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The structure of hessite, Ag_2Te-III

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With 3 figures

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Auszug

Als Raumgruppe eines einheitlichen Hessitkristalls (Ag_2Te-III) von Bótes, Transsylvanien, wurde $P2_1/c$ gefunden; die Gitterkonstanten wurden zu $a = 8{,}09$, $b = 4{,}48$, $c = 8{,}96$ Å, $\beta = 123°20'$ bestimmt. Die Elementarzelle enthält 4 Ag_2Te. Alle Atome befinden sich in allgemeinen Lagen; ihre Parameter sind:

$x = 0{,}018$, $y = 0{,}152$, $z = 0{,}371$ für Ag(I),
$x = 0{,}332$, $y = 0{,}837$, $z = 0{,}995$ für Ag(II),
$x = 0{,}272$, $y = 0{,}159$, $z = 0{,}243$ für Te.

Symmetrie und Dimensionen der Zelle stimmen nicht mit den Literaturangaben überein. Es wird angenommen, daß die früheren Untersuchungen an verzwillingten Kristallen durchgeführt wurden.

Abstract

The space group of a single crystal of naturally occurring hessite (Ag_2Te-III) from Bótes, Transylvania, was found to be monoclinic $P2_1/c$; the cell constants were determined as follows: $a = 8.09$, $b = 4.48$, $c = 8.96$ Å, $\beta = 123°20'$. There are 4 (Ag_2Te) per cell, and all atoms lie on the following fourfold general positions: Ag(I) at $x = 0.018$, $y = 0.152$, $z = 0.371$; Ag(II) at $x = 0.332$, $y = 0.837$, $z = 0.995$; and Te at $x = 0.272$, $y = 0.159$, $z = 0.243$.

This cell and the symmetry differ from those previously reported for hessite in the literature. It is believed that the other recent determinations have been based upon misleading data from twinned crystals.

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Introduction

The mineral hessite, Ag_2Te, and its polymorphs have been the subject of several crystallographic investigations. Results have been conflicting and confusing. Part of the confusion arises out of the notation used to identify the different polymorphs. In this paper the notation used by KRACEK and KSANDA[1], utilizing Roman numerals, will be followed. The polymorph whose stability range lies between 690° to 802°C and the melting point will be referred to as Ag_2Te-I. The polymorph stable between 105° to 145° and 690° to 802°C, listed as α-hessite or α-Ag_2Te in many texts, will be called Ag_2Te-II. The polymorph stable from room temperature up to 105° to 145°C, called β-Ag_2Te in earlier literature, will be labeled Ag_2Te-III. These labels should not be confused with the notation used by ROWLAND and BERRY[2], where Ag_2Te "type I" and "type II" refer to morphological examples.

A conflict exists in that the symmetry and unit-cell dimensions reported by three different investigators for Ag_2Te-III do not agree; nor does the lattice type arrived at by two workers for Ag_2Te-II. There has been no crystallographic study of Ag_2Te-I reported in the literature.

Ag_2Te-III: hessite

The most recent crystallographic investigation of the room-temperature polymorph, Ag_2Te-III, is that of ROWLAND and BERRY[2]. From material synthesized from aqueous sodium-sulfide solution in a graphite-lined steel bomb at several different temperatures from 350° to 490°C, crystals were obtained from which morphological data and some single-crystal x-ray data could be taken. It is to be noted that the temperatures utilized were at least 200°C above the stability range of Ag_2Te-III at normal pressures. Unless the effect of the pressure that existed within the steel bomb was to increase the stability range of Ag_2Te-III by more than 200°, it seems unlikely that the morphology of the crystals grown under these conditions represents the morphology of the Ag_2Te-III phase. However, as the powder diffraction record of the products of these runs was identical with that of natural

[1] F. C. KRACEK and C. J. KSANDA, A paper on the Ag — Te system; in preparation.

[2] J. F. ROWLAND and L. G. BERRY, The structural lattice of hessite. Amer. Mineral. **36** (1951) 471—479.

hessite, there is little doubt that the internal structure at room temperature was that of Ag_2Te-III.

From one of these crystals exhibiting orthorhombic morphology, ROWLAND and BERRY obtained Weißenberg and rotation films that lead to the following unit-cell and space group: orthorhombic *Immm*; $a = 16.28$, $b = 26.68$, $c = 7.55$ Å. But here again it must be pointed out that since the crystals were grown at temperatures above the stability field of Ag_2Te-III, there is a possibility that, during the transformation, twinning took place that resulted in additional symmetry and an apparent cell larger than that which would be exhibited by a true single crystal.

ROWLAND and BERRY's cell does not agree with that described by TOKODY[3,4]. TOKODY found Ag_2Te-III to be monoclinic with a cell size of $a = 6.57$, $b = 6.14$, $c = 6.10$ Å, $\beta = 61° 15'$. From the cell content of 3 (Ag_2Te) he concluded that the space group must be *Pm*, *P*2, or *P*2/*m*. However, this cell was determined principally from the powder diffraction record, and to index all the reflections it was necessary to consider that some reflections were due to β radiation. Powder photographs taken on natural samples during the present investigation indicate that the lines considered by TOKODY to be due to β radiation were clearly due to Cu$K\alpha$. THOMPSON[5] also reports that the powder pattern of hessite could not be indexed on the monoclinic elements of TOKODY.

Structure determination

Small crystals of hessite from Bótes, Transylvania, obtained both from the U. S. National Museum (U.S.N.M.No.R9556) and from the Harvard University Museum (No. 99348), were found to contain small inclusions of petzite[6]. By fracturing these small crystals at liquid nitrogen temperatures, it was possible to obtain fragments of hessite free from any petzite. The diffraction record of these fragments showed them to be single, undeformed crystals. The x-ray powder diagram

[3] L. TOKODY, Über Hessit. Z. Kristallogr. **82** (1932) 154–157.

[4] L. TOKODY, Berichtigung zu meiner Mitteilung „Über Hessit". Z. Kristallogr. **89** (1934) 416.

[5] R. M. THOMPSON, The telluride minerals and their occurrence in Canada. Amer. Mineral. **34** (1949) 342–382.

[6] A. J. FRUEH, The crystallography of petzite, Ag_3AuTe_2. Amer. Mineral. **44** (1959), in press.

Table 1

I	d	I	d	I	d	I	d
2	3.16	2	2.14	2	1.445	1	1.127
5	2.98	2	2.116	8	1.393	1	1.115
5	2.87	1	2.022	6	1.302	3	1.104
10	2.30	1	1.930	1	1.280	1	1.077
8	2.24	1	1.773	1	1.245	1	1.050
2	2.18	1	1.693	2	1.192	7	1.001

prepared from some of these fragments, using Fe$K\alpha$ = 1.937 Å, is tabulated in Table 1. It can be seen that this pattern is in close agreement with the hessite pattern reported by ROWLAND and BERRY[2].

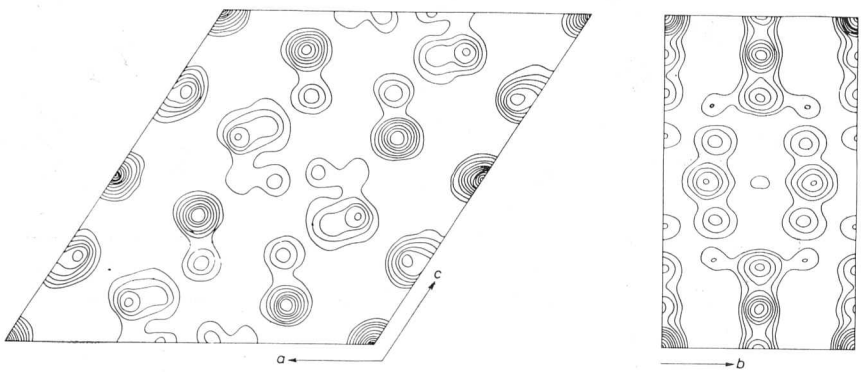

Fig. 1. Patterson projections of hessite on (010) and on plane perpendicular to [100]

The space group symmetry was determined as monoclinic $P2_1/c$, The cell constants measured from Buerger precession photographs, using Mo$K\alpha$ radiation, were as follows: $a = 8.09$, $b = 4.48$, $c = 8.96$ Å. $\beta = 123° 20'$. By using the specific gravity of 8.21 as determined by THOMPSON[5], and the cell volume of 271.4 Å^3 as computed from the above dimensions, it is ascertained that the cell contains 4 (Ag_2Te).

Intensity data for the b axis zero, first, second, third and fourth levels were gathered by an equi-inclination Geiger-counter spectrometer, using Mo$K\alpha$ radiation. The data were corrected for Lorentz and polarization factors by the accepted method[7].

[7] M. J. BUERGER and G. KLEIN, Correction of x-ray diffraction intensities for Lorentz and polarization factors. J. Appl. Physics **16** (1945) 406–418.

The positions of all the atoms were located (Fig. 1) from Patterson projections on (010) and on the plane perpendicular to [100], with the aid of a Harker-Patterson section $P(x, \frac{1}{2}, z)$. From these positions signs were calculated and combined with observed intensities to make electron-density projections on (010) and on the plane perpendicular to [100] (Fig. 2). These projections confirmed the validity of the initial positions, and further refinement was accomplished by least-squares utilizing the Service Bureau Corporation's (IBM) NY-XR2 program.

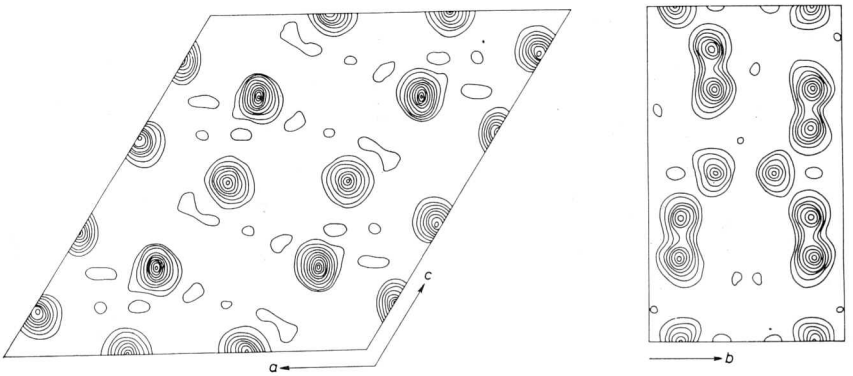

Fig. 2. Electron-density projections of hessite on (010) and on plane perpendicular to [100]

All atoms are located on the fourfold general positions: x, y, z; $\bar{x}, \bar{y}, \bar{z}$; $\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$; $x, \frac{1}{2}-y, \frac{1}{2}+z$. The final refined parameters are listed in Table 2. In Table 3 the intensities from all reflections as

Table 2

	x	y	z
Ag_I	0.018	0.152	0.371
Ag_{II}	0.332	0.837	0.995
Te	0.272	0.159	0.243

calculated from these parameters are compared with those observed. The final standard discrepancy factor R for the three-dimensional data is 0.157; and the final isotropic temperature factors are:

$$B_{Ag_I} = 2.02,\ B_{Ag_{II}} = 2.75, \text{ and } B_{Te} = 1.07\ .$$

Table 3

h k l	sin θ	$F_{calc.}$	$F_{obs.}$	h k l	sin θ	$F_{calc.}$	$F_{obs.}$	h k l	sin θ	$F_{calc.}$	$F_{obs.}$	h k l	sin θ	$F_{calc.}$	$F_{obs.}$
1 0 0	.053	61	71	$\bar{9}$ 0 8	.413	− 21	39	$\bar{4}$ 1 3	.195	− 14	28	$\bar{2}$ 1 8	.344	21	28
2 0 0	.105	− 97	114	$\bar{10}$ 0 8	.449	− 1	−	$\bar{5}$ 1 3	.234	− 10	−	$\bar{3}$ 1 8	.331	− 38	36
3 0 0	.158	307	300	$\bar{11}$ 0 8	.487	47	51	$\bar{6}$ 1 3	.277	132	142	$\bar{4}$ 1 8	.328	59	59
4 0 0	.210	160	169	0 0 10	.475	− 37	36	$\bar{7}$ 1 3	.323	45	43	$\bar{5}$ 1 8	.332	120	114
5 0 0	.263	− 40	59	$\bar{1}$ 0 10	.449	− 1	−	$\bar{8}$ 1 3	.371	− 21	−	$\bar{6}$ 1 8	.345	− 37	32
6 0 0	.315	49	55	$\bar{2}$ 0 10	.427	23	−	$\bar{9}$ 1 3	.420	34	−	$\bar{7}$ 1 8	.364	− 7	−
7 0 0	.368	83	79	$\bar{3}$ 0 10	.411	− 45	51	$\bar{10}$ 1 3	.470	42	43	$\bar{8}$ 1 8	.390	132	122
8 0 0	.420	38	36	$\bar{4}$ 0 10	.401	− 99	99	0 1 4	.206	− 2	−	$\bar{9}$ 1 8	.421	26	32
0 0 2	.095	− 31	35	$\bar{5}$ 0 10	.397	22	−	1 1 4	.237	− 30	36	$\bar{10}$ 1 8	.456	− 39	36
1 0 2	.131	− 43	55	$\bar{6}$ 0 10	.401	18	−	2 1 4	.275	− 32	43	$\bar{11}$ 1 8	.494	54	55
2 0 2	.176	97	103	$\bar{7}$ 0 10	.412	−134	130	3 1 4	.319	82	83	$\bar{12}$ 1 8	.534	52	51
3 0 2	.224	83	91	$\bar{8}$ 0 10	.428	− 48	51	4 1 4	.361	29	47	0 1 9	.435	17	−
4 0 2	.274	− 93	99	$\bar{9}$ 0 10	.450	52	47	5 1 4	.408	− 58	67	1 1 9	.466	− 45	43
5 0 2	.325	51	43	$\bar{10}$ 0 10	.478	− 62	63	6 1 4	.456	42	43	2 1 9	.500	− 23	39
6 0 2	.376	133	138	$\bar{11}$ 0 10	.512	− 79	87	7 1 4	.510	61	71	$\bar{1}$ 1 9	.409	8	−
7 0 2	.427	− 34	47	$\bar{4}$ 0 12	.488	14	−	$\bar{1}$ 1 4	.185	15	12	$\bar{2}$ 1 9	.389	− 39	47
$\bar{1}$ 0 2	.079	− 76	75	$\bar{5}$ 0 12	.478	− 76	79	$\bar{2}$ 1 4	.178	5	−	$\bar{3}$ 1 9	.374	− 13	−
$\bar{2}$ 0 2	.095	52	55	$\bar{6}$ 0 12	.477	− 7	−	$\bar{3}$ 1 4	.186	−151	138	$\bar{4}$ 1 9	.367	16	−
$\bar{3}$ 0 2	.132	4	−	$\bar{7}$ 0 12	.480	24	−	$\bar{4}$ 1 4	.206	− 44	43	$\bar{5}$ 1 9	.368	15	−
$\bar{4}$ 0 2	.177	−237	237	$\bar{8}$ 0 12	.489	− 17	−	$\bar{5}$ 1 4	.238	84	83	$\bar{6}$ 1 9	.375	− 13	−
$\bar{5}$ 0 2	.225	− 17	−	$\bar{9}$ 0 12	.504	− 37	47	$\bar{6}$ 1 4	.276	−128	134	$\bar{7}$ 1 9	.390	− 15	−
$\bar{6}$ 0 2	.278	83	91	1 1 0	.095	− 48	47	$\bar{7}$ 1 4	.318	−119	118	$\bar{8}$ 1 9	.411	42	51
$\bar{7}$ 0 2	.325	−158	162	2 1 0	.132	− 90	95	$\bar{8}$ 1 4	.362	62	67	$\bar{9}$ 1 9	.437	24	−
$\bar{8}$ 0 2	.377	− 95	99	3 1 0	.175	75	75	$\bar{9}$ 1 4	.409	− 27	−	$\bar{10}$ 1 9	.468	− 28	−
$\bar{9}$ 0 2	.428	59	67	4 1 0	.225	− 21	16	$\bar{10}$ 1 4	.457	− 97	95	$\bar{11}$ 1 9	.500	17	−
$\bar{10}$ 0 2	.480	− 35	39	5 1 0	.274	−158	154	0 1 5	.250	88	91	$\bar{12}$ 1 9	.538	39	39
0 0 4	.191	130	118	6 1 0	.325	19	32	1 1 5	.282	− 37	39	0 1 10	.482	− 2	−
1 0 4	.223	−131	138	7 1 0	.376	39	47	2 1 5	.318	13	24	1 1 10	.538	77	39
2 0 4	.263	−244	245	8 1 0	.428	− 99	99	3 1 5	.359	96	103	$\bar{1}$ 1 10	.456	− 30	−
3 0 4	.306	14	32	9 1 0	.480	− 39	47	4 1 5	.402	6	−	$\bar{2}$ 1 10	.434	91	87
4 0 4	.352	6	−	0 1 1	.092	23	−	5 1 5	.448	− 19	−	$\bar{3}$ 1 10	.418	57	59
5 0 4	.400	−102	107	1 1 1	.119	−192	197	6 1 5	.494	43	55	$\bar{4}$ 1 10	.408	− 43	39
6 0 4	.449	− 53	43	2 1 1	.158	− 79	83	$\bar{1}$ 1 5	.228	61	55	$\bar{5}$ 1 10	.405	30	36
$\bar{1}$ 0 4	.167	−241	213	3 1 1	.204	64	67	$\bar{2}$ 1 5	.216	− 27	24	$\bar{6}$ 1 10	.409	69	71
$\bar{2}$ 0 4	.159	−306	268	4 1 1	.252	− 98	107	$\bar{3}$ 1 5	.216	13	−	$\bar{2}$ 1 11	.480	37	51
$\bar{3}$ 0 4	.168	89	83	5 1 1	.302	−102	103	$\bar{4}$ 1 5	.227	28	28	$\bar{3}$ 1 11	.463	52	55
$\bar{4}$ 0 4	.191	− 58	59	6 1 1	.353	24	32	$\bar{5}$ 1 5	.252	25	32	$\bar{4}$ 1 11	.451	− 18	−
$\bar{5}$ 0 4	.224	−212	209	7 1 1	.404	− 12	−	$\bar{6}$ 1 5	.283	− 14	24	$\bar{5}$ 1 11	.445	6	−
$\bar{6}$ 0 4	.264	− 42	59	8 1 1	.455	− 57	59	$\bar{7}$ 1 5	.320	− 43	47	$\bar{6}$ 1 11	.445	69	67
$\bar{7}$ 0 4	.308	9	20	$\bar{1}$ 1 1	.093	− 2	−	$\bar{8}$ 1 5	.360	24	32	$\bar{4}$ 1 12	.494	11	−
$\bar{8}$ 0 4	.354	− 28	32	$\bar{2}$ 1 1	.119	−108	110	$\bar{9}$ 1 5	.404	13	−	$\bar{5}$ 1 12	.486	14	−
$\bar{9}$ 0 4	.401	− 53	55	$\bar{3}$ 1 1	.159	− 39	39	$\bar{10}$ 1 5	.449	− 52	55	$\bar{6}$ 1 12	.484	− 74	71
$\bar{10}$ 0 4	.450	− 27	24	$\bar{4}$ 1 1	.204	− 5	−	0 1 6	.296	− 94	91	0 2 0	.159	−161	189
$\bar{11}$ 0 4	.503	37	51	$\bar{5}$ 1 1	.253	15	32	1 1 6	.327	68	71	1 2 0	.167	− 6	−
0 0 6	.285	− 18	12	$\bar{6}$ 1 1	.303	− 10	−	2 1 6	.363	− 75	79	2 2 0	.190	44	12
1 0 6	.317	− 27	39	$\bar{7}$ 1 1	.353	− 35	43	3 1 6	.402	−105	91	3 2 0	.222	− 95	107
2 0 6	.354	46	43	$\bar{8}$ 1 1	.404	29	39	4 1 6	.444	8	−	4 2 0	.263	− 48	59
3 0 6	.394	19	39	$\bar{9}$ 1 1	.455	29	43	5 1 6	.489	5	−	5 2 0	.307	21	36
4 0 6	.437	− 81	83	0 1 2	.124	97	107	6 1 6	.502	− 40	47	6 2 0	.353	− 14	−
$\bar{1}$ 0 6	.260	16	16	1 1 2	.153	333	308	$\bar{1}$ 1 6	.272	−196	181	7 2 0	.400	− 28	35
$\bar{2}$ 0 6	.244	108	99	2 1 2	.193	− 5	20	$\bar{2}$ 1 6	.256	47	43	0 2 1	.165	−225	233
$\bar{3}$ 0 6	.238	58	55	3 1 2	.238	− 28	32	$\bar{3}$ 1 6	.251	− 2	−	1 2 1	.180	30	32
$\bar{4}$ 0 6	.245	− 80	67	4 1 2	.285	151	150	$\bar{4}$ 1 6	.257	−180	170	2 2 1	.209	− 15	20
$\bar{5}$ 0 6	.261	122	122	5 1 2	.334	69	63	$\bar{5}$ 1 6	.273	− 42	55	3 2 1	.246	− 82	83
$\bar{6}$ 0 6	.286	174	170	$\bar{1}$ 1 2	.112	−125	118	$\bar{6}$ 1 6	.297	26	39	4 2 1	.287	− 52	51
$\bar{7}$ 0 6	.319	− 68	63	$\bar{2}$ 1 2	.124	271	249	$\bar{7}$ 1 6	.328	− 42	39	5 2 1	.331	− 6	−
$\bar{8}$ 0 6	.356	17	−	$\bar{3}$ 1 2	.154	207	221	$\bar{8}$ 1 6	.364	− 51	63	6 2 1	.378	41	47
$\bar{9}$ 0 6	.396	157	146	$\bar{4}$ 1 2	.194	− 66	75	$\bar{9}$ 1 6	.404	− 22	−	7 2 1	.426	− 22	−
$\bar{10}$ 0 6	.439	16	−	$\bar{5}$ 1 2	.239	57	59	$\bar{10}$ 1 6.	.446	25	36	8 2 1	.475	− 39	36
$\bar{11}$ 0 6	.484	− 32	43	$\bar{6}$ 1 2	.286	114	118	0 1 7	.342	− 18	−	9 2 1	.530	44	39
0 0 8	.380	164	154	$\bar{7}$ 1 2	.335	31	36	1 1 7	.373	12	−	$\bar{1}$ 2 1	.165	−162	−
1 0 8	.411	52	55	0 1 3	.163	109	110	2 1 7	.408	− 30	43	$\bar{2}$ 2 1	.181	114	114
2 0 8	.447	− 45	51	1 1 3	.194	97	99	3 1 7	.446	− 32	20	$\bar{3}$ 2 1	.210	−146	154
3 0 8	.485	55	71	2 1 3	.233	− 4	−	$\bar{1}$ 1 7	.317	−102	154	$\bar{4}$ 2 1	.246	−236	237
$\bar{1}$ 0 8	.354	− 19	−	3 1 3	.276	6	−	$\bar{2}$ 1 7	.299	− 20	−	$\bar{5}$ 2 1	.288	43	51
$\bar{2}$ 0 8	.334	− 28	−	4 1 3	.322	24	−	$\bar{3}$ 1 7	.290	33	28	$\bar{6}$ 2 1	.332	− 7	36
$\bar{3}$ 0 8	.322	177	162	5 1 3	.370	31	−	$\bar{4}$ 1 7	.290	−109	110	$\bar{7}$ 2 1	.379	−143	150
$\bar{4}$ 0 8	.318	70	75	6 1 3	.419	− 2	−	$\bar{5}$ 1 7	.300	− 82	83	$\bar{8}$ 2 1	.427	− 39	39
$\bar{5}$ 0 8	.323	− 49	51	7 1 3	.469	− 25	43	$\bar{6}$ 1 7	.318	37	36	$\bar{9}$ 2 1	.476	20	32
$\bar{6}$ 0 8	.335	58	59	$\bar{1}$ 1 3	.145	− 57	55	$\bar{7}$ 1 7	.344	− 39	47	$\bar{10}$ 2 1	.530	− 29	36
$\bar{7}$ 0 8	.356	78	83	$\bar{2}$ 1 3	.146	74	79	$\bar{8}$ 1 7	.374	− 79	39	0 2 2	.185	9	−
$\bar{8}$ 0 8	.382	17	28	$\bar{3}$ 1 3	.164	201	205	$\bar{1}$ 1 8	.363	47	47	1 2 2	.206	15	−

Table 3 *(continued)*

h k l	sin θ	$F_{calc.}$	$F_{obs.}$
2 2 2	.237	- 31	32
3 2 2	.275	- 27	-
4 2 2	.316	37	39
5 2 2	.361	- 16	-
6 2 2	.408	- 47	47
$\bar{1}$ 2 2	.177	22	16
$\bar{2}$ 2 2	.185	- 20	-
$\bar{3}$ 2 2	.206	- 6	-
$\bar{4}$ 2 2	.237	76	67
$\bar{5}$ 2 2	.275	1	-
$\bar{6}$ 2 2	.317	- 35	43
$\bar{7}$ 2 2	.362	54	47
$\bar{8}$ 2 2	.409	31	36
$\bar{9}$ 2 2	.457	- 26	36
0 2 3	.213	43	39
1 2 3	.238	6	16
2 2 3	.270	-214	221
3 2 3	.308	- 41	39
4 2 3	.350	60	67
5 2 3	.394	-107	110
6 2 3	.441	- 85	80
7 2 3	.488	26	39
$\bar{1}$ 2 3	.200	-167	158
$\bar{2}$ 2 3	.200	- 75	75
$\bar{3}$ 2 3	.214	19	20
$\bar{4}$ 2 3	.238	- 2	-
$\bar{5}$ 2 3	.271	- 22	-
$\bar{6}$ 2 3	.309	- 54	59
$\bar{7}$ 2 3	.351	37	43
$\bar{8}$ 2 3	.395	63	63
$\bar{9}$ 2 3	.442	- 45	43
$\bar{10}$ 2 3	.489	- 7	-
$\bar{11}$ 2 3	.540	65	63
0 2 4	.247	- 55	51
1 2 4	.274	38	16
2 2 4	.307	81	245
3 2 4	.345	- 12	43
4 2 4	.386	- 7	63
5 2 4	.430	34	110
$\bar{1}$ 2 4	.230	72	63
$\bar{2}$ 2 4	.224	94	95
$\bar{3}$ 2 4	.231	- 40	36
$\bar{4}$ 2 4	.248	12	-
$\bar{5}$ 2 4	.275	68	87
$\bar{6}$ 2 4	.308	10	16
0 2 5	.285	- 43	43
1 2 5	.313	91	95
2 2 5	.346	80	75
3 2 5	.384	6	-
4 2 5	.425	- 12	-
5 2 5	.468	18	-
6 2 5	.523	39	39
$\bar{1}$ 2 5	.266	51	-
$\bar{2}$ 2 5	.255	234	217
$\bar{3}$ 2 5	.256	8	-
$\bar{4}$ 2 5	.266	- 46	-
$\bar{5}$ 2 5	.286	204	197
$\bar{6}$ 2 5	.314	102	99
$\bar{7}$ 2 5	.348	- 52	51
$\bar{8}$ 2 5	.386	63	59
$\bar{9}$ 2 5	.426	94	87
0 2 6	.326	7	-
1 2 6	.354	10	-
2 2 6	.388	- 17	-
$\bar{1}$ 2 6	.305	- 3	-
$\bar{2}$ 2 6	.291	- 35	28
$\bar{3}$ 2 6	.286	- 17	-
$\bar{4}$ 2 6	.291	34	24
$\bar{5}$ 2 6	.305	- 39	28
$\bar{6}$ 2 6	.327	- 59	-
$\bar{7}$ 2 6	.356	30	28
$\bar{8}$ 2 6	.389	- 2	-
$\bar{9}$ 2 6	.427	- 55	51
0 2 7	.369	89	83
1 2 7	.397	74	75
2 2 7	.431	- 51	51
3 2 7	.467	25	-
4 2 7	.518	84	87
$\bar{1}$ 2 7	.346	- 41	39
$\bar{2}$ 2 7	.329	1	-
$\bar{3}$ 2 7	.321	60	59
$\bar{4}$ 2 7	.322	24	28
$\bar{5}$ 2 7	.330	- 21	28
$\bar{6}$ 2 7	.347	- 47	51
$\bar{7}$ 2 7	.370	28	32
$\bar{8}$ 2 7	.399	28	28
$\bar{9}$ 2 7	.432	- 80	83
$\bar{10}$ 2 7	.470	- 28	20
$\bar{11}$ 2 7	.513	44	43
0 2 8	.412	- 57	55
1 2 8	.441	- 15	-
2 2 8	.474	20	-
3 2 8	.517	- 18	39
$\bar{1}$ 2 8	.388	12	-
$\bar{2}$ 2 8	.370	16	-
$\bar{3}$ 2 8	.359	- 61	55
$\bar{4}$ 2 8	.355	- 21	36
$\bar{5}$ 2 8	.359	22	36
$\bar{6}$ 2 8	.371	- 18	16
$\bar{7}$ 2 8	.389	- 26	36
0 2 9	.456	- 87	87
$\bar{1}$ 2 9	.432	- 24	32
$\bar{2}$ 2 9	.412	39	36
$\bar{3}$ 2 9	.399	-102	99
$\bar{4}$ 2 9	.392	-110	103
$\bar{5}$ 2 9	.392	47	39
$\bar{6}$ 2 9	.399	- 31	39
$\bar{7}$ 2 9	.413	-125	114
$\bar{8}$ 2 9	.433	- 13	-
$\bar{9}$ 2 9	.458	19	-
$\bar{10}$ 2 9	.487	- 48	43
$\bar{11}$ 2 9	.526	- 45	47
$\bar{1}$ 2 10	.476	- 1	-
$\bar{2}$ 2 10	.455	- 11	-
$\bar{3}$ 2 10	.440	15	-
$\bar{4}$ 2 10	.431	34	24
$\bar{5}$ 2 10	.428	- 11	-
$\bar{6}$ 2 10	.431	- 10	-
$\bar{7}$ 2 10	.441	47	39
$\bar{5}$ 2 11	.466	- 24	24
$\bar{6}$ 2 11	.466	- 14	-
$\bar{7}$ 2 11	.472	47	51
$\bar{8}$ 2 11	.484	31	32
$\bar{9}$ 2 11	.510	- 38	-
$\bar{10}$ 2 11	.531	17	28
$\bar{11}$ 2 11	.545	63	51
1 3 0	.243	- 14	-
2 3 0	.260	- 6	-
3 3 0	.284	6	16
4 3 0	.317	- 11	28
5 3 0	.354	- 21	36
0 3 1	.242	- 29	-
1 3 1	.253	215	209
2 3 1	.274	82	79
3 3 1	.303	- 91	91
4 3 1	.338	122	118
5 3 1	.376	136	134
6 3 1	.418	- 39	43
7 3 1	.462	9	-
8 3 1	.518	81	79
$\bar{1}$ 3 1	.242	- 15	-
$\bar{2}$ 3 1	.254	118	114
$\bar{3}$ 3 1	.275	53	55
$\bar{4}$ 3 1	.303	- 2	-
$\bar{5}$ 3 1	.338	- 27	28
$\bar{6}$ 3 1	.376	19	-
$\bar{7}$ 3 1	.418	50	51
$\bar{8}$ 3 1	.462	- 45	43
$\bar{9}$ 3 1	.518	- 40	51
0 3 2	.256	23	20
1 3 2	.272	44	47
$\bar{1}$ 3 2	.250	3	-
$\bar{2}$ 3 2	.256	35	39
$\bar{3}$ 3 2	.272	35	28
$\bar{4}$ 3 2	.296	5	-
$\bar{5}$ 3 2	.327	9	-
$\bar{6}$ 3 2	.363	21	-
$\bar{7}$ 3 2	.403	11	-
$\bar{8}$ 3 2	.445	- 1	32
0 3 3	.277	-117	114
1 3 3	.296	-121	114
2 3 3	.323	9	-
3 3 3	.355	3	-
4 3 3	.392	- 33	28
5 3 3	.432	- 46	36
6 3 3	.475	7	-
7 3 3	.540	37	43
$\bar{1}$ 3 3	.267	80	71
$\bar{2}$ 3 3	.267	- 83	79
$\bar{3}$ 3 3	.277	-234	217
$\bar{4}$ 3 3	.297	29	32
$\bar{5}$ 3 3	.324	24	24
$\bar{6}$ 3 3	.356	-170	170
$\bar{7}$ 3 3	.393	- 59	55
$\bar{8}$ 3 3	.433	37	43
$\bar{3}$ 3 4	.291	- 22	36
$\bar{4}$ 3 4	.305	- 5	-
$\bar{5}$ 3 4	.327	1	-
$\bar{6}$ 3 4	.355	- 22	39
0 3 5	.336	-109	110
1 3 5	.360	59	59
2 3 5	.389	- 15	-
3 3 5	.423	-132	138
4 3 5	.460	- 3	-
5 3 5	.502	33	43
$\bar{1}$ 3 5	.319	- 82	75
$\bar{2}$ 3 5	.311	40	39
$\bar{3}$ 3 5	.311	- 5	-
$\bar{4}$ 3 5	.320	- 40	43
$\bar{5}$ 3 5	.337	- 37	39
$\bar{6}$ 3 5	.361	26	28
$\bar{7}$ 3 5	.390	59	55
$\bar{8}$ 3 5	.424	- 40	39
0 3 6	.371	- 19	28
1 3 6	.396	0	-
2 3 6	.426	- 14	43
$\bar{1}$ 3 6	.352	- 30	28
0 3 7	.409	23	24
$\bar{1}$ 3 7	.388	137	130
$\bar{2}$ 3 7	.374	18	-
$\bar{3}$ 3 7	.367	- 52	-
$\bar{4}$ 3 7	.367	143	138
$\bar{5}$ 3 7	.375	107	99
$\bar{6}$ 3 7	.389	- 59	47
$\bar{7}$ 3 7	.410	45	43
$\bar{8}$ 3 7	.436	109	107
$\bar{4}$ 3 8	.397	15	24
$\bar{5}$ 3 8	.401	18	28
$\bar{6}$ 3 8	.411	0	-
$\bar{7}$ 3 8	.428	6	-
$\bar{8}$ 3 8	.450	20	35
0 4 0	.317	-150	154
1 4 0	.321	- 27	27
2 4 0	.334	24	24
3 4 0	.353	- 94	91
4 4 0	.380	- 68	59
5 4 0	.411	11	-
6 4 0	.447	- 12	-
7 4 0	.485	- 40	39
0 4 1	.320	102	95
1 4 1	.329	- 20	-
2 4 1	.345	- 7	-
3 4 1	.368	39	47
4 4 1	.397	30	32
$\bar{1}$ 4 1	.320	61	51
$\bar{2}$ 4 1	.329	- 69	63
$\bar{3}$ 4 1	.345	63	51
$\bar{4}$ 4 1	.368	114	83
$\bar{5}$ 4 1	.397	- 34	36
$\bar{6}$ 4 1	.431	- 6	-
$\bar{7}$ 4 1	.468	75	71
0 4 2	.331	29	32
1 4 2	.343	7	-
2 4 2	.363	- 45	51
3 4 2	.388	- 19	24
4 4 2	.419	35	36
5 4 2	.454	- 27	32
6 4 2	.492	- 52	51
$\bar{1}$ 4 2	.327	14	-
$\bar{2}$ 4 2	.331	- 26	31
$\bar{3}$ 4 2	.343	16	-
$\bar{4}$ 4 2	.363	79	87
$\bar{5}$ 4 2	.389	0	-
$\bar{6}$ 4 2	.419	- 24	-
$\bar{7}$ 4 2	.454	64	71
0 4 3	.347	- 35	35
1 4 3	.363	- 9	-
2 4 3	.385	108	107
3 4 3	.413	13	-
4 4 3	.445	- 43	47
5 4 3	.480	55	55
6 4 3	.515	46	47
$\bar{1}$ 4 3	.339	74	67
$\bar{2}$ 4 3	.340	39	39
0 4 4	.369	- 35	39
1 4 4	.388	46	43
2 4 4	.412	93	95
$\bar{1}$ 4 4	.358	77	79
$\bar{2}$ 4 4	.354	104	83
$\bar{3}$ 4 4	.358	- 17	-
$\bar{4}$ 4 4	.370	12	35
$\bar{5}$ 4 4	.388	78	63
0 4 5	.396	35	-
1 4 5	.416	- 41	47
2 4 5	.442	- 45	47
$\bar{1}$ 4 5	.382	- 22	24
$\bar{2}$ 4 5	.375	-115	99
$\bar{3}$ 4 5	.375	8	-
$\bar{4}$ 4 5	.382	36	36
$\bar{5}$ 4 5	.397	-102	91
$\bar{6}$ 4 5	.417	- 49	55
$\bar{7}$ 4 5	.443	39	36
$\bar{8}$ 4 5	.473	- 27	-
$\bar{9}$ 4 5	.505	- 52	59
$\bar{2}$ 4 6	.400	- 48	51
$\bar{3}$ 4 6	.396	- 10	-
$\bar{4}$ 4 6	.400	25	-
$\bar{5}$ 4 6	.410	- 54	63
$\bar{6}$ 4 6	.427	- 63	63
$\bar{7}$ 4 6	.449	24	39
$\bar{8}$ 4 6	.476	- 10	-
$\bar{9}$ 4 6	.509	- 64	63
0 4 7	.459	- 50	47
1 4 7	.483	- 37	39
$\bar{1}$ 4 7	.441	26	39
$\bar{2}$ 4 7	.429	7	-
$\bar{3}$ 4 7	.422	- 34	39
$\bar{4}$ 4 7	.423	- 16	-
$\bar{5}$ 4 7	.429	17	16
0 4 8	.495	- 66	71
$\bar{1}$ 4 8	.475	3	-
$\bar{2}$ 4 8	.461	11	-
$\bar{3}$ 4 8	.452	- 68	63
$\bar{4}$ 4 8	.449	- 36	32
$\bar{3}$ 4 9	.484	54	43
$\bar{4}$ 4 9	.478	57	51
$\bar{5}$ 4 9	.479	- 35	-
$\bar{6}$ 4 9	.485	10	-
$\bar{7}$ 4 9	.496	68	59

The structure of hessite is illustrated in Figs. 3a and 3b. There are two structurally different types of silver atoms. One (Ag_I) is surrounded by four tellurium atoms at 2.87, 2.91, 3.04 and 2.99 Å, making a somewhat distorted tetrahedron. The average Ag—Te distance of this tetrahedron is 2.95 Å. The other type of silver atom (Ag_{II}) has five close tellurium neighbors at 3.04, 3.01, 2.95, 2.90 and 2.85 Å, again giving an average Ag—Te distance of 2.95 Å. Each Te atom has nine

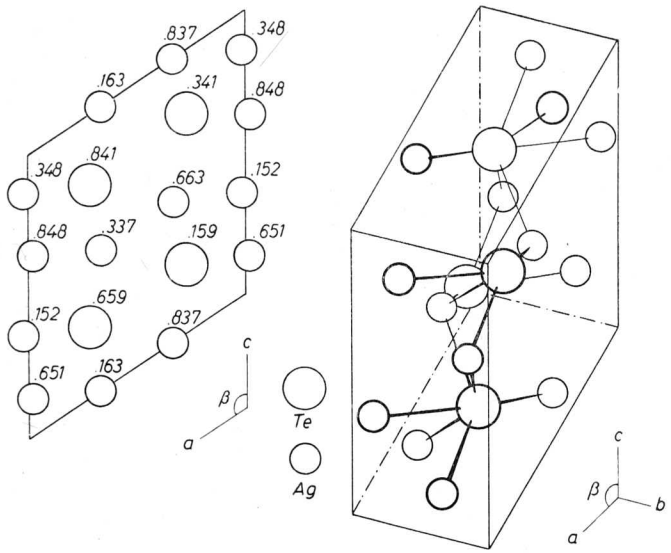

Fig. 3. The structure of hessite, Ag_2Te-III. (*a*) Orthographic projection. (*b*) Clinographic projection

fairly evenly spaced silver atoms around it. Although little significance can be attached to the average bond length, it is interesting to note that in the gold-silver telluride, sylvanite ($AuAgTe_4$), the silver atom has six tellurium neighbors, two at 2.69, two at 2.96, and two at 3.20 Å, again averaging 2.95 Å[8]. In petzite (Ag_3AuTe_2) the silver is tetrahedrally coordinated to two tellurium atoms at 2.90 Å and two at 2.95 Å[6].

It should also be pointed out that in the other gold and gold-silver tellurides every tellurium atom has one close tellurium neighbor, but in hessite there are no tellurium — tellurium distances closer than 4.26 Å.

[8] G. Tunnel and L. Pauling, The atomic arrangement and bonds of the gold-silver ditellurides. Acta Crystallogr. **5** (1952) 375—381.

Attempts to find the relations between this structure and the orthorhombic cell of ROWLAND and BERRY were unsuccessful. Although their orthorhombic cell is the cell best fitting the Weissenberg and rotation record of their crystal (hessite, type I), there still remain quite a number of reflections that do not fall on the reciprocal lattice points based on this cell. In so far as the powder diffraction records of the two crystals are identical, it is felt that their single crystal diffraction record was produced by a composite of several crystals of monoclinic Ag_2Te-III of different orientations. An investigation is presently under way on Ag_2Te-II and Ag_2Te-I, including a study of the transformation twinning and domain orientation resulting from cooling Ag_2Te-II to Ag_2Te-III. This may throw some light on the above relations.

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