottom of the drawing; the positive direction of the b -axis is from left to right; the positive direction of the c -axis (which is perpendicular to the plane of the paper) is upward from the plane of the paper.

ture are given in Fig. 1, and a model of the structure is shown in Fig. 2. The intensities calculated from this structure are compared with those observed in Tables 5, 6 and 7. Table 5 contains the observed and calculated intensities of diffraction lines in a powder photograph taken with Co K-radiation filtered through iron foil. The indexing of the powder photograph was carried out rigorously by use of the unit cell dimensions obtained from the single crystal Weissenberg photographs. Table 5 lists in decreasing order the calculated and observed spacings and intensities of all planes the spacings of which are greater than 1.28 Å, together with the observed spacings and intensities of the remaining lines of the powder photographs. The intensities I_p of the lines on the powder diffraction film taken with filtered radiation were calculated from the formula

$$I_p = \frac{1 + \cos^2 2\theta}{\sin 2\theta \sin \theta} j |F|^2,$$

where 2θ denotes the angle between the incident and diffracted beams, F the structure factor, and j the number of cooperating planes. On the powder photograph the α_1 and α_2 lines were not resolved. Tables 6 and 7 contain the observed and calculated intensities of diffraction spots in

TABLE 5. RELATIVE INTENSITIES* OF THE X-RAY DIFFRACTION LINES OF KRENNERITE FROM A POWDER PHOTOGRAPH TAKEN WITH FILTERED COBALT K-RADIATION

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
100	16.54 Å	0.00		
010	8.82	.03		
200	8.27	.00		
110	7.79	.02		
210	6.04	.61	6.08 Å	$\frac{1}{2}$
300	5.51	.00		
310	4.69	.68	4.69	1
001	4.46	.10	4.47	$\frac{1}{2}$
020	4.41	.00		
101	4.31	.00		
120	4.26	.01		
400	4.14	.00		
011	3.98	.18		
201	3.93	.00	3.94	2
220	3.89	.00		
111	3.87	.55	3.88	2
410	3.75	.14		
211	3.59	.15		
301	3.47	.00		
320	3.44	.00		
500	3.31	.00		
311	3.23	.02		
021	3.14	.00		
510	3.10	.09		
121	3.08	.02		
401	3.03	10.00		
420	3.02	.00	3.03	10
030	2.94	3.62		
221	2.93	.03	2.94	6
130	2.89	.04		
411	2.87	.02		
230	2.76	.00		
600	2.76	.00		
321	2.73	.00		
501	2.66	.00		
520	2.65	.02		
610	2.63	.00		
330	2.59	.01		
511	2.54	.00		
421	2.50	.00		
031	2.45	.03		
131	2.43	.04		
430	2.39	.00		

TABLE 5—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
700	2.36	.00		
231	2.35	.00		
601	2.35	.00	2.35	$\frac{1}{2}$
620	2.34	.02		
710	2.28	.01		
521	2.28	.01		
611	2.27	.19		
331	2.24	.07		
002	2.23	1.97	2.23	5
102	2.21	.00		
040	2.20	.00		
530	2.19	.02		
140	2.18	.00		
012	2.16	.00	2.16	1
202	2.15	.00		
112	2.14	.00		
240	2.13	.14		
431	2.11	5.42	2.11	7
212	2.09	.09		
701	2.09	.00		
720	2.08	.00		
621	2.07	.02		
800	2.07	1.59	2.07	4
302	2.07	.00		
340	2.04	.39		
711	2.03	.21		
810	2.01	.00		
312	2.01	.15	2.01	1
630	2.00	.00		
022	1.99	.00		
041	1.98	.23		
122	1.98	.01		
531	1.97	.01	1.97	2
402	1.96	.08		
141	1.96	.57		
440	1.94	.21		
222	1.93	.04		
241	1.92	.10		
412	1.92	.05	1.92	2
721	1.89	.00		
801	1.88	.02		
322	1.87	.00		
820	1.87	.00		
341	1.86	.01		

TABLE 5—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
502	1.85	.00		
900	1.84	.00		
730	1.84	.03		
811	1.84	.04	1.84	1
631	1.83	.00		
540	1.83	.24		
512	1.81	.04		
910	1.80	.00		
422	1.79	.00		
441	1.78	.00		
032	1.78	1.52	1.78	4
132	1.77	.02		
050	1.76	.00		
150	1.75	.00		
232	1.74	.00		
602	1.73	.00	1.74	1
821	1.73	.00		
250	1.72	.01		
640	1.72	.02		
522	1.71	.01		
731	1.70	.01		
612	1.70	.01		
901	1.70	.00		
541	1.70	.00		
920	1.70	.00	1.69	4
332	1.69	.01		
830	1.69	1.28		
350	1.68	.01		
911	1.67	.02		
10.0.0	1.65	.00		
051	1.64	.00		
432	1.63	.06		
151	1.63	.02		
10.1.0	1.63	.05		
702	1.62	.00		
450	1.62	.00		
622	1.61	.02		
740	1.61	.00		
251	1.61	.02		
641	1.61	.16		
712	1.60	.00		
921	1.59	.01		
831	1.58	.01		
351	1.57	.00		

TABLE 5—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
042	1.57	.00		
532	1.57	.01		
142	1.56	.01		
930	1.56	.00		
550	1.55	.01		
10.0.1	1.55	.00		
10.2.0	1.55	.00		
242	1.54	.09		
10.1.1	1.53	.00		
451	1.52	.00		
722	1.52	.00	1.52	4
802	1.52	1.11		
741	1.52	.34		
342	1.51	.28		
840	1.51	.00		
11.0.0	1.50	.00	1.50	$\frac{1}{2}$
812	1.49	.00		
632	1.49	.00		
003	1.49	.03		
650	1.48	.01		
11.1.0	1.48	.05		
103	1.48	.00		
931	1.47	.02		
551	1.47	.01		
442	1.47	.17		
013	1.47	.01	1.47	3
10.2.1	1.46	.01		
060	1.47	.19		
203	1.46	.00		
160	1.46	.01		
113	1.46	.04		
260	1.45	.00		
213	1.44	.02		
10.3.0	1.44	.00		
303	1.44	.00		
822	1.43	.00		
841	1.43	.08		
11.0.1	1.43	.00		
11.2.0	1.42	.00		
732	1.42	.03		
360	1.42	.00		
902	1.42	.00		
542	1.42	.17		
313	1.42	.00		

TABLE 5—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
750	1.41	.00		
651	1.41	.02		
940	1.41	.00		
023	1.41	.00		
11.1.1	1.41	.01		
123	1.40	.00	1.40	2
912	1.40	.00		
403	1.40	.83		
061	1.40	.01		
161	1.39	.01		
223	1.39	.03		
052	1.38	.00		
460	1.38	.00		
413	1.38	.00		
12.0.0	1.38	.00		
152	1.38	.01		
261	1.38	.00		
10.3.1	1.37	.00		
323	1.37	.00		
252	1.36	.03		
642	1.36	.02		
12.1.0	1.36	.01		
11.2.1	1.36	.00		
503	1.36	.00		
361	1.35	.02		
922	1.35	.00		
832	1.35	1.18	1.35	4
751	1.35	.01		
941	1.35	.13		
352	1.34	.01		
560	1.34	.01		
850	1.34	.00		
513	1.34	.00		
11.3.0	1.34	.00		
423	1.33	.00		
10.0.2	1.33	.00		
033	1.33	.03		
461	1.32	.34	1.33	2
133	1.32	.01		
10.4.0	1.32	.06		
12.0.1	1.32	.70	1.32	3
12.2.0	1.32	.00		
10.1.2	1.31	.06		
452	1.31	.00		

TABLE 5—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity (calculated)	Spacing (measured)	Relative intensity (observed)
233	1.31	.00		
603	1.31	.00		
742	1.31	.01		
12.1.1	1.30	.00		
523	1.30	.01		
660	1.30	.00		
613	1.30	.04		
333	1.29	.01		
561	1.29	.00		
851	1.29	.00		
11.3.1	1.28	.03		
			1.268	3
			1.251	$\frac{1}{2}$
			1.232	2
			1.212	2
			1.202	4
			1.179	$\frac{1}{2}$
			1.165	$\frac{1}{2}$
			1.120	1
			1.089	$\frac{1}{2}$
			1.082	2
			1.074	1
			1.061	1 Broad
			1.048	2
			1.036	1
			1.015	3
			.999	$\frac{1}{2}$
			.983	2
			.977	1
			.971	$\frac{1}{2}$
			.965	1
			.959	2
			.941	2
			.935	1

* The intensities were estimated visually on a scale of ten, where ten represents the intensity of the strongest line.

two Weissenberg equator photographs with the crystals rotating about the *b*- and *c*-axes. The intensities I_w of the α_1 spots (where the α_1 and α_2 spots were resolved) on the Weissenberg equator films were calculated from the formula

$$I_w = \frac{1 + \cos^2 2\theta}{\sin 2\theta} |F|^2$$

TABLE 6. RELATIVE INTENSITIES OF X-RAY DIFFRACTION SPOTS FROM A WEISSENBERG EQUATOR PHOTOGRAPH OF KRENNERITE TAKEN WITH THE CRYSTAL ROTATING AROUND THE *b*-AXIS

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation †
		(Observed)*	(Calculated)	
005	0.89Å	w	.15	α_1
205	0.89	w	.00	α_1
405	0.87	w	.61	α_1
605	0.85	w	.00	α_1
805	0.82	m	.22	α_1
004	1.11	m	.72	α_1
204	1.10	w	.00	α_1
404	1.08	w	.08	α_1
604	1.03	w	.00	α_1
804	0.98	w	.62	α_1
10.0.4	0.93	w	.00	α_1
12.0.4	0.87	w	.10	α_1
14.0.4	0.81	w	.00	α_1
003	1.49	m	.14	$\alpha_1 + \alpha_2$
203	1.46	w	.00	$\alpha_1 + \alpha_2$
403	1.40	m	1.77	$\alpha_1 + \alpha_2$
603	1.31	w	.00	$\alpha_1 + \alpha_2$
803	1.21	w	.08	$\alpha_1 + \alpha_2$
10.0.3	1.11	w	.00	$\alpha_1 + \alpha_2$
12.0.3	1.01	w	.65	α_1
14.0.3	0.93	w	.00	α_1
16.0.3	0.85	w	.06	α_1
002	2.23	s	5.53	$\alpha_1 + \alpha_2$
202	2.15	w	.00	$\alpha_1 + \alpha_2$
402	1.96	w	.13	$\alpha_1 + \alpha_2$
602	1.73	w	.00	$\alpha_1 + \alpha_2$
802	1.52	w	2.26	$\alpha_1 + \alpha_2$
10.0.2	1.33	w	.00	$\alpha_1 + \alpha_2$
12.0.2	1.17	w	.04	$\alpha_1 + \alpha_2$
14.0.2	1.04	w	.00	$\alpha_1 + \alpha_2$
16.0.2	0.94	m	.68	α_1
18.0.2	0.85	w	.00	α_1
001	4.46	w	.13	$\alpha_1 + \alpha_2$
201	3.93	0	.00	$\alpha_1 + \alpha_2$
401	3.03	m	10.00	$\alpha_1 + \alpha_2$
601	2.35	0	.00	$\alpha_1 + \alpha_2$
801	1.88	0	.03	$\alpha_1 + \alpha_2$
10.0.1	1.55	w	.00	$\alpha_1 + \alpha_2$
12.0.1	1.32	m	1.57	$\alpha_1 + \alpha_2$
14.0.1	1.14	w	.00	$\alpha_1 + \alpha_2$
16.0.1	1.01	0	.01	$\alpha_1 + \alpha_2$
18.0.1	0.90	0	.00	α_1
20.0.1	0.81	s	1.23	α_1
200	8.27	0	.00	$\alpha_1 + \alpha_2$
400	4.14	0	.00	$\alpha_1 + \alpha_2$
600	2.76	0	.00	$\alpha_1 + \alpha_2$
800	2.07	s	4.81	$\alpha_1 + \alpha_2$
10.0.0	1.65	0	.00	$\alpha_1 + \alpha_2$
12.0.0	1.38	0	.00	$\alpha_1 + \alpha_2$
14.0.0	1.18	0	.00	$\alpha_1 + \alpha_2$
16.0.0	1.03	m	1.03	$\alpha_1 + \alpha_2$
18.0.0	0.92	0	.00	α_1
20.0.0	0.83	w	.01	α_1

* Denotation of symbols: s, strong; m, medium; w, weak.

† The symbol $\alpha_1 + \alpha_2$ denotes an unresolved spot resulting from α_1 and α_2 rays together; the symbol α_1 denotes a spot resulting from α_1 rays alone.

TABLE 7. RELATIVE INTENSITIES OF X-RAY DIFFRACTION SPOTS FROM A WEISSENBERG EQUATOR PHOTOGRAPH OF KRENNERITE TAKEN WITH THE CRYSTAL ROTATING AROUND THE *c*-AXIS

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation†
		(Observed)*	(Calculated)	
0.11.0	0.80 Å	w	.03	α_1
1.11.0	0.80	w	.01	α_1
2.11.0	0.80	w	.03	α_1
3.11.0	0.79	w	.01	α_1
4.11.0	0.79	w	.02	α_1
0.10.0	0.88	0	.01	α_1
1.10.0	0.88	w	.01	α_1
2.10.0	0.88	w	.03	α_1
3.10.0	0.87	s	.36	α_1
4.10.0	0.86	s	.60	α_1
5.10.0	0.85	s	.41	α_1
6.10.0	0.84	m	.03	α_1
7.10.0	0.83	w	.00	α_1
8.10.0	0.81	0	.01	α_1
9.10.0	0.79	w	.01	α_1
090	0.98	m	.06	α_1
190	0.98	0	.00	α_1
290	0.97	0	.00	α_1
390	0.96	0	.00	α_1
490	0.95	0	.00	α_1
590	0.94	0	.00	α_1
690	0.92	0	.00	α_1
790	0.90	w	.01	α_1
890	0.88	m	.18	α_1
990	0.86	0	.02	α_1
10.9.0	0.84	0	.00	α_1
11.9.0	0.82	0	.00	α_1
12.9.0	0.80	w	.00	α_1
080	1.10	0	.00	$\alpha_1 + \alpha_2$
180	1.10	0	.00	$\alpha_1 + \alpha_2$
280	1.09	w	.00	$\alpha_1 + \alpha_2$
380	1.08	w	.00	$\alpha_1 + \alpha_2$
480	1.06	0	.00	$\alpha_1 + \alpha_2$
580	1.04	0	.00	$\alpha_1 + \alpha_2$
680	1.02	0	.00	$\alpha_1 + \alpha_2$
780	1.00	0	.00	$\alpha_1 + \alpha_2$
880	0.97	0	.00	$\alpha_1 + \alpha_2$
980	0.94	0	.00	$\alpha_1 + \alpha_2$
10.8.0	0.92	0	.01	α_1
11.8.0	0.89	w	.00	α_1
12.8.0	0.86	0	.00	α_1
13.8.0	0.83	w	.00	α_1
14.8.0	0.80	0	.02	α_1
070	1.26	0	.00	$\alpha_1 + \alpha_2$

TABLE 7—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation
		(Observed)	(Calculated)	
170	1.26	0	.00	$\alpha_1 + \alpha_2$
270	1.24	w	.08	$\alpha_1 + \alpha_2$
370	1.23	m	.48	$\alpha_1 + \alpha_2$
470	1.20	m	.48	$\alpha_1 + \alpha_2$
570	1.18	m	.40	$\alpha_1 + \alpha_2$
670	1.14	w	.04	$\alpha_1 + \alpha_2$
770	1.11	0	.00	$\alpha_1 + \alpha_2$
870	1.07	0	.00	$\alpha_1 + \alpha_2$
970	1.04	w	.01	$\alpha_1 + \alpha_2$
10.7.0	1.00	w	.10	$\alpha_1 + \alpha_2$
11.7.0	0.96	m	.28	α_1
12.7.0	0.93	m	.26	α_1
13.7.0	0.89	m	.22	α_1
14.7.0	0.86	w	.01	α_1
15.7.0	0.83	0	.00	α_1
16.7.0	0.80	w	.01	α_1
060	1.47	s	1.02	$\alpha_1 + \alpha_2$
160	1.46	w	.02	$\alpha_1 + \alpha_2$
260	1.45	0	.00	$\alpha_1 + \alpha_2$
360	1.42	w	.01	$\alpha_1 + \alpha_2$
460	1.38	w	.00	$\alpha_1 + \alpha_2$
560	1.34	w	.02	$\alpha_1 + \alpha_2$
660	1.30	w	.00	$\alpha_1 + \alpha_2$
760	1.25	w	.05	$\alpha_1 + \alpha_2$
860	1.20	m	.63	$\alpha_1 + \alpha_2$
960	1.15	0	.00	$\alpha_1 + \alpha_2$
10.6.0	1.10	0	.00	$\alpha_1 + \alpha_2$
11.6.0	1.05	w	.00	$\alpha_1 + \alpha_2$
12.6.0	1.00	w	.00	$\alpha_1 + \alpha_2$
13.6.0	0.96	0	.03	$\alpha_1 + \alpha_2$
14.6.0	0.92	0	.00	α_1
15.6.0	0.88	m	.08	α_1
16.6.0	0.84	m	.50	α_1
17.6.0	0.81	w	.01	α_1
050	1.76	0	.00	$\alpha_1 + \alpha_2$
150	1.75	0	.01	$\alpha_1 + \alpha_2$
250	1.72	w	.03	$\alpha_1 + \alpha_2$
350	1.68	w	.02	$\alpha_1 + \alpha_2$
450	1.62	0	.00	$\alpha_1 + \alpha_2$
550	1.55	w	.02	$\alpha_1 + \alpha_2$
650	1.48	w	.01	$\alpha_1 + \alpha_2$
750	1.41	w	.00	$\alpha_1 + \alpha_2$
850	1.34	w	.00	$\alpha_1 + \alpha_2$
950	1.27	0	.00	$\alpha_1 + \alpha_2$

TABLE 7—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation
		(Observed)	(Calculated)	
10.5.0	1.20	w	.01	$\alpha_1 + \alpha_2$
11.5.0	1.14	w	.02	$\alpha_1 + \alpha_2$
12.5.0	1.08	0	.00	$\alpha_1 + \alpha_2$
13.5.0	1.03	w	.00	$\alpha_1 + \alpha_2$
14.5.0	0.98	w	.01	$\alpha_1 + \alpha_2$
15.5.0	0.93	w	.00	$\alpha_1 + \alpha_2$
16.5.0	0.89	w	.00	$\alpha_1 + \alpha_2$
17.5.0	0.85	0	.00	α_1
18.5.0	0.81	0	.01	α_1
040	2.20	0	.01	$\alpha_1 + \alpha_2$
140	2.18	w	.01	$\alpha_1 + \alpha_2$
240	2.13	w	.26	$\alpha_1 + \alpha_2$
340	2.04	m	.80	$\alpha_1 + \alpha_2$
440	1.94	m	.48	$\alpha_1 + \alpha_2$
540	1.83	m	.54	$\alpha_1 + \alpha_2$
640	1.72	w	.06	$\alpha_1 + \alpha_2$
740	1.61	0	.01	$\alpha_1 + \alpha_2$
840	1.51	w	.00	$\alpha_1 + \alpha_2$
940	1.41	w	.00	$\alpha_1 + \alpha_2$
10.4.0	1.32	m	.17	$\alpha_1 + \alpha_2$
11.4.0	1.24	m	.32	$\alpha_1 + \alpha_2$
12.4.0	1.17	m	.13	$\alpha_1 + \alpha_2$
13.4.0	1.10	w	.10	$\alpha_1 + \alpha_2$
14.4.0	1.04	w	.00	$\alpha_1 + \alpha_2$
15.4.0	0.98	0	.00	$\alpha_1 + \alpha_2$
16.4.0	0.93	w	.00	$\alpha_1 + \alpha_2$
17.4.0	0.89	w	.00	$\alpha_1 + \alpha_2$
18.4.0	0.85	m	.18	α_1
19.4.0	0.81	m	.46	α_1
030	2.94	s	10.00	$\alpha_1 + \alpha_2$
130	2.89	w	.05	$\alpha_1 + \alpha_2$
230	2.76	0	.00	$\alpha_1 + \alpha_2$
330	2.59	0	.02	$\alpha_1 + \alpha_2$
430	2.39	0	.00	$\alpha_1 + \alpha_2$
530	2.19	w	.04	$\alpha_1 + \alpha_2$
630	2.01	0	.00	$\alpha_1 + \alpha_2$
730	1.84	w	.07	$\alpha_1 + \alpha_2$
830	1.69	s	3.21	$\alpha_1 + \alpha_2$
930	1.56	0	.01	$\alpha_1 + \alpha_2$
10.3.0	1.44	0	.00	$\alpha_1 + \alpha_2$
11.3.0	1.34	w	.00	$\alpha_1 + \alpha_2$
12.3.0	1.24	w	.00	$\alpha_1 + \alpha_2$
13.3.0	1.16	0	.02	$\alpha_1 + \alpha_2$
14.3.0	1.09	0	.00	$\alpha_1 + \alpha_2$

TABLE 7—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation
		(Observed)	(Calculated)	
15.3.0	1.03	w	.05	$\alpha_1 + \alpha_2$
16.3.0	0.97	s	1.09	$\alpha_1 + \alpha_2$
17.3.0	0.92	0	.00	$\alpha_1 + \alpha_2$
18.3.0	0.87	w	.00	$\alpha_1 + \alpha_2$
19.3.0	0.83	w	.00	α_1
20.3.0	0.79	w	.02	α_1
020	4.41	0	.00	$\alpha_1 + \alpha_2$
120	4.26	0	.00	$\alpha_1 + \alpha_2$
220	3.89	0	.00	$\alpha_1 + \alpha_2$
320	3.44	0	.00	$\alpha_1 + \alpha_2$
420	3.02	0	.00	$\alpha_1 + \alpha_2$
520	2.65	w	.03	$\alpha_1 + \alpha_2$
620	2.34	w	.03	$\alpha_1 + \alpha_2$
720	2.08	0	.00	$\alpha_1 + \alpha_2$
820	1.87	0	.00	$\alpha_1 + \alpha_2$
920	1.70	w	.00	$\alpha_1 + \alpha_2$
10.2.0	1.55	0	.00	$\alpha_1 + \alpha_2$
11.2.0	1.42	0	.01	$\alpha_1 + \alpha_2$
12.2.0	1.32	0	.01	$\alpha_1 + \alpha_2$
13.2.0	1.22	w	.01	$\alpha_1 + \alpha_2$
14.2.0	1.14	w	.01	$\alpha_1 + \alpha_2$
15.2.0	1.07	w	.00	$\alpha_1 + \alpha_2$
16.2.0	1.00	0	.00	$\alpha_1 + \alpha_2$
17.2.0	0.95	w	.00	$\alpha_1 + \alpha_2$
18.2.0	0.90	w	.01	$\alpha_1 + \alpha_2$
19.2.0	0.85	0	.02	α_1
20.2.0	0.81	w	.00	α_1
010	8.82	0	.03	$\alpha_1 + \alpha_2$
110	7.79	0	.01	$\alpha_1 + \alpha_2$
210	6.04	w	.40	$\alpha_1 + \alpha_2$
310	4.69	w	.57	$\alpha_1 + \alpha_2$
410	3.75	w	.16	$\alpha_1 + \alpha_2$
510	3.10	w	.12	$\alpha_1 + \alpha_2$
610	2.63	0	.01	$\alpha_1 + \alpha_2$
710	2.28	0	.01	$\alpha_1 + \alpha_2$
810	2.01	0	.00	$\alpha_1 + \alpha_2$
910	1.80	w	.00	$\alpha_1 + \alpha_2$
10.1.0	1.63	w	.13	$\alpha_1 + \alpha_2$
11.1.0	1.48	w	.15	$\alpha_1 + \alpha_2$
12.1.0	1.36	w	.02	$\alpha_1 + \alpha_2$
13.1.0	1.26	0	.01	$\alpha_1 + \alpha_2$
14.1.0	1.17	0	.00	$\alpha_1 + \alpha_2$
15.1.0	1.09	0	.01	$\alpha_1 + \alpha_2$
16.1.0	1.03	0	.00	$\alpha_1 + \alpha_2$
17.1.0	0.97	w	.00	$\alpha_1 + \alpha_2$
18.1.0	0.91	w	.11	$\alpha_1 + \alpha_2$

TABLE 7—Continued

Indices (<i>hkl</i>)	Spacing (calculated)	Relative intensity		CuK-radiation
		(Observed)	(Calculated)	
19.1.0	0.87	m	.12	α_1
20.1.0	0.82	w	.01	α_1
100	16.54	0	.01	$\alpha_1 + \alpha_2$
200	8.27	0	.00	$\alpha_1 + \alpha_2$
300	5.51	0	.00	$\alpha_1 + \alpha_2$
400	4.14	0	.00	$\alpha_1 + \alpha_2$
500	3.31	0	.00	$\alpha_1 + \alpha_2$
600	2.76	0	.00	$\alpha_1 + \alpha_2$
700	2.36	0	.00	$\alpha_1 + \alpha_2$
800	2.07	m	6.43	$\alpha_1 + \alpha_2$
900	1.84	0	.00	$\alpha_1 + \alpha_2$
10.0.0	1.65	0	.00	$\alpha_1 + \alpha_2$
11.0.0	1.50	0	.00	$\alpha_1 + \alpha_2$
12.0.0	1.38	0	.00	$\alpha_1 + \alpha_2$
13.0.0	1.27	0	.00	$\alpha_1 + \alpha_2$
14.0.0	1.18	0	.00	$\alpha_1 + \alpha_2$
15.0.0	1.10	0	.00	$\alpha_1 + \alpha_2$
16.0.0	1.03	s	1.38	$\alpha_1 + \alpha_2$
17.0.0	0.97	0	.00	$\alpha_1 + \alpha_2$
18.0.0	0.92	0	.00	$\alpha_1 + \alpha_2$
19.0.0	0.87	0	.00	α_1
20.0.0	0.83	w	.02	α_1

* Denotation of symbols: s, strong; m, medium; w, weak.

† The symbol $\alpha_1 + \alpha_2$ denotes an unresolved spot resulting from α_1 and α_2 rays together; the symbol α_1 denotes a spot resulting from α_1 rays alone.

and the intensities I_w of the unresolved α_1 and α_2 spots on the same films from the formula

$$I_w = 1.5 \frac{1 + \cos^2 2\theta}{\sin 2\theta} |F|^2.$$

The atomic f -values of James and Brindley²⁴ were used except that in view of the substitution of silver atoms for some of the gold atoms, a composite value made up of 79 per cent of the f -value of gold and 21 per cent of the f -value of silver was used in place of the f -value of gold. No correction was made for absorption. However, it was observed that an equator Weissenberg photograph of a very small crystal (of cross section 0.04 mm. by 0.08 mm.) exhibited relative intensities closely similar to those of a considerably larger one (of cross section 0.36 mm. by 0.60 mm.), both crystals being oscillated about the c -axis. The intensities used are relative and were estimated visually. For computation of a Fourier series leading to the construction of the projection of the struc-

²⁴ James, R. W., and Brindley, G. W.: *Z. Krist.*, **78**, 475 (1931).

ture on the plane 001, the intensities on the Weissenberg equator photograph taken with the crystal rotating around the c -axis were used, and these were obtained by visual comparison of the diffraction spots on the film with a standard scale of spots prepared in the Department of Chemistry of The Johns Hopkins University.²⁵ On this standard scale the intensities are taken to be proportional to the exposure times of the spots to a beam of constant energy output. The observed intensities obtained by comparison with the standard scale were multiplied by $2/3$ for the spots in which the $\alpha_1\alpha_2$ -doublet is not resolved to reduce them to the same basis as the spots due to α_1 -radiation alone. The resulting values divided by the Lorentz and polarization factors yielded numbers proportional to the squares of the absolute values of the structure factors. The square roots of these numbers were extracted and positive and negative signs were affixed in accordance with the signs of the F 's obtained from the structure arrived at by comparison of observed and calculated intensities. The experimental F -values are listed in Table 8, along with the calculated F -values, which are given for comparison. The synthesis of the two-dimensional Fourier series was carried out by the method devised by Patterson²⁶ and improved by Patterson and Tunell.²⁷ The values of $A(x, y) = \rho(x, y) + K$, where $\rho(x, y)$ denotes the projected electron density and K denotes a constant, were computed at 900 points in the quarter projection, corresponding to division of each of the unit cell edges into 60 parts. Vertical sections were drawn along the lines of the grid work parallel to the b -axis, and from them a contour map of $A(x, y)$ was plotted (Fig. 3). The positions of the atoms found from the contour map are as given at the beginning of this section.

DISCUSSION OF THE ATOMIC ARRANGEMENT

In the krennerite structure each gold (or silver) atom is surrounded by six tellurium atoms. The orientation of the distorted octahedra is most easily seen from Fig. 1A. Two neighbors of each gold (or silver) atom have their centers situated nearly on a line passing through the center of the gold (or silver) atom parallel to the b -axis; the other four neighbors have their centers not far from a plane passing through the center of the gold (or silver) atom perpendicular to the b -axis. The tellurium atoms also are surrounded by six neighbors, in some cases by three gold (or silver) atoms and three tellurium atoms, in others by five gold (or silver) atoms and one tellurium atom, and in still others by one

²⁵ The writers are indebted to Dr. David Harker for the use of this scale.

²⁶ Patterson, A. L.: *Phil. Mag.* (7), **22**, 753-754 (1936).

²⁷ Patterson, A. L., and Tunell, G.: *Am. Mineral.*, **27**, 655-679 (1942).

TABLE 8. OBSERVED AND CALCULATED VALUES OF THE STRUCTURE FACTOR F (The upper figure in each square is the observed value; the lower figure in each square is the calculated value.)

h k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
11	$\begin{matrix} -8. \\ -8.7 \end{matrix}$	$\begin{matrix} -8. \\ -4.7 \end{matrix}$	$\begin{matrix} +13. \\ +8.2 \end{matrix}$	$\begin{matrix} -7. \\ -5.1 \end{matrix}$	$\begin{matrix} +6. \\ +6.4 \end{matrix}$																
10	$\begin{matrix} 0. \\ +5.7 \end{matrix}$	$\begin{matrix} +11. \\ +5.3 \end{matrix}$	$\begin{matrix} +23. \\ +12.3 \end{matrix}$	$\begin{matrix} +105. \\ +42.6 \end{matrix}$	$\begin{matrix} +128. \\ +54.2 \end{matrix}$	$\begin{matrix} -110. \\ -42.7 \end{matrix}$	$\begin{matrix} +27. \\ +10.9 \end{matrix}$	$\begin{matrix} -9. \\ -3.7 \end{matrix}$	$\begin{matrix} 0. \\ +6.3 \end{matrix}$	$\begin{matrix} +7. \\ +4.8 \end{matrix}$											
9	$\begin{matrix} +22. \\ +21.4 \end{matrix}$	$\begin{matrix} 0. \\ +1.7 \end{matrix}$	$\begin{matrix} 0. \\ +1.0 \end{matrix}$	$\begin{matrix} 0. \\ -2.7 \end{matrix}$	$\begin{matrix} 0. \\ -1.3 \end{matrix}$	$\begin{matrix} 0. \\ -2.9 \end{matrix}$	$\begin{matrix} +2.3 \\ +0.4 \end{matrix}$	$\begin{matrix} -2.3 \\ +2.1 \end{matrix}$	$\begin{matrix} +66. \\ +31.4 \end{matrix}$	$\begin{matrix} 0. \\ -9.3 \end{matrix}$	$\begin{matrix} 0. \\ +0.2 \end{matrix}$	$\begin{matrix} +1.8 \\ +0.2 \end{matrix}$	$\begin{matrix} -7. \\ -1.9 \end{matrix}$								
8	$\begin{matrix} -1.5 \\ +0.9 \end{matrix}$	$\begin{matrix} 0. \\ +3.3 \end{matrix}$	$\begin{matrix} -8. \\ +3.6 \end{matrix}$	$\begin{matrix} +8. \\ +1.4 \end{matrix}$	$\begin{matrix} 0. \\ +2.5 \end{matrix}$	$\begin{matrix} 0. \\ +0.4 \end{matrix}$	$\begin{matrix} 0. \\ +2.1 \end{matrix}$	$\begin{matrix} 0. \\ -2.0 \end{matrix}$	$\begin{matrix} 0. \\ -2.2 \end{matrix}$	$\begin{matrix} 0. \\ +2.7 \end{matrix}$	$\begin{matrix} 0. \\ -8.1 \end{matrix}$	$\begin{matrix} +12. \\ +1.4 \end{matrix}$	$\begin{matrix} 0. \\ +3.9 \end{matrix}$	$\begin{matrix} +9. \\ +3.4 \end{matrix}$	$\begin{matrix} 0. \\ +6.4 \end{matrix}$						
7	$\begin{matrix} 0. \\ +0.9 \end{matrix}$	$\begin{matrix} 0. \\ +4.3 \end{matrix}$	$\begin{matrix} +21. \\ +20.9 \end{matrix}$	$\begin{matrix} +98. \\ +50.2 \end{matrix}$	$\begin{matrix} +49.6 \\ +20.3 \end{matrix}$	$\begin{matrix} -99. \\ -20.3 \end{matrix}$	$\begin{matrix} +20. \\ +14.5 \end{matrix}$	$\begin{matrix} 0. \\ -3.9 \end{matrix}$	$\begin{matrix} 0. \\ +2.0 \end{matrix}$	$\begin{matrix} +8. \\ +8.4 \end{matrix}$	$\begin{matrix} +21. \\ +23.3 \end{matrix}$	$\begin{matrix} +115. \\ +45.4 \end{matrix}$	$\begin{matrix} +110. \\ +41.5 \end{matrix}$	$\begin{matrix} -102. \\ -24.8 \end{matrix}$	$\begin{matrix} +11. \\ +8.0 \end{matrix}$	$\begin{matrix} 0. \\ -2.3 \end{matrix}$	$\begin{matrix} +7. \\ +4.1 \end{matrix}$				
6	$\begin{matrix} +106. \\ +65.2 \end{matrix}$	$\begin{matrix} -10. \\ +8.5 \end{matrix}$	$\begin{matrix} 0. \\ +2.1 \end{matrix}$	$\begin{matrix} -7. \\ -6.0 \end{matrix}$	$\begin{matrix} +7. \\ -2.3 \end{matrix}$	$\begin{matrix} +8. \\ +9.2 \end{matrix}$	$\begin{matrix} -8. \\ +3.6 \end{matrix}$	$\begin{matrix} -21. \\ -16.8 \end{matrix}$	$\begin{matrix} +103. \\ +58.0 \end{matrix}$	$\begin{matrix} 0. \\ -0.3 \end{matrix}$	$\begin{matrix} 0. \\ +0.3 \end{matrix}$	$\begin{matrix} +8. \\ +4.6 \end{matrix}$	$\begin{matrix} +8. \\ +0.9 \end{matrix}$	$\begin{matrix} +11. \\ +11.9 \end{matrix}$	$\begin{matrix} 0. \\ +4.1 \end{matrix}$	$\begin{matrix} -31. \\ -21.2 \end{matrix}$	$\begin{matrix} +02. \\ +46.0 \end{matrix}$	$\begin{matrix} -8. \\ -5.1 \end{matrix}$			
5	$\begin{matrix} 0. \\ +2.0 \end{matrix}$	$\begin{matrix} 0. \\ +5.6 \end{matrix}$	$\begin{matrix} -9. \\ -9.6 \end{matrix}$	$\begin{matrix} +6. \\ +7.3 \end{matrix}$	$\begin{matrix} 0. \\ -1.7 \end{matrix}$	$\begin{matrix} -7. \\ -8.1 \end{matrix}$	$\begin{matrix} -10. \\ -7.8 \end{matrix}$	$\begin{matrix} +7. \\ -2.6 \end{matrix}$	$\begin{matrix} -8. \\ +1.0 \end{matrix}$	$\begin{matrix} 0. \\ +4.3 \end{matrix}$	$\begin{matrix} -8. \\ -8.2 \end{matrix}$	$\begin{matrix} +8. \\ +2.6 \end{matrix}$	$\begin{matrix} 0. \\ +0.5 \end{matrix}$	$\begin{matrix} -8. \\ -4.8 \end{matrix}$	$\begin{matrix} -11. \\ -5.2 \end{matrix}$	$\begin{matrix} +7. \\ +1.4 \end{matrix}$	$\begin{matrix} -7. \\ -0.8 \end{matrix}$	$\begin{matrix} 0. \\ +1.0 \end{matrix}$	$\begin{matrix} -6.3 \\ -6.3 \end{matrix}$		
4	$\begin{matrix} -3.8 \\ +74. \\ +127.3 \end{matrix}$	$\begin{matrix} +5. \\ +3.7 \end{matrix}$	$\begin{matrix} +14. \\ +25.5 \end{matrix}$	$\begin{matrix} +22. \\ +45.4 \end{matrix}$	$\begin{matrix} +35.7 \\ +13.5 \end{matrix}$	$\begin{matrix} -47. \\ -40.8 \end{matrix}$	$\begin{matrix} +17. \\ +13.5 \end{matrix}$	$\begin{matrix} 0. \\ -5.4 \end{matrix}$	$\begin{matrix} -7. \\ -2.3 \end{matrix}$	$\begin{matrix} +10. \\ +1.8 \end{matrix}$	$\begin{matrix} +29. \\ +29.1 \end{matrix}$	$\begin{matrix} +72. \\ +41.2 \end{matrix}$	$\begin{matrix} +31. \\ +26.4 \end{matrix}$	$\begin{matrix} -22. \\ -23.8 \end{matrix}$	$\begin{matrix} +8. \\ +3.6 \end{matrix}$	$\begin{matrix} 0. \\ -5.0 \end{matrix}$	$\begin{matrix} -7. \\ +0.2 \end{matrix}$	$\begin{matrix} +104. \\ +73.7 \end{matrix}$	$\begin{matrix} -10. \\ -3.9 \end{matrix}$	$\begin{matrix} +28. \\ +27.8 \end{matrix}$	$\begin{matrix} +71. \\ +35.9 \end{matrix}$
3	$\begin{matrix} +74. \\ +127.3 \end{matrix}$	$\begin{matrix} -4. \\ +9.4 \end{matrix}$	$\begin{matrix} 0. \\ +0.6 \end{matrix}$	$\begin{matrix} -6.1 \\ -6.1 \end{matrix}$	$\begin{matrix} -0.8 \\ -0.8 \end{matrix}$	$\begin{matrix} +5. \\ +9.6 \end{matrix}$	$\begin{matrix} +2.9 \\ +2.9 \end{matrix}$	$\begin{matrix} -16. \\ -14.9 \end{matrix}$	$\begin{matrix} +106. \\ +103.9 \end{matrix}$	$\begin{matrix} 0. \\ +1.9 \end{matrix}$	$\begin{matrix} -1.6 \\ -1.6 \end{matrix}$	$\begin{matrix} +8. \\ -1.4 \end{matrix}$	$\begin{matrix} +8. \\ +2.2 \end{matrix}$	$\begin{matrix} +6.5 \\ +6.5 \end{matrix}$	$\begin{matrix} 0. \\ +3.3 \end{matrix}$	$\begin{matrix} -21. \\ -16.0 \end{matrix}$	$\begin{matrix} +104. \\ +73.7 \end{matrix}$	$\begin{matrix} -1.9 \\ -1.9 \end{matrix}$	$\begin{matrix} +6. \\ -3.9 \end{matrix}$	$\begin{matrix} +10. \\ +10.2 \end{matrix}$	$\begin{matrix} +13. \\ +5.7 \end{matrix}$
2	$\begin{matrix} +0.8 \\ -3.9 \end{matrix}$	$\begin{matrix} +2.2 \\ +2.8 \end{matrix}$	$\begin{matrix} -2.4 \\ +17.1 \end{matrix}$	$\begin{matrix} 0. \\ +23.3 \end{matrix}$	$\begin{matrix} -1.1 \\ +13.7 \end{matrix}$	$\begin{matrix} -5. \\ -13.5 \end{matrix}$	$\begin{matrix} -5. \\ +3.7 \end{matrix}$	$\begin{matrix} +1.6 \\ -5.5 \end{matrix}$	$\begin{matrix} 0. \\ -2.8 \end{matrix}$	$\begin{matrix} +6. \\ +0.9 \end{matrix}$	$\begin{matrix} +4.1 \\ +21.7 \end{matrix}$	$\begin{matrix} 0. \\ +19. \\ +24.8 \end{matrix}$	$\begin{matrix} +0. \\ +11. \\ +9.8 \end{matrix}$	$\begin{matrix} +0.7 \\ -5.6 \end{matrix}$	$\begin{matrix} -8. \\ -8.8 \end{matrix}$	$\begin{matrix} +8. \\ +5.0 \end{matrix}$	$\begin{matrix} -7. \\ -0.6 \end{matrix}$	$\begin{matrix} +10. \\ +6.8 \end{matrix}$	$\begin{matrix} -11. \\ -10.1 \end{matrix}$	$\begin{matrix} +19. \\ +21.7 \end{matrix}$	$\begin{matrix} +30. \\ +24.3 \end{matrix}$
1	$\begin{matrix} 0. \\ -3.9 \end{matrix}$	$\begin{matrix} 0. \\ +2.8 \end{matrix}$	$\begin{matrix} +8. \\ +17.1 \end{matrix}$	$\begin{matrix} +9. \\ +23.3 \end{matrix}$	$\begin{matrix} +5. \\ +13.7 \end{matrix}$	$\begin{matrix} -6. \\ -13.5 \end{matrix}$	$\begin{matrix} +3.7 \\ -5.5 \end{matrix}$	$\begin{matrix} 0. \\ -2.8 \end{matrix}$	$\begin{matrix} +0. \\ +0.9 \end{matrix}$	$\begin{matrix} +9. \\ +21.7 \end{matrix}$	$\begin{matrix} +19. \\ +24.8 \end{matrix}$	$\begin{matrix} +11. \\ +9.8 \end{matrix}$	$\begin{matrix} -6.1 \\ -6.1 \end{matrix}$	$\begin{matrix} -3.8 \\ -6.8 \end{matrix}$	$\begin{matrix} 0. \\ -6.8 \end{matrix}$	$\begin{matrix} -1.3 \\ -1.2 \end{matrix}$	$\begin{matrix} +107. \\ +86.2 \end{matrix}$	$\begin{matrix} 0. \\ -3.4 \end{matrix}$	$\begin{matrix} +10. \\ +21.7 \end{matrix}$	$\begin{matrix} +30. \\ +24.3 \end{matrix}$	$\begin{matrix} +7.0 \\ +7.5 \end{matrix}$
0	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ -0.9 \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} +0.7 \\ +0.7 \end{matrix}$	$\begin{matrix} 0. \\ +2.0 \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} +68. \\ +128.0 \end{matrix}$	$\begin{matrix} 0. \\ -3.0 \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ +4.0 \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ +4.8 \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} 0. \\ 0. \end{matrix}$	$\begin{matrix} +107. \\ +86.2 \end{matrix}$	$\begin{matrix} 0. \\ -3.4 \end{matrix}$	$\begin{matrix} +10. \\ +21.7 \end{matrix}$	$\begin{matrix} +30. \\ +24.3 \end{matrix}$	$\begin{matrix} +7.0 \\ +7.5 \end{matrix}$

gold (or silver) atom and five tellurium atoms. In all cases two neighbors of each tellurium atom have their centers situated nearly on a line through the center of the tellurium atom parallel to the b -axis; the other four neighbors have their centers not far from a plane through the center of the tellurium atom perpendicular to the b -axis. The distances between the gold (or silver) and the tellurium atoms are 2.66, 2.99, 2.99, 2.67, 2.63, 2.87, 3.15, 2.95, 3.22, 2.66, 2.63, 2.94, and 3.04 Å. The distances between the tellurium atoms are 3.51, 3.08, 3.34, 3.54, 3.02, 3.28, and 3.54 Å. All these distances are shown in Fig. 1A. The structure can be described as consisting of lines of atoms parallel to the b -axis. These lines are at $x=0, z=0$, at $x=0.124, z=0.500$, and at $x=0.250, z=0.014$. Along each of these lines gold (or silver) atoms are separated by pairs of tellurium atoms, the gold (or silver) atoms lying exactly on the line and the tellurium atoms close to it. The gold (or silver) atoms also lie in corrugated sheets with two layers of tellurium atoms, in similar corrugated sheets, between successive corrugated sheets of gold (or silver) atoms. The zigzag pattern of the corrugated sheets is clearly shown in projection on the basal plane in Fig. 1A.

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