the hydrogen atom found by the least-squares refinement. The highest background peaks had heights of 0·12, 0·38 and 0·36 respectively of the hydrogen peak heights in the three projections. But none of the background peaks in the three projections is close to the hydrogen peak.

There are close-packed layers of (two-dimensional black-and-white space group) symmetry $2_1t[\bar{1}]$ (notation of Kitaigorodskii, 1955) parallel to the (100) plane with a sixfold coordination of each molecule. These layers are stacked parallel to one another and neighbouring layers are connected by hydrogen bonds. There are also hydrogen-bonded layers parallel to the $(10\bar{2})$ plane. The interaction between neighbouring layers of the latter type involves only van der Waals forces, which incidentally explains the easy cleavage of the crystal along the $(10\bar{2})$ plane (as well as the twinning across this plane, referred to earlier).

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The Crystal Structure of In_6S_7

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The crystal structure of In_6S_7 has been determined from powder and single-crystal X-ray diffraction data. The unit cell is monoclinic with $a=9{\cdot}090$, $b=3{\cdot}887$, $c=17{\cdot}705$ Å, $\beta=108{\cdot}20°$ and the space group $P2_1/m$. There are 2 formula units per cell and all In and S atoms are in special positions 2(*e*). The structure consists basically of two separate sections both consisting of almost cubic close-packed arrays of S atoms with In atoms in octahedral coordination, the two sections having equivalent directions at 61·5° to each other.

Introduction

A black crystalline phase occurring in the system In–In_2S_3 has from time to time been allocated various chemical formulae, including both In_4S_5 and In_5S_6. In a recent general survey of the system, however, Duffin & Hogg (1966) presented evidence showing that the phase is in fact In_6S_7.

Direct analysis to decide between the various formulae proved quite impossible, partly because some methods were inherently incapable of achieving the necessary accuracy but mostly because specimens sufficiently free from contamination by other phases could not be prepared. However, none of the ranges of composition yielded by analysis was in conflict with the formula finally adopted and this also applies to those

analyses of the phase given by other authors, including the recent estimate by Miller & Searcy (1965).

Positive evidence for the formula In_6S_7 is contained in the structure analysis described in this paper and is reinforced by density measurements which rule out the other formulae quoted above. An account of the experimental procedure used to obtain specimens and of the density determinations is given by the authors in the paper referred to above.

Unit cell and space group

The unit cell of In_6S_7 is monoclinic with lattice parameters $a=9{\cdot}090\pm0{\cdot}005$, $b=3{\cdot}887\pm0{\cdot}001$, $c=17{\cdot}705\pm0{\cdot}004$ Å, $\beta=108{\cdot}20\pm0{\cdot}05°$. These parameters are those giving a least-squares fit with the powder data given by Duffin & Hogg (1966) and they allow 2 formula units per cell, yielding a calculated density of 5·11 compared with a measured value of 5·08 g.cm^{-3}.

Because the material is opaque, twinned crystals cannot be eliminated by optical methods and in practice nearly all single crystals were found to be twinned when X-ray photographs were taken. The first suitable crystal was unfortunately very irregular in cross-section but was nevertheless used to obtain equi-inclination Weissenberg photographs about the *b* and *a* axes. These showed that the only systematic absences were those of $0k0$ with k odd and thus indicated a space group of either $P2_1$ or $P2_1/m$.

An important feature of the *b*-axis photographs was that the relative intensities of corresponding $h0l$ and $h2l$ reflexions were to a first approximation the same, as were those of $h1l$ and $h3l$. This suggested strongly that all the atoms lay on or near planes separated by $\frac{1}{2}$ in y.

Structure determination

First crystal

The intensities of reflexions from Weissenberg photographs were obtained from multiple-film exposures and visual comparison with a standard set of spots. After correction for Lorentz and polarization factors and for spot elongation on the upper layer lines, isotropic temperature and scale factors were obtained by means of a Wilson plot.

In an attempt to decide whether or not the structure was centred, the statistical distribution of intensities was examined by the $N(z)$ functions of Howells, Phillips & Rogers (1950). Fig. 1 shows that the $h0l$ points correspond almost exactly to the centric distribution, as is expected whether the space group is $P2_1$ or $P2_1/m$. The $0kl$ points, however, lie marginally nearer the centred curve for low z but do not yield an unequivocal answer. This could be explained if in this projection the atoms all lie in special positions since the theory is not then strictly valid. In view of the uncertainty in the space group, the structure analysis was performed on the assumption that it was $P2_1$ using initial y coordinates of 0 or $\frac{1}{2}$, for the atoms were not then constrained to lie in special positions and deviations of the y coordinates would be allowed if the structure were non-centrosymmetric. In fact during the refinement of the structure the least-squares program made no attempt to change the y coordinates and it is concluded that the true space group is $P2_1/m$, with $y=\frac{1}{4}$ or $\frac{3}{4}$, so that all atoms are in special positions 2(*e*).

The corrected intensities were used to obtain a Patterson projection on (010) [Fig. 2(*a*)] and the main peaks were taken as being due to In–In vectors because they would have a volume at least three times that of an In–S peak and nine times that of an S–S peak. The positions of 12 In atoms which completely accounted for the main peaks were determined by triangulation of the vectors, and these positions were then used in conjunction with a sharpened Patterson projection to obtain possible In–S vectors. This proved an uncertain process, and although 16 possible sites were obtained for the S atoms, one or two of these seemed somewhat dubious. To check these sites, the observed $h0l$ structure factors were used together with the phases from the provisional positions of the 12 In atoms to obtain an electron-density projection on to (010). The positions of S atoms showed up quite clearly and except in two cases coincided with the positions deduced from the sharpened Patterson function: no S atoms appeared in the two doubtful positions. The number of S atoms was thus established at this stage as 14 and the chemical formula very probably In_6S_7.

The y coordinates were found by means of the Patterson function

$$P_1(x,z)=\sum_h \sum_l |F_{o_{h1l}}|^2 \cos 2\pi(hx+lz)$$

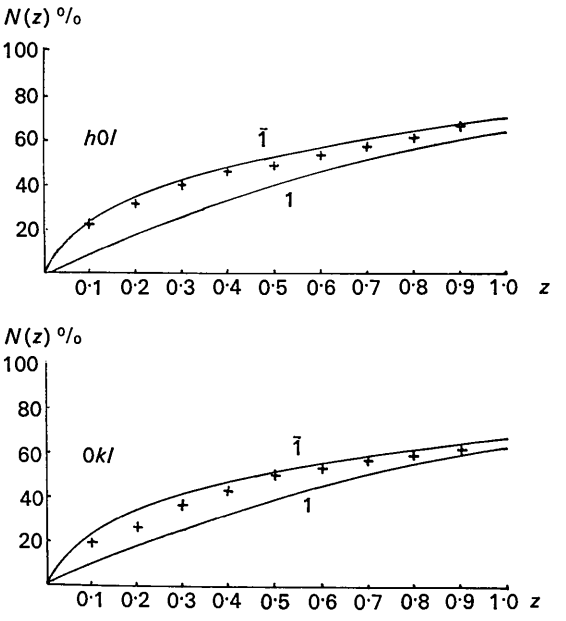

Fig. 1. The experimental $N(z)$ distributions given by $h0l$ and $0kl$ intensities. Full curves are theoretical distributions for centrosymmetric (upper) and non-centrosymmetric (lower) structures.

which differs from the projection on (010) used above in that the peaks due to vectors between atoms with the same y coordinate are weighted $+1$ and those due to vectors between atoms with y coordinates differing by $\frac{1}{2}$ are weighted -1 (Dyer, 1951). The y coordinates to be allocated to the In atoms were easily found on plotting this function [Fig. 2(*b*)], and those of the S atoms were allocated from considerations of packing in the unit cell. Structure factors calculated with the allocated y coordinates using the $h1l$ reflexions gave an R index of 0·22, sufficiently low to indicate that they were correct.

Second crystal

Another crystal was found, untwinned and of more regular shape – needle-like with a roughly rectangular cross-section. A completely fresh set of intensities was obtained and corrected as before. An absorption correction was then made with the use of the factors given by Bond (1959) with an equivalent radius of 0·0014 cm. The atomic coordinates obtained using the first crystal provided the starting point for the refinement of the structure. The scattering factors used to obtain calculated structure amplitudes were those for un-ionized atoms taken from *International Tables for X-ray Crystallography* (1962).

Structure refinement

The structure was initially refined in two dimensions, using the $h0l$ reflexions, several cycles being necessary to reduce the R index from 0·19 to 0·14. The refined x and z coordinates were used together with the y coordinates 0 or $\frac{1}{2}$ to calculate structure amplitudes F_c, for the $h1l$, $h2l$ and $h3l$ reflexions. These F_c's were then used to scale the F_o's of these layers. The refinement was continued in three dimensions, using all the data in space group $P2_1$. After several cycles the observed structure amplitudes were again scaled to the calculated ones for each layer separately and the refinement continued until the shifts in coordinates were small compared with the standard deviations. The atomic positions are given in Table 1, all atoms being in the special positions 2(*e*). Calculated structure amplitudes were then computed in space group $P2_1/m$ and compared with F_o's as in Table 2. The R value yielded by these data is 0·129.

Table 1. *Atomic parameters with standard deviations*

Values of x, z, σ_x and σ_z are fractions of the unit cell-edges multiplied by 10^4. The last two columns give the parameter B of the temperature factor $\exp[-B(\sin\theta/\lambda)^2]$ and its standard deviation.

	x	σ_x	z	σ_z	B	σ_B
In(1)	552	2	1214	1	1·76 Å²	0·03 Å²
In(2)	3708	2	1889	1	1·34	0·03
In(3)	5831	2	6044	1	1·48	0·03
In(4)	1401	2	4682	1	1·48	0·03
In(5)	8043	3	2747	1	2·35	0·04
In(6)	3088	2	9535	1	1·33	0·03
S(1)	8293	8	9947	4	1·28	0·10
S(2)	2287	8	3461	4	1·34	0·10
S(3)	4880	8	7283	4	1·33	0·10
S(4)	5344	8	906	4	1·39	0·11
S(5)	694	8	8257	4	1·42	0·11
S(6)	536	8	5895	4	1·26	0·10
S(7)	6364	8	4675	4	1·40	0·11

An electron-density projection was made on to the (010) plane (Fig. 3), and contained no spurious peaks other than those due to series-termination effects. A difference electron-density map was almost featureless: the exceptions were two small negative regions lying on either side of an In atomic site and two small positive regions similarly situated but at right angles to the negative ones. These effects are probably due to the assumptions either that the temperature factor is isotropic, that the crystal has a cylindrical cross section, or that no extinction occurred.

Because all the low angle strong reflexions have observed structure amplitudes about 70% of the calcu-

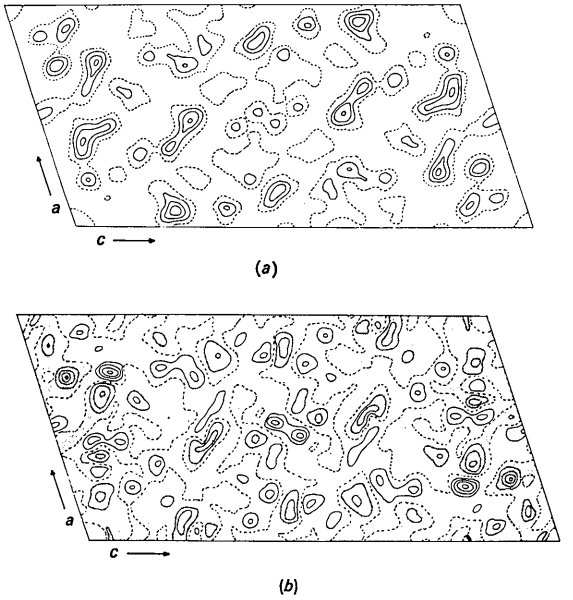

Fig. 2. (*a*) Patterson projection on the (010) plane. The zero level is indicated by the dashed line. (*b*) General Patterson projection $P_1(x,z)$ on the 010 plane. Shaded areas are negative, unshared areas positive.

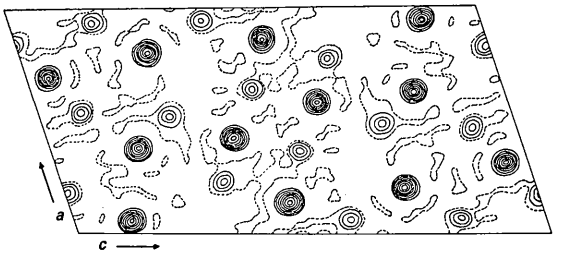

Fig. 3. Electron density projection on the (010) plane. Solid contours are drawn at intervals of 5 e.Å^{-2} for S atoms, and of 7 e.Å^{-2} for In atoms. The broken contour is at 2 e.Å^{-2}.

Table 2. *Observed and calculated structure factors*

Reflexions too weak to record photographically were allocated an intensity $I_o = I_{min}/2$, where I_{min} is the smallest intensity on the scale used for visual estimates.

H	K	L	F_o	F_c
0	0	-2	78	63
0	0	-3	79	-69
0	0	-4	14	11
0	0	-5	24	13
0	0	-6	40	-31
0	0	-7	65	56
0	0	-8	12	10
0	0	-9	140	-125
0	0	-10	55	46
0	0	-11	97	72
0	0	-12	117	-111
0	0	-13	110	-99
0	0	-14	140	-134
0	0	-15	153	155
0	0	-16	62	-45
0	0	-17	93	91
0	0	-18	27	23
0	0	-19	9	-6
0	0	-20	5	-7
0	0	-21	37	39
1	0	0	17	-6
1	0	-1	20	22
1	0	1	11	-7
1	0	-2	7	-5
1	0	2	89	71
1	0	-3	12	-9
1	0	3	147	-148
1	0	-4	159	-205
1	0	4	157	195
1	0	-5	235	-298
1	0	5	23	13
1	0	-6	62	57
1	0	6	50	49
1	0	-7	109	121
1	0	7	86	81
1	0	-8	63	-57
1	0	8	210	221
1	0	-9	106	102
1	0	9	144	135
1	0	-10	59	-47
1	0	10	65	-56
1	0	-11	66	74
1	0	11	79	-76
1	0	-12	49	-44
1	0	12	7	-10
1	0	-13	80	69
1	0	13	88	-78
1	0	-14	55	43
1	0	14	25	28
1	0	-15	17	-14
1	0	15	17	15
1	0	-16	53	52
1	0	16	36	-34
1	0	-17	126	146
1	0	17	6	9
1	0	-18	91	91
1	0	18	75	-84
1	0	-19	25	24
1	0	19	49	49
1	0	-20	66	-73
1	0	20	44	-59
1	0	-21	12	-12
1	0	21	30	-69
2	0	0	17	4
2	0	-1	103	-128
2	0	1	109	99
2	0	-2	59	62
2	0	2	90	-84
2	0	-3	36	38
2	0	3	200	-258
2	0	-4	71	-80
2	0	4	201	-282
2	0	-5	126	139
2	0	5	103	-93
2	0	-6	181	-232
2	0	6	86	85
2	0	-7	133	151
2	0	7	86	-56
2	0	-8	100	-101
2	0	8	195	213
2	0	-9	236	270
2	0	9	161	-145
2	0	-10	167	189
2	0	10	42	37
2	0	-11	24	-14
2	0	11	50	-45
2	0	-12	47	-44
2	0	12	96	91
2	0	-13	18	-19
2	0	13	60	65
2	0	-14	32	-31
2	0	14	43	-35
2	0	-15	7	10
2	0	15	7	1
2	0	-16	45	-35
2	0	16	70	76
2	0	-17	7	-11
2	0	17	14	14
2	0	-18	19	-33
2	0	18	14	14
2	0	-19	69	-61
2	0	19	16	-22
2	0	-20	43	41
2	0	20	45	-74
2	0	-21	73	-86
2	0	-22	15	2
3	0	0	4	-0
3	0	-1	181	277
3	0	1	4	4
3	0	-2	59	63
3	0	2	4	-3
3	0	-3	19	10
3	0	3	121	-129
3	0	-4	141	-166
3	0	4	88	-76
3	0	-5	128	162
3	0	5	82	76
3	0	-6	31	30
3	0	6	46	32
3	0	-7	116	-131
3	0	7	40	-32
3	0	-8	41	-36
3	0	8	166	-146
3	0	-9	9	9
3	0	9	40	-34
3	0	-10	35	-27
3	0	10	24	13
3	0	-11	6	3
3	0	11	187	-222
3	0	-12	82	-78
3	0	12	29	-22
3	0	-13	104	-108
3	0	13	58	-61
3	0	-14	145	-168
3	0	14	22	26
3	0	-15	147	-150
3	0	15	36	35
3	0	-16	143	135
3	0	16	46	51
3	0	-17	7	11
3	0	17	40	39
3	0	-18	16	19
3	0	18	29	-34
3	0	-19	22	-20
3	0	19	19	-31
3	0	-20	23	19
3	0	20	17	14
4	0	0	104	-113
4	0	-1	96	115
4	0	1	45	48
4	0	-2	42	42
4	0	2	123	-160
4	0	-3	12	-10
4	0	3	207	260
4	0	-4	19	19
4	0	4	100	-89
4	0	-5	171	-167
4	0	5	41	-33
4	0	-6	264	-300
4	0	6	124	104
4	0	-7	94	-89
4	0	7	136	133
4	0	-8	9	11
4	0	8	98	92
4	0	-9	16	18
4	0	9	17	14
4	0	-10	50	-46
4	0	10	51	-53
4	0	-11	54	-42
4	0	11	54	-48
4	0	-12	173	183
4	0	12	66	-65
4	0	-13	130	-135
4	0	13	7	6
4	0	-14	108	99
4	0	14	75	79
4	0	-15	42	-43
4	0	15	67	-78
4	0	-16	21	22
4	0	16	34	-32
4	0	-17	11	8
4	0	17	57	-64
4	0	-18	43	55
4	0	-19	90	87
4	0	-20	17	8
4	0	-21	78	-80
4	0	21	13	3
5	0	0	50	51
5	0	-1	98	-100
5	0	1	84	-83
5	0	-2	105	-111
5	0	2	90	-90
5	0	-3	84	69
5	0	3	46	-37
5	0	-4	95	89
5	0	4	121	-115
5	0	-5	18	15
5	0	5	107	110
5	0	-6	28	-26
5	0	6	20	9
5	0	-7	95	-82
5	0	7	132	141
5	0	-8	100	98
5	0	8	7	1
5	0	-9	35	32
5	0	9	73	-68
5	0	-10	227	234
5	0	10	7	3
5	0	-11	90	88
5	0	11	54	52
5	0	-12	7	9
5	0	12	56	55
5	0	-13	69	-68
5	0	13	52	58
5	0	-14	12	-12
5	0	14	30	27
5	0	-15	50	44
5	0	15	63	73
5	0	-16	7	-13
5	0	-17	66	-63
5	0	-18	18	18
5	0	-19	28	-20
5	0	-20	5	1
5	0	-21	37	31
5	0	-22	76	-82
6	0	0	26	22
6	0	-1	97	91
6	0	1	11	-6
6	0	-2	182	183
6	0	2	118	-113
6	0	-3	79	62
6	0	3	40	-34
6	0	-4	233	217
6	0	4	98	103
6	0	-5	178	-154
6	0	5	19	12
6	0	-6	179	148
6	0	6	67	-71
6	0	-7	22	5
6	0	7	12	-8
6	0	-8	59	-46
6	0	8	36	-38
6	0	-9	74	-69
6	0	9	29	35
6	0	-10	24	22
6	0	10	95	-109
6	0	-11	87	76
6	0	11	42	47
6	0	-12	34	26
6	0	12	64	-71
6	0	-13	64	-56
6	0	13	17	20
6	0	-14	12	-16
6	0	14	37	46
6	0	-15	101	-98
6	0	-16	58	-58
6	0	-17	45	38
6	0	-18	33	-20
6	0	-19	75	66
6	0	-20	101	-84
6	0	-21	98	95
6	0	-22	18	20
7	0	0	51	-39
7	0	-1	151	-149
7	0	1	21	20
7	0	-2	165	167
7	0	2	105	105
7	0	-3	53	42
7	0	3	60	56
7	0	-4	7	0
7	0	4	48	36
7	0	-5	56	-43
7	0	5	85	80
7	0	-6	122	-103
7	0	6	39	39
7	0	-7	103	-77
7	0	7	7	-7
7	0	-8	68	-61
7	0	8	51	57
7	0	-9	29	19
7	0	9	38	-42
7	0	-10	66	54
7	0	10	64	-68
7	0	-11	88	-76
7	0	11	55	-54
7	0	-12	51	-39
7	0	12	4	-7
7	0	-13	133	118
7	0	13	16	9
7	0	-14	19	7
7	0	14	16	-60
7	0	-15	72	55
7	0	15	31	30
7	0	-16	78	79
7	0	16	101	98
7	0	-17	31	36
7	0	17	70	-63
7	0	-18	37	-30
7	0	18	130	-115
7	0	-19	57	-46
7	0	19	7	-2
7	0	-20	42	-39
7	0	20	105	-114
7	0	-21	38	24
7	0	21	66	63
8	0	-1	37	-30
8	0	1	130	-115
8	0	-2	57	-46
8	0	2	7	-2
8	0	-3	42	-39
8	0	3	105	-114
8	0	-4	38	24
8	0	4	66	63
8	0	-5	63	51
8	0	5	18	-20
8	0	-6	27	24
8	0	6	96	104
8	0	-7	126	-113
8	0	7	20	-19
8	0	-8	71	-66
8	0	8	44	-44
8	0	-9	93	78
8	0	9	14	17
8	0	-10	68	-59
8	0	10	30	37
8	0	-11	186	169
8	0	-12	22	-10
8	0	-13	104	90
8	0	-14	15	-17
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8	2	2	6	4
8	2	4	53	-53
8	2	5	16	18
8	2	7	16	16
8	2	8	30	36
[illegible]	2	1	[illegible]	[illegible]
[illegible]	2	2	36	[illegible]
[illegible]	2	3	57	-59
9	2	4	14	-9
9	2	5	34	46
0	2	2	51	-44
0	2	3	62	50
0	2	7	48	-38
0	2	5	117	97
0	2	11	71	-66
0	2	12	94	98
0	2	13	88	79
0	2	14	108	112
0	2	15	135	-128
1	2	-4	151	146
1	2	-5	191	218
1	2	-6	46	-35
1	2	-7	100	-88
1	2	-9	95	-80
1	2	-17	111	-122
1	2	-18	70	-76
2	2	-1	84	91
2	2	-2	45	-43
2	2	-4	58	52
2	2	-5	100	-102
2	2	-6	145	160
2	2	-7	118	-114
2	2	-8	88	73
2	2	-9	180	-209
2	2	-10	146	-147
3	2	-1	160	-212
3	2	-2	45	-42
3	2	-4	112	122
3	2	-5	103	-119
3	2	-7	93	96
3	2	-13	94	90
3	2	-14	137	137
3	2	-15	130	125
3	2	-16	114	-111
4	2	0	82	89
4	2	-1	79	-85
4	2	-5	136	130
4	2	-6	206	229
4	2	-7	81	67
4	2	-12	120	-147

Table 2 (*cont.*)

H	K	L	F_o	F_c
3	3	-17	31	-30
3	3	-16	50	-62
4	3	0	144	167
4	3	-1	95	56
4	3	-2	39	34
4	3	-3	19	14
4	3	-4	122	-118
4	3	-5	96	74
4	3	-6	99	-35
4	3	-7	150	157
4	3	-8	18	-16
4	3	-9	66	-59
4	3	-10	27	-25
4	3	-11	14	-2
4	3	-12	19	-19
4	3	-13	53	-49
4	3	-14	85	-71
4	3	-15	7	3
4	3	-16	5	7
4	3	-17	41	47
4	3	-18	49	65
5	3	0	15	-10
5	3	-1	25	-22
5	3	-2	72	-66
5	3	-3	95	-85
5	3	-4	104	-96
5	3	-5	104	-84
5	3	-6	25	-20
5	3	-7	14	-10
5	3	-8	23	22
5	3	-9	46	39
5	3	-10	25	23
5	3	-11	7	4
5	3	-12	60	-56
5	3	-13	14	11
5	3	-14	110	113
5	3	-15	10	1
5	3	-16	64	56
5	3	-17	33	37
6	3	0	7	-3
6	3	-1	30	21
6	3	-2	14	2
6	3	-3	77	-65
6	3	-4	45	-39
6	3	-5	55	46
6	3	-6	29	25
6	3	-7	11	5
6	3	-8	14	-12
6	3	-9	108	85
6	3	-10	152	143
6	3	-11	42	-33
6	3	-12	85	65
6	3	-13	108	-100
6	3	-14	5	-7
6	3	-15	27	-25
6	3	-16	32	35
6	3	-17	17	20
7	3	0	21	14
7	3	-1	73	66
7	3	-2	75	66
7	3	-3	42	32
7	3	-4	27	-19
7	3	-5	31	-21
7	3	-6	22	15
7	3	-7	36	-27
7	3	-8	60	54
7	3	-9	61	-44
7	3	-10	6	-8
7	3	-11	70	-59
7	3	-12	27	-19
7	3	-13	33	-29
7	3	-14	75	-64
7	3	-15	47	-51
8	3	0	11	7
8	3	-1	17	-15
8	3	-2	45	33
8	3	-3	91	-86
8	3	-4	80	82
8	3	-5	103	-93
8	3	-6	102	-95
8	3	-7	103	-102
8	3	-8	5	-3
8	3	-9	44	36
8	3	-10	9	7
8	3	-11	5	-6
8	3	-12	4	4
8	3	-13	45	-44
8	3	-14	16	14
8	3	-15	36	-55
9	3	-1	11	6
9	3	-2	9	-11
9	3	-3	6	-5
9	3	-4	10	12
9	3	-5	13	-11
9	3	-7	25	27
9	3	-8	10	10
9	3	-9	10	-12
9	3	-10	50	66
1	3	1	50	61
1	3	2	17	12
1	3	3	6	-3
1	3	4	34	31
1	3	5	47	41
1	3	6	7	1
1	3	7	132	-138
1	3	8	54	-46
1	3	9	101	95
1	3	10	45	-39
1	3	11	31	27
1	3	12	92	-92
1	3	13	80	-75
1	3	14	87	-84
1	3	15	31	-29
1	3	16	29	31
2	3	1	117	-105
2	3	2	132	127
2	3	3	12	9
2	3	4	36	-32
2	3	5	50	-43
2	3	6	19	-16
2	3	7	37	31
2	3	8	43	37
2	3	9	69	56
2	3	10	85	77
2	3	11	23	-19
2	3	12	23	-21
2	3	13	50	48
2	3	14	35	-38
2	3	15	10	-10
3	3	1	34	26

H	K	L	F_o	F_c
4	2	-13	103	109
5	2	-11	83	79
5	2	-9	90	86
5	2	-8	67	-52
5	2	-7	83	-87
5	2	-6	82	66
5	2	-5	91	-77
6	2	-10	186	-189
6	2	-9	86	-77
6	2	-8	153	-140
6	2	-7	143	122
6	2	-6	183	-176
6	2	-5	137	-119
7	2	-11	116	122
7	2	-9	140	-135
7	2	-8	92	66
7	2	-7	71	62
8	2	-13	98	-97
8	2	-12	99	92
8	2	-11	139	-144
8	2	-10	73	-74
9	2	-7	74	-69
9	2	-6	72	79
10	2	-9	81	87
10	2	-8	90	-96
10	2	-6	66	69
10	2	-10	49	59
1	2	2	62	-49
1	2	3	107	103
1	2	4	137	-147
1	2	8	158	-170
1	2	9	121	-107
2	2	1	74	-66
2	2	3	157	144
2	2	4	184	209
2	2	5	83	72
2	2	6	77	-66
2	2	8	169	-167
2	2	9	133	120
3	2	3	109	97
3	2	4	64	55
3	2	5	69	-60
3	2	8	113	118
3	2	11	164	182
5	2	1	71	64
5	2	2	83	75
5	2	4	86	95
5	2	5	91	-91
6	2	2	86	90
6	2	10	83	90
7	2	2	69	-88
8	2	1	114	96
8	2	3	90	97
8	2	6	109	-87
4	2	2	114	123
4	2	3	179	-203
4	2	4	72	69
4	2	6	80	-61
4	2	7	104	-107
4	2	8	85	-77
0	3	2	66	66
0	3	3	52	-54
0	3	4	57	-52
0	3	5	26	-22
0	3	6	142	-163
0	3	7	49	44
0	3	8	149	-147
0	3	9	46	36
0	3	10	64	-55
0	3	11	56	53
0	3	12	95	84
0	3	13	13	-10
0	3	14	30	-38
0	3	15	21	14
0	3	16	17	15
0	3	17	40	56
1	3	0	79	79
1	3	-1	6	6
1	3	-2	83	89
1	3	-3	108	-127
1	3	-4	53	-53
1	3	-5	28	-20
1	3	-6	106	121
1	3	-7	13	-8
1	3	-8	117	-109
1	3	-9	81	-74
1	3	-10	79	-71
1	3	-11	94	-84
1	3	-12	6	1
1	3	-13	23	-22
1	3	-14	6	-5
1	3	-15	14	14
1	3	-16	10	4
1	3	-17	75	99
2	3	0	42	35
2	3	-1	67	-79
2	3	-2	33	-29
2	3	-3	89	-122
2	3	-4	109	-130
2	3	-5	40	-39
2	3	-6	42	-44
2	3	-7	6	-7
2	3	-8	113	114
2	3	-9	27	23
2	3	-10	72	-67
2	3	-11	46	-44
2	3	-12	7	1
2	3	-13	118	127
2	3	-14	83	-70
2	3	-15	86	88
2	3	-16	21	-19
2	3	-17	12	15
2	3	-18	7	7
3	3	0	46	43
3	3	-1	40	34
3	3	-2	92	-96
3	3	-3	64	-60
3	3	-4	90	90
3	3	-5	58	55
3	3	-6	32	30
3	3	-7	84	82
3	3	-8	8	10
3	3	-9	80	80
3	3	-10	27	-22
3	3	-11	48	43
3	3	-12	68	-62
3	3	-13	62	-61
3	3	-14	6	-5
3	3	-15	40	41
3	3	-16	17	15

H	K	L	F_o	F_c
3	3	2	20	-15
3	3	3	121	-137
3	3	4	42	-32
3	3	5	112	-125
3	3	6	43	42
3	3	7	25	16
3	3	8	16	-18
3	3	9	14	-13
3	3	10	47	39
3	3	11	80	83
3	3	12	20	21
3	3	13	36	-40
3	3	14	10	11
4	3	1	50	46
4	3	2	14	-10
4	3	3	54	53
4	3	4	31	30
4	3	5	27	-22
4	3	6	37	-32
4	3	7	44	-45
4	3	8	56	55
4	3	9	64	-66
4	3	10	75	93
4	3	11	57	-62
4	3	12	32	-33
4	3	13	36	-51
5	3	1	79	88
5	3	2	27	25
5	3	3	33	-29
5	3	4	7	10
5	3	5	11	11
5	3	6	15	14
5	3	7	97	113
5	3	8	63	65
5	3	9	43	44
5	3	10	35	-35
5	3	11	35	-45
6	3	1	66	64
6	3	2	95	-105
6	3	3	38	-33
6	3	4	131	-160
6	3	5	41	-45
6	3	6	14	13
6	3	7	19	-21
6	3	8	4	2
6	3	9	14	14
7	3	1	58	-51
7	3	2	15	20
7	3	3	14	-9
7	3	4	49	-46
7	3	5	21	24
7	3	6	53	-68
7	3	7	21	26
8	3	1	25	24
8	3	2	13	14
8	3	3	14	14
8	3	4	21	-25

lated values in Table 2, it was suspected that extinction was occurring. That such a reduction was possible was confirmed by a calculation of the attenuation factor for the $30\bar{1}$ reflexion on the assumption that the crystal was composed of 5 mosaic blocks. This factor turned out to be 0·37, even smaller than the actual value of 0·65. In all, 51 reflexions are seriously affected in this way but a further refinement of the structure using F_c's for F_o's in these 51 cases did not shift the atomic parameters by amounts exceeding the standard deviations, even though the R value was thereby further lowered to 0·098, and the remaining features on the difference projection were further reduced.

Powder pattern intensities were calculated from the structure and compared with observed values (Table 3).

Table 3. *Powder pattern intensities*

I_o are scaled so that $I_{212}=100$. I_c are calculated from $p|F_c|^2 f_1(\theta)$, where p is the multiplicity and $f_1(\theta)$ is the angular factor for the de Wolff camera as defined by Goodyear & Duffin (1957). The I_c are then scaled so that $\Sigma I_o=\Sigma I_c$. Spacings are given in Duffin & Hogg (1966).

hkl	I_o	I_c	
002	21	23	
003	10	13	
102	15	13	
$20\bar{1}$	26	29	
$20\bar{2}$	9	9	
$10\bar{4}$	50	59	
103	26	28	
$20\bar{3}$	2	1	
301	7	13	
011	36	42	
$20\bar{4}$	5	11	
110	123	25	127
$10\bar{5}$		76	
012		26	
202	53	5	55
$11\bar{2}$		50	
104	65	30	63
111		33	
013	92	6	92
$11\bar{3}$		74	
$20\bar{5}$		12	
$30\bar{2}$	5	2	
203	93	43	109
301		66	
$21\bar{1}$	27	22	
$21\bar{2}$	8	5	
$11\bar{4}$	10	16	
210	5	7	
014	10	7	
$30\bar{4}$	63	7	67
$21\bar{3}$		60	
$20\bar{6}$	29	25	
211	91	93	
$21\bar{4}$	54	45	
$30\bar{5}$	48	13	52
204		39	
212	100	107	
$10\bar{7}$	7	5	
106	12	1	11
$20\bar{7}$		10	
$31\bar{2}$	23	21	
$31\bar{3}$	35	9	41
$11\bar{6}$		32	
$31\bar{4}$	70	16	72
016		56	
$40\bar{1}$	4	3	
$30\bar{7}$	6	7	
$31\bar{5}$	8	4	11
214		3	
$20\bar{8}$		4	
400	6	4	
107	10	2	15
$40\bar{5}$		13	
$40\bar{6}$	30	28	
313	31	24	
$20\bar{9}$	136	9	118
402		25	
020		84	
$41\bar{1}$	53	7	32
$41\bar{4}$		15	
$31\bar{7}$		10	
$11\bar{8}$	19	16	
108	13	14	
$21\bar{8}$	16	21	
410	44	36	
117	33	25	29
$41\bar{5}$		4	
009	6	4	5
207		1	
018	21	23	
403	23	16	
$41\bar{6}$	11	10	13
$50\bar{2}$		3	
$22\bar{1}$	4	2	
$12\bar{4}$	11	9	
$2,0,1\bar{0}$	8	7	
$41\bar{7}$	20	33	
315	22	19	
$12\bar{5}$	19	18	
208	10	11	
124	12	7	
$31\bar{9}$	4	7	9
$50\bar{7}$		2	
413	6	2	5
$22\bar{5}$		3	
$51\bar{3}$	12	6	
$51\bar{2}$	16	7	
223	21	14	35
$32\bar{1}$		21	

Description of the structure

Distances between atoms up to a maximum of 4·25 Å were calculated and are given with standard deviations in Table 4. The positions of the atoms referred to in this table are shown in Fig. 4, which is a projection on to (010) of the contents of four unit cells. The radii of the indium and sulphur atoms have been taken as those of In^{3+} and S^{2-} because the S–S and In–S bond lengths agree quite closely with those given for β-In_2S_3 by Steigmann, Sutherland & Goodyear (1965): these radii are 0·81 Å and 1·90 Å respectively.

The structure basically consists of two separate sections, both consisting of almost cubic close-packed arrays of sulphur atoms with indium atoms in octahedral coordination. The limits of these sections, which for convenience will be called the centre and end sections, are marked in the Figure. The two sections could be brought into the same orientation if one of them were rotated through 61·5° about an axis parallel to the b axis.

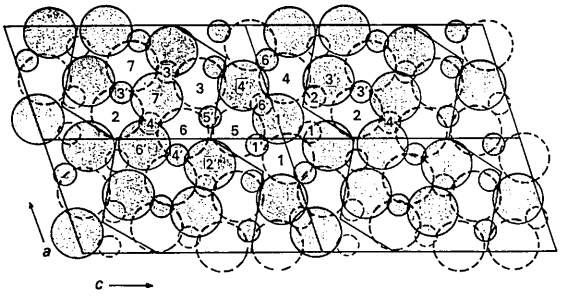

Fig. 4. Structure of In_6S_7. The contents of 4 unit cells projected on to the (010) face. Atoms having y coordinates of $\frac{3}{4}$ are shaded, those with $y=\frac{1}{4}$ are drawn with broken lines and unshaded. Small circles are In atoms, large circles S atoms. The numbers refer to the designations in Tables 1 and 4.

Table 4. *Interatomic distances*

Standard deviations for In–In distances are 0·002 Å, for In–S 0·006 Å, and for S–S, 0·008 Å.

In(1)–In(2)	2·741 Å
In(1)–In(5)	4·054
In(1)–In(6′)	3·707
In(2)–In(3′)	4·047
In(2)–In(6)	4·028
In(3)–In(3′)	4·030
In(3)–In(4)	3·995
In(3)–In(4′)	3·713
In(4)–In(4′)	3·651
In(4)–In(5)	3·811
In(6)–In(6′)	3·873
In(1)–S(1)	2·524
In(1)–S(1′)	3·234
In(1)–S(2)	3·794
In(1)–S(5′)	2·569
In(2)–S(1′)	3·737
In(2)–S(2)	3·414
In(2)–S(3′)	2·530
In(2)–S(4)	2·619
In(3)–S(2′)	2·557
In(3)–S(3′)	2·596
In(3)–S(7)	2·617
In(3)–S(7′)	2·791
In(4)–S(2)	2·532
In(4)–S(6)	2·507
In(4)–S(6′)	2·608
In(4)–S(7′)	2·785
In(5)–S(2)	3·665
In(5)–S(3′)	3·279
In(5)–S(4)	3·412
In(5)–S(5′)	3·087
In(5)–S(6′)	3·047
In(5)–S(7)	4·151
In(6)–S(1′)	2·629
In(6)–S(4)	2·644
In(6)–S(4′)	2·668
In(6)–S(5)	2·604
S(1)–S(1′)	3·617
S(1)–S(4)	3·594
S(1)–S(4′)	3·724
S(1)–S(5)	4·219
S(1)–S(5′)	3·593
S(2)–S(3′)	3·776

Table 4 (*cont.*)

S(2)–S(5′)	3·901
S(2)–S(6′)	3·673
S(2)–S(7)	3·658
S(2)–S(7′)	3·695
S(3)–S(4′)	3·809
S(3)–S(6)	3·945
S(3)–S(7′)	3·823
S(4)–S(4′)	3·636
S(4)–S(5′)	3·952
S(5)–S(6)	4·139
S(6)–S(6′)	3·584
S(6)–S(7)	3·733
S(6)–S(7′)	3·809
S(7)–S(7′)	3·611

The centre section of close-packing is continuous throughout the whole structure whereas the end section suffers considerable distortion when it is inverted across the origin of the unit cell. The close packing in both sections is distorted, as the S–S distance in the y direction is 3·89 Å while the averages for the centre and end sections respectively are 3·74 and 3·76 Å.

The indium atom I(5), I(5′) could fit in with the close packing of either section, given slight shifts in its x and z coordinates. In this it is unique since the other In atoms can all be said to belong to one or other of the sections. This results in its being rather loosely bound with an average distance from nearest sulphur neighbours of 3·18 Å and probably also accounts for the very high temperature factor assigned to it.

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