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The crystal structure of synthetic christite, HgTlAsS₃

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Auszug

Die Kristallstruktur von synthetischem Christit, HgTlAsS₃, wurde bestimmt und bis zu R = 0.044 verfeinert. Die Gitterkonstanten sind $a = 6.113 \pm 0.001$, $b = 16.188 \pm 0.004$, $c = 6.111 \pm 0.001$ Å, $\beta = 96.71 \pm 0.02^{\circ}$; Z = 4; Raumgruppe $P2_1/n$.

Die Struktur besteht aus AsS_3 -Pyramiden, die durch HgS_4 -Tetraeder zu einer zweidimensionalen Schicht parallel {010} verbunden werden. Die Tl-Atome liegen zwischen den Schichten; sie halten diese durch schwache Bindungen zusammen, was die beobachtete vollkommene Spaltbarkeit nach {010} erklärt. Die aus Pulveraufnahmen berechneten Daten stimmen gut mit denen des natürlichen Christits überein.

Abstract

The crystal structure of synthetic christite, HgTlAsS₃ has been determined. The crystal is monoclinic with the space group $P2_1/n$. Four formula units are contained in a unit cell of dimensions $a = 6.113 \pm 0.001$, $b = 16.188 \pm 0.004$, $c = 6.111 \pm 0.001$ Å, $\beta = 96.71 \pm 0.02^{\circ}$. The structure was refined by fullmatrix least-squares methods using diffractometer data to a conventional discrepancy index, R, of 0.044.

The structure consists of AsS_3 pyramids connected by HgS_4 tetrahedra to form a polymeric two-dimensional sheet structure parallel to $\{010\}$. The thallium atoms lie between the sheets, connecting them together with weak bonds, which gives the perfect $\{010\}$ cleavage observed. The calculated powder diffraction pattern agrees well with that of natural christite.

Introduction

This investigation was prompted by a study of the new mineral christite (RADTKE, DICKSON, SLACK and BROWN, 1976), from the Carlin gold mine, Nevada, U.S.A., where several other rare thallium

minerals occur (RADTKE and DICKSON, 1975). As the natural material proved unsuitable for a single-crystal analysis, synthetic christite was prepared for single-crystal study.

Experimental

Crystals were prepared by recrystallizing synthetic HgTlAsS₃ powder in contact with a $1^{0}/_{0}$ Na₂B₄O₇ solution in a sealed gold tube at 285 °C and 250 bars pressure for 4 days. Individual euhedral crystals grew on the tube wall, but most of the product was a porous holocrystalline cake. The atomic spacings of ground individual crystals were identical to spacings of the holocrystalline mass and of the new mineral, christite.

The crystals obtained were plate-like and orange in colour. After considerable difficulty with multiple and curved crystals, a crystal suitable for an x-ray diffraction analysis was found.

The synthetic crystal of christite selected for single-crystal study was tabular, flattened parallel to $\{010\}$, slightly elongated parallel to the *c* axis, and was enclosed by the $\{010\}$, $\{\overline{1}01\}$ pinacoids and the $\{110\}$ and $\{011\}$ prisms. Overall dimensions were $0.07 \times 0.03 \times 0.11$ mm. The crystal is bright orange, in contrast to the deep red shown by large crystals and thick plates. HgTlAsS₃ is soft and shows a perfect cleavage parallel to $\{010\}$ along with several other less developed cleavages. The crystals deform easily in a ductile manner. Approximate unit-cell constants and space-group absences were obtained from Weissenberg and precession photographs. The systematic absences 0k0, k = 2n + 1; h0l, h + l = 2n + 1 found are consistent with space group $P 2_1/n$.

The unit-cell parameters were refined by a least-squares treatment of the setting angles of 12 reflections centred automatically on a Hilger and Watts Y290 automatic diffractometer, using zirconium-filtered molybdenum radiation ($\lambda = 0.71069$ Å). Crystal data are given in

HgTlAsS₃, Formula weight = 576.07 Monoclinic, $P 2_1/n$ $a = 6.113(1), b = 16.188(4), c = 6.111(1) \text{ Å}, \beta = 96.71(2)^{\circ}$ $V = 600.6 \text{ Å}^3, Z = 4$ $D_c = 6.37 \text{ g} \cdot \text{em}^{-3}$ $\mu (\text{MoK}\alpha) = 596 \text{ cm}^{-1}$

Table 1. In this and following tables, estimated standard deviations in the least significant figures are given in parentheses.

The intensities were measured by the $\omega/2\theta$ scan technique with a scan step of 0.01° and a counting time of 1.5 sec/step. Each reflection was scanned through a range of 0.8° centred on the peak. The local background was measured for 25 seconds at each end of the scan using the stationary-counter/stationary-crystal technique. To monitor the crystal and electronic stability, the intensities of three reflections were measured periodically throughout the data collection, but only random fluctuations of $\pm 3^{0}/_{0}$ were observed. All independent reflections in the sphere with $\theta < 25^{\circ}$ were measured. The integrated intensities and their standard deviations were calculated as described by CORFIELD *et al.* (1967). The 702 reflections for which $I > 3\sigma_{\rm I}$ were used in the subsequent analysis.

Structure determination and refinement

A three-dimensional Patterson synthesis enabled the positions of the mercury, thallium and arsenic atoms to be found. Least-squares refinement followed by a difference Fourier synthesis revealed the positions of the three sulphur atoms. All atoms were then refined by full-matrix least-squares (STEWART *et al.*, 1972), the mercury, thallium and arsenic atoms having anisotropic and the sulphur atoms having isotropic thermal parameters. Scattering factors were those of CROMER and MANN (1968) with the anomalous dispersion corrections for mercury, thallium and arsenic of CROMER (1965). The function minimized in the least-squares refinement was $\Sigma w_i (|F_0| - |F_c|)^2$, where F_0 and F_c are the observed and calculated structure factors and the weight $w_i = 4F_0^2/\sigma(I)^2$. At this stage $R_1 = \Sigma ||F_0| - |F_c||/\Sigma |F_0| =$ 0.115 and $R_2 = [\Sigma w_i (|F_0| - |F_c|)^2 / \Sigma w_i |F_0|^2]^{1/2} = 0.150$.

Corrections for absorption were applied (TEMPLETON and TEM-PLETON, 1974) by the analytical method of DE MEULENAER and TOMPA (1965); the transmission coefficients ranging from 0.204 to 0.042. Three further cycles of full-matrix least squares with the temperature factors refined as above the discrepancy indices $R_1 = 0.046$ and $R_2 = 0.050$. The mercury and thallium positions were now interchanged and the atom parameters were refined as above to convergence resulting in $R_1 = 0.045$ and $R_2 = 0.049$. A test on the ratio of the weighted residuals (HAMILTON, 1965) showed that the second refinement was not significantly better at the $90^{0}/_{0}$ confidence level. The mercury and thallium positions were again interchanged

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 Table 2. Positional parameters for synthetic christite

Atom	<i>x</i>	y	2		
Tl	0.1633(2)	0.45039(8)	0.3366(2)		
Hg	0.0793(2)	0.25013(8)	0.9207(2)		
As	0.5759(5)	0.3916(2)	0.9254(5)		
S(1)	0.2046(10)	0.3917(5)	0.8587(12)		
S(2)	0.1419(12)	0.2408(5)	0.3559(14)		
S(3)	0.1421(11)	0.1077(4)	0.7962(12)		

Table 3. Thermal parameters ($\times 10^2$). The form of the thermal ellipsoids is given by exp $-2\pi^2(U_{11}h^2a^{*2}...+...+2\ U_{12}hka^*b^*+...)$

Atom	U_{11}	U_{22}	U33	U_{12}	U13	U_{23}
Tl	2.79(6)	3.82(8)	3.50(7)	0.25(6)	0.73(5)	-0.38(7)
Hg	3.03(7)	2.94(7)	4.07(8)	-0.33(5)	0.01(6)	-0.27(6)
As	1.95(15)	2.21(17)	3.09(18)	-0.18(13)	0.59(13)	0.22(14)
S(1)	1.8(4)	3.2(5)	2.9(5)	0.2(3)	-0.5(3)	-0.3(4)
S(2)	1.9(4)	3.1(5)	2.4(5)	-0.4(3)	0.2(3)	0.4(4)
S(3)	1.9(4)	2.2(4)	3.3(5)	0.1(3)	-0.1(3)	0.2(4)

and the sulphur atoms were now refined to convergence with anisotropic thermal parameters which gave final values of $R_1 = 0.044$ and $R_2 = 0.048$, which is significantly better at the $95^{0}/_{0}$ confidence level. An analysis of the weighting scheme showed that the average $w_i(|F_0| - |F_c|)^2$ was approximately constant over a range of $\sin \theta$ and $|F_0|$ values. A final difference Fourier showed no residual density greater than $10^{0}/_{0}$ of that expected for a sulphur atom. The final positional parameters are given in Table 2 and their thermal parameters in Table 3. Observed and calculated structure-factor amplitudes for the observed reflections are given in Table 4.

Results and discussion

As the x-ray scattering factors for mercury and thallium atoms are very similar, it was not possible to distinguish them by an x-ray diffraction analysis. The two "heavy" atom sites in this structure are in different coordination environments. One site (A) provides the bridge between AsS₃ pyramids and is tetrahedral in coordination with shorter bond lengths (2.46–2.66 Å), the second site (B) shows no clear-cut coordination and the bonding is much weaker (3.11–3.52 Å). In the crystal structure of vrbaite (OHMASA and NOWACKI, 1971), a mercury or thallium atom is in a similar environment to site A; strong

h k l	F _o F _c	ħ k	I P F	с в 1	، ۱	F _o F _c	b k l	P _o F _c	h	k 1	F _o F _c	h	k 1	F	Fe	ь	k l	F,	Fc
-7 1 1	65 70	-4 6	4 97 94	4 -2 4	4 2	102 100	-1 12 3	83 82	1	2 1	392 437	2	84	107	104	4	12	215	225
-7 2 1	58 57 84 86	-4 7	2 37 39	9	3	53 52	-1 13 1	46 32		5	50 51 89 79	2	90	49 197	51 199	4	22	116	52 120
-732	51 55 59 63		4 149 139 5 35 4	9	5	86 89 37 15	2 4	89 83 31 41	1	30	94 87 146 142		1 3	123	123	4	30	33 223	219
-7 5 1	133 139	-4 8	1 39 3	2 -2 5	5 1 3	19 21	-1 14 4	74 73		2	97 93		4 5	120	121		1	85	86
	53 56		3 59 5	6	5	35 37	-1 16 1	72 68		- í	83 82	2	10 2	201	207		5	41	44
-0 1 1	31 32	-4 9	5 88 81	5 -2 (ь 51	44 42 63 66	2	42 34 81 71	1	40	206 203	2	11 0	60	96 63	4	4 0	34	32
3	76 81	-4 11	1 46 3	5	3	170 164 98 99	-1 17 1 2	132 125 28 30		1 2	146 147		34	71 64	71		4	100	102 60
-621	38 48 63 63	-4 12	2 152 15	3	4 5	77 80 78 71	-1 18 1	66 67 46 55		3	193 194	2	5 12 0	44 116	46	4	52	219 40	228 48
4 3 9	40 51		3 72 6	6 1 _2 ·	6	65 66	002	21 22	1	50	99 99		1	90 71	85 69	4	6 0	128	129
. , ,	60 63	-4 14	1 76 7	4	2	277 288	0 1 1	54 43		3	18 27		5	58	50		3	107	113
-641	79 78		2 59 58 3 58 54	6 4	5	28 32 104 105	23	368 414 191 199	1	60	198 200 206 206	2	13 0	89 43	81 23		9 5	149	147
-651	49 42 82 76	-4 16 -3 0	1 81 8	1-28 5	31	54 56 36 41	4 5	106 106 102 96		1 2	110 111 197 197	2	4 14 1	59 84	44 78	4	70	232 75	241 72
2	34 43	-3 1	3 223 22	5	3	56 57	0 2 0	44 41		3	72 77		23	208	207	4	2	94	95
-6 6 1	67 65	-, .	2 132 13	0	5	38 42	1	89 93	1	70	64 62		4	27	36		2	104	110
-672	120 124		5 42 4 4 140 130	6 -2 9) 1	151 151	3	102 109		3	186 194	2	3	235 52	41		4	66	- 74 59
-6 B 1	42 40 51 47		5 90 89	9 3	2 5	87 84 49 39	5	73 76	1	80	70 67	2	16 0	50 48	40 34	4	90	72 93	68 97
-6 10 2	51 51	-3 2	1 154 144	8 =2 10 8	2	36 41 124 126	0 3 1	29 38 145 143		1	295 301 127 129	2	18 0	100 57	103		2	124	129
-5 0 1	185 191		3 59 50	6 -2 1	1	113 113	2	55 59	1	5	60 61	3	0 1	141	131	4	10 0	106	103
5	88 87		5 121 11	1	3	43 35	4	191 201		2	118 121	_	5	71	73	4	11 0	51	53
-5 1 1	42 39	-33	1 186 18	4 -2 1; 4	21	48 50	040	213 212 206 205		- 4	65 63 89 93	3	10	213	204 62		2	77	85 73
3	89 94 81 81		3 32 31 5 46 4	3 -2 13 2	51 2	88 85 168 169	2 4	64 64 78 76	1	5 10 3	112 116		4	44 73	49 65	4	12 2	66 58	73 59
-5 2 1	51 42 49 48	-3 4	6 57 5	7	3	55 59 36 43	5	111 113	1	11 0	98 93	3	20	120	116	4	13 1	57	57
2	77 75		2 187 18	6 -2 1/	12	98 92	0 5 1	97 96		3	65 73		2	71	70	4	14 0	80	77
4	46 46		4 108 10	3	_ 4	52 53	5	47 48		5	116 124		5	36	25	4	16 0	52	43
-5 3 1	33 31 34 34		5 71 69	9 -2 10 6	52	65 58 68 70	0 6 6	429 463 199 204	1	12 0	78 77 239 239	3	30	132 297	125	5	01	54 81	54 74
3	47 48 73 70	-3 5	1 353 360	6 -2 17 2	712	29 33	2	90 88 92 88		25	83 85 59 50		24	103	100	5	10	104	110
-5 h 1	129 130		3 58 6	2 -1 0	1	171 165	4	111 118	1	13 5	128 130		5	149	141		2	102	103
2	95 96		5 195 19	0	5	174 176	6	45 53	1	14 0	97 95	3	4 0	36	34	,	1	88	91
4	74 75 51 36	-3 0	2 95 99	0 -1	2	103 98 251 246	0 7 1	63 61 160 169		2	58 55 79 76		1 2	203 135	199 134		2	77	85 31
-551	49 48 45 51		4 92 80	6 3	3	156 159 88 85	3	72 79	1	15 0 16 1	43 42 57 66		34	110	110	5	31	99 65	101
2	37 41	-3 7	1 72 6	9	5	37 33	080	176 185	1	17 3	56 54	٦	5 0	81	82 16		3	158	156
-561	111 113		3 18 19	9	7	45 58	2	164 166	i	18 0	48 39	,	1	22	25	5	4 0	123	124
3	63 57		5 39 4	, -, . !	2	74 72	5	51 52	2	0 0	29 23	3	60	95	95		3	90	87
-573	48 47 50 45	-38	6 29 30 1 113 112	2	3	142 142	091	120 128		4	547 588 26 30		2	113	82 117	5	50	56 56	61 59
4	45 46 96 96		2 63 6	3	5	40 40	23	185 196 124 139	2	10	396 424 86 79		3	47 107	52 110	5	6 0	220 77	224 80
-582	42 43		4 64 51	6 2 - 1 ·	, 7	58 68	4 0 10 0	57 60		4	219 211	7	- 5	36	44		2	70	68
-592	47 42	-3 9	1 202 20	1	2	140 138	3	54 52		6	68 60	,	1	201	201	_	4	49	46
	95 92		5 93 9	1	5	42 28	0 11 1	85 88	2	2 0	51 49		5	75	4) 78	5	13	>> 85	40 82
-5 10 1	246 247 36 41	-3 10	1 37 3 3 295 30	4 -1 × 1	4	275 288 162 164	23	90 96 92 92		2	52 48 70 70	3	802	78 88	81 87	5	80	56 70	61 65
-5 11 1	37 39	-3 11	5 45 30	6 1	56	216 224 70 68	0 12 1	54 47 69 70		4 5	116 111		3	158	165	5	9 1	67	61 127
-5 12 1	27 40 79 78		3 40 4	5	7	48 48	2	113 114	2	30	63 60	3	90	146	148	-	23	85	89
-5 13 2	58 50	7 10	5 107 110	0	2	18 21	0 13 2	78 77		3	99 97		2	134	142	5	10 2	43	37
- 6	59 53	-) 12	3 43 4	5) 5	48 47	3	128 132		6	57 62 87 78		5	53	33	5	11-1	143	142
-4 11	95 91 141 141	-3 13	5 67 73	3	6 7	57 63	0 14 0	47 48 273 270	2	40	74 70	3	10 0	54 175	50 178	5	2 12 1	51 50	50 58
4	36 30 84 79	-3 14	4 63 64	6 -1 (0	51 2	95 99 63 65	1 2	96 95 50 48		2	176 171	3	11 0	83	80 97	5	2 13 0	62	56
-4 2 1	113 102	-	3 44 44	8	4	73 69		68 66 30 52		- 6 - 0	40 42		1	80	78	6	0 2	106	111
2	255 258	-3 15	1 109 10	5.	6	45 59	2	213 215	4	1	40 33	_	4	23	27	0	2	70	74
5	53 44	-5 10	3 97 8	9 - I., 9	2	98 98	0 16 0	43 43		ر 4	92 91 209 215	,	12 0	27	74 38	6	20	158	73
-4 3 1	39 46 29 29	-3 17	1 75 74	0 0	3	66 67 45 22	23	28 41 58 52	2	60 1	90 90		2	46 140	38 152	6	1	102	103
4	142 147	-2 1	6 123 110	9 –1 8 9	32	47 53	4 0 18 1	42 48		2	317 326	7	13 0	61	55	6	3	29	36
- 4 1	40 43		2 138 130	6 6 _1 4	. 4 . 0	28 34	2	51 53		4	67 59	,	1	137	135	4	2	49	51
2	57 57		5 89 9	5	3	195 195	3	137 129	2	70	174 175	3	14 1	78	>) 73	0	ь 0 1	38	33
35	105 107 40 35	-2 2	1 74 7	9 -1 10 4) 1 2	239 235 27 38	5 7	54 45 111 98		1	51 47 36 43	3	15 2 16 0	44 58	39 52	6	7^{2}_{2}	68 147	65 142
-4 5 2	30 23 67 73		3 146 146	6 3 - 1 1'	5 1	212 220 89 87	1 1 0 2	51 43 81 78		4	89 87 31 36	3	17 1	65 104	55 107	6 7	80	153	155
4	55 52 92 89	-2 3	5 63 6	7	23	106 114	3	66 60	,	6 8.0	127 121	á	0 0	229	233	ż	20	50	50
-4 6 1	71 74	- /	2 301 298	- 8 1	5	32 37	5	106 102	-	1	129 129		4	255	249	'	40	8ر	27
3	86 87		7 48 4	7	2	51 52	120	37 34 101 93		3	86 85	4	+ 0	165	163				

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Fig. 1. A stereoscopic view of the unit cell

space-group evidence exists for vrbaite that mercury occupies this position. Consequently, we have assigned site A as a mercury atom and site B as a thallium atom.

The crystal structure consists of trigonal pyramids of AsS₃ linked together by mercury atoms to form a two-dimensional sheet-like network (see Figs. 1 and 2). The sheets are parallel to $\{010\}$ and occur every b/2 in the y direction. The thallium atoms are located between the sheets, bonded weakly to their nearest neighbours. The structure falls into the category IIa, ($\phi = 3$) of sulphosalt classification suggested by NOWACKI (1969, 1970). Bond lengths and angles are given in Table 5.

The AsS₃ pyramid is similar to that found in other sulphosalts [e.g. FLEET (1973), TAKÉUCHI, OHMASA and NOWACKI (1968)]. The As—S bond lengths of 2.258(10), 2.232(7) and 2.255(10) Å come into

The crystal structure of synthetic christite



OHg ⊙As OS

Fig. 2. A view projected down (010) of one sheet

the "non-bridge" category described by TAKÉUCHI and SADANAGA (1969). The S—As—S bond angles are slightly larger (mean = 101.3°) than the mean observed (98.66°) by TAKÉUCHI and SADANAGA. An As—Tl contact of 3.50(1) Å occurs in the fourth tetrahedral coordination position of the arsenic atom.

The sulphur atoms S(1) and S(3) each have only two nearest neighbours: one mercury and one arsenic atom. The S(2) sulphur atom has three nearest neighbours: two mercury atoms and one arsenic atom. This difference in coordination is reflected in the Hg—S(2) bond lengths of 2.65(1) and 2.66(1) Å compared with Hg—S(1) and Hg—S(3)bond lengths of 2.461(7) and 2.472(7) Å respectively. The four sulphur atoms around the mercury atom form a distorted tetrahedron, similar to that found in other mercury compounds (GRDENIĆ, 1965). There are no other contacts less than 3.5 Å around the mercury atom. The expected tetrahedral covalent Hg—S bond length (PAULING, 1960) is 2.52 Å which is intermediate between the two different types found here.

The arrangement of atoms around the thallium atom shows no systematic coordination geometry, with seven Tl—S contacts ranging from 3.11—3.52 Å. This is typical of thallium atoms (OHMASA and NOWACKI, 1971) which are loosely bound in 'holes' formed in a poly-

Bond	Length	Bond	Length			
$\begin{array}{c} {\rm Hg-S(1)} \\ {\rm Hg-S(3)} \\ {\rm Hg-S(2)} \\ {\rm Hg-S(2')} \\ {\rm As-S(1)} \\ {\rm As-S(2)} \\ {\rm As-S(3)} \\ {\rm As-Tl} \end{array}$	$\begin{array}{c} 2.460(9) \text{ \AA}\\ 2.471(8)\\ 2.646(11)\\ 2.661(11)\\ 2.258(10)\\ 2.232(8)\\ 2.255(11)\\ 3.499(12)\end{array}$	$ \begin{array}{c c} Tl - S(1) \\ Tl - S(1') \\ Tl - S(1'') \\ Tl - S(2) \\ Tl - S(3) \\ Tl - S(3') \\ Tl - S(3'') \\ Tl - S(3'') \end{array} $	$\begin{array}{c} 3.310(9) \text{ \AA} \\ 3.110(9) \\ 3.520(9) \\ 3.397(7) \\ 3.111(8) \\ 3.303(8) \\ 3.509(8) \end{array}$			
Bond	Angle	Bond	Angle			
$\begin{array}{c} S(1)-Hg-S(3)\\ S(1)-Hg-S(2)\\ S(1)-Hg-S(2)\\ S(2)-Hg-S(2')\\ S(2)-Hg-S(3)\\ S(2')-Hg-S(3)\\ S(1)-As-S(2)\\ S(1)-As-S(3)\\ S(1)-As-Tl\\ S(2)-As-S(3)\\ S(2)-As-Tl\\ S(2)-As-Tl\\ S(2)-As-Tl\\ Hg-S(1)-As\\ Hg-S(2)-As\\ Hg'-S(2)-As\\ Hg'-S(2)-As\\ \end{array}$	$\begin{array}{c} 139.4(3) \\ ^{\circ}\\ 101.3(2)\\ 104.6(2)\\ 100.2(2)\\ 104.3(2)\\ 101.2(2)\\ 99.6(3)\\ 103.9(3)\\ 114.8(2)\\ 100.4(3)\\ 120.8(2)\\ 114.7(2)\\ 107.2(3)\\ 103.8(8)\\ 103.0(3) \end{array}$	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	99.9(3)° 106.8(3)			

Table 5. Bond lengths and anglesPrimed symbols refer to atoms in different asymmetric units

meric network of AsS_3 pyramids. As in lorandite (FLEET, 1973), the thallium atom is more closely associated with one sheet than the other. All five Tl—S contacts of less than 3.45 Å are to one sheet, the remaining two Tl—S contacts to the other sheet are 3.51 and 3.52 Å. There is however a Tl—Tl bond of 3.39 Å between sheets and a Tl—As contact of 3.50 Å. The former distance is similar to the Tl—Tl distance in elemental thallium (3.40 Å; WELLS, 1962), and the thallium atoms probably provide the principal cohesive force between sheets.

Two properties of monoclinic $HgTlAsS_3$ follow from the proposed sheet structure. The first is the perfect {010} cleavage observed in synthetic crystals and in the mineral. The polymeric $HgAsS_3$ sheets are linked to one another mainly by long Tl—Tl contacts which would be considerably weaker than the bonds within the sheets resulting in the micaceous cleavage. Secondly, it is possible to deform $\{010\}$ cleavage fragments ductily to smooth curved surfaces. This is a consequence of the ease with which the sheets slip past one another, *i.e.* the intersheet bonds break and then reform.

The structure is pseudo-tetragonal as evidenced both by the equality of the a and c axial lengths and also by the relationship of the x and z atom coordinates. However the cell-constants do not show any relationship to routhierite (JOHAN, MANTIENNE and PICOT, 1974) which is reported as a tetragonal form of HgTlAsS₃, but which contains noteworthy amounts of copper, silver, zinc and antimony.

The calculated x-ray powder diffraction data agree well with the observed data for natural christite (RADTKE *et al.*, 1976).

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