quoted. Exposures should, ideally, give a maximum density of 1·0 on the second film of the pack.

Before photometry the film should be carefully scrutinized for any signs (such as irregularities in the spots or unusual shadows in the background) that the experimental arrangements were faulty in any way.

If the photometer errors are comparable with absorption errors the films should be photometered twice, on different occasions, and any measurements which disagree by more than twice the expected standard deviation repeated until consistent results are obtained.

Correlation of layers

Correlation should be achieved by the use of data collected about two axes (Rollett & Sparks, 1960; Hamilton, Rollett & Sparks, 1965). Such data would normally be necessary in any case if all independent reflexions are to be measured. In order to get as many corresponding pairs of reflexions from the two sets as possible and also increase the accuracy of the correlation, the symmetry-related reflexions in the layers should be averaged before correlation (Whitaker, 1965) and the weights already assigned to the intensities (Jeffery & Rose, 1964) adjusted accordingly. If symmetry-related reflexions occur on different films these should be utilized in the correlation.

Extinction

Data from more than one crystal should enable extinction to be detected, but for a quantitative estimate some of the single-crystal intensity values should be compared with those measured on a diffractometer using very fine ($<1\mu$) powder, or Chandresekhar's method using polarized X-rays should be applied to the single-crystal specimen.

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The Crystal Structure of β-In_2S_3

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A structural analysis of β-In_2S_3, using Weissenberg data, has confirmed the cation-deficient spinel structure proposed by Rooymans. The absence of some of the tetrahedrally coordinated cations, found in spinel, leads to appreciable atomic displacements from idealized positions.

Introduction

On the basis of accurate powder data, Rooymans (1959) proposed that β-In_2S_3 has a spinel-type structure with ordered vacant tetrahedrally coordinated cation sites. Rooymans found a body-centred tetragonal supercell, containing 16 In_2S_3 molecules, which was related to the spinel-type cell by $a=d_{(110)}/2=7\cdot62$ Å and $c=3d_{(001)}=32\cdot32$ Å, $d_{(110)}$ and $d_{(001)}$ being planar spacings of the spinel lattice. The space group suggested by Rooymans was $I4_122$ with the four cation vacancies per cell located at the equivalent positions of the 4_1 screw axes.

A more detailed investigation of the space group was undertaken by King (1962) using a single-crystal technique. Systematically absent reflexions on Weissenberg photographs, taken about the [110] axis, suggested the more highly symmetrical space group $I4_1/amd$, which is indeed the space group of the structure proposed by Rooymans. King also calculated the unit-cell parameters from the Weissenberg data and found $a=7\cdot61$, $c=32\cdot24$ Å.

Goodyear & Steigmann (1961) carried out a single-crystal examination of twinned crystals of β-In_2S_3 and were able to explain the twinning mechanism in terms of a cation-deficient spinel model. The twin components of the material available for this work were sufficiently large to enable a suitable single crystal to be selected for the present structural analysis. Accurate powder data published by Goodyear & Steigmann were in agreement with those of Rooymans, and their lattice parameters, $a=7{\cdot}623$, $c=32{\cdot}36$ Å, have been assumed in this paper.

Intensity measurements

A single crystal of approximately square cross-section, 0·03 mm × 0·03 mm, and elongated parallel to the a axis was chosen for the analysis. Six layer lines were recorded on equi-inclination Weissenberg photographs taken about the a axis with Cu $K\alpha$ radiation.

The intensities of nearly 750 independently recorded reflexions were estimated visually from multiple film exposures with a calibrated scale. To compare the strong principal with the weaker superlattice reflexions ($l \neq 3n$), it was necessary to pack six films into the camera. The systematically absent reflexions were hkl with $h+k+l=2n+1$, $hk0$ with $h(k)=2n+1$, hhl with $l \neq 4n$. These are the same conditions as found by King, thus confirming the space group $I4_1/amd$. About 150 reflexions were too weak to be observed.

The observed intensities were corrected for Lorentz & polarization factors and adjusted for spot shape on the upper layer lines (Phillips, 1954). Absorption corrections were made by assuming the specimen to be cylindrical, of average radius 0·017 mm with $\mu r=1{\cdot}6$, and applying the correction factors given by Bond (1959).

The determination of the structure

Atomic scattering factors listed by Wilson (1960) were used in the intensity calculations.

In the idealized structure the atoms are distributed among the equipoints as follows. Indium in tetrahedral coordination at 8(e), indium in octahedral coordination at 8(c) and 16(h), S in three sets at 16(h). Assuming idealized parameters [Table 1, column (i)] and temperature factors of 0·8 Å^2 for In and 1·0 Å^2 for S, initial intensity calculations for $0kl$ reflexions yielded a value of the reliability index, $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ of 40%. A close examination of the discrepancy between the observed and calculated structure factors suggested that the principal and superlattice reflexions needed to be scaled separately. When this was done the value of R reduced considerably.

At this stage, a two-dimensional least-squares refinement of both atomic coordinates and isotropic temperature factors was carried out with a program by Daly, Stephens & Wheatley (1963) on the Elliot 803 computer installed at the University of Hull. After several cycles of refinement, the R index was reduced to 16·8% for the $0kl$ reflexions. This was followed by a three-dimensional least-squares refinement with structure factors determined from 741 observed intensities, giving a final R value of 15·4%. The refinement was stopped when the changes in the atomic parameters were significantly less than the standard deviations. As a check on the structure, a (100) electron-density projection was made, and this did not reveal any spurious peaks.

The final parameters with their standard deviations are listed in column (ii) of Table 1. The observed and calculated structure factors are compared in Table 2, the mean value of $|F_o|$ for hkl and khl reflexions being given. Calculated structure factors of unobserved reflexions were all less than the lowest value of $|F_o|$, and these data have not been included in Table 2.

Discussion of the structure

The single-crystal data have fully confirmed the basic structure proposed by Rooymans. Since the sequence of atomic layers parallel to the (013) planes of close-packed sulphur atoms has been described previously by Goodyear & Steigmann, it is not proposed to deal with such general features of the structure in this paper, but rather with atomic displacements from idealized spinel positions as revealed by the present analysis. These can be described readily with reference to layers of atoms parallel to the (001) face of the unit cell, as vacant tetrahedral sites are most densely populated in this plane. Fig. 1 shows the directions of the shifts of sulphur and octahedrally coordinated In1, In2, atoms in three successive layers in the unit cell, and of tetrahedrally coordinated In3 atoms situated between the layers.

The In1 atoms are centres of symmetry and, as might be expected, are situated at the ideal positions in the spinel structure. In diagram (a) of Fig. 1 it will be seen that the In1 atoms are linked to S1 atoms, and that the tetrahedral sites on either side of the layer are filled. The displacements of the S1 atoms are thus comparatively small and are mainly due to the large shifts of In3 atoms away from the layer. In the next layer [dia-

Table 1. *Atomic parameters and temperature factors*

Origin at centre (2/m)

		(i) Preliminary			(ii) Final			
Atom	Equipoint	x/a	y/b	z/c	x/a	y/b	z/c	B(Å^2)
In1	8(c)	0	0	0	0	0	0	1·00 ± 0·06
In2	16(h)	0	0	$\frac{1}{3}$	0	−0·0181 ± 0·0004	0·3324 ± 0·0001	1·14 ± 0·05
In3	8(e)	0	$\frac{1}{4}$	$\frac{5}{24}$	0	$\frac{1}{4}$	0·2046 ± 0·0001	1·10 ± 0·06
S1	16(h)	0	0	$\frac{1}{4}$	0	−0·0034 ± 0·0016	0·2506 ± 0·0003	1·83 ± 0·21
S2	16(h)	0	0	$\frac{1}{12}$	0	0·0086 ± 0·0017	0·0785 ± 0·0003	1·83 ± 0·20
S3	16(h)	0	0	$\frac{5}{12}$	0	0·0237 ± 0·0017	0·4131 ± 0·0004	1·79 ± 0·19

Table 2. *Observed and calculated structure factors*

H	K	L	F_c	F_o
0	0	4	181	230
0	0	8	-258	332
0	0	12	1095	1015
0	0	16	36	56
0	0	20	153	142
0	0	24	1032	810
0	0	28	70	58
0	0	32	-177	172
0	0	36	[illegible]	371
0	0	40	133	92
0	1	1	[illegible]	75
0	1	3	-336	333
0	1	5	112	114
0	1	7	128	139
0	1	9	673	645
0	1	11	-137	140
0	1	13	103	118
0	1	15	-600	591
0	1	17	-164	154
0	1	21	139	176
0	1	23	163	145
0	1	25	72	73
0	1	27	-233	272
0	1	29	103	125
0	1	33	240	232
0	1	37	-277	230
0	1	41	-63	50
0	2	0	[illegible]	425
0	2	4	-130	115
0	2	6	424	443
0	2	8	206	153
0	2	12	252	312
0	2	16	42	49
0	2	18	372	338
0	2	20	-181	157
0	2	24	-169	222
0	2	26	-47	50
0	2	30	290	259
0	2	32	144	127
0	2	36	82	115
0	3	1	164	148
0	3	3	194	201
0	3	5	-223	186
0	3	7	33	47
0	3	9	-523	504
0	3	11	38	39
0	3	15	518	554
0	3	17	52	59
0	3	19	96	103
0	3	21	-95	98
0	3	23	-206	130
0	3	27	176	232
0	3	29	-150	156
0	3	31	39	95
0	3	33	-218	191
0	3	39	234	169
0	4	0	1406	894
0	4	4	144	124
0	4	8	-164	150
0	4	12	763	765
0	4	16	44	53
0	4	20	136	145
0	4	24	823	833
0	4	28	69	70
0	4	32	-144	118
0	4	36	352	307
0	5	3	-248	234
0	5	7	175	172
0	5	9	478	485
0	5	11	-152	151
0	5	13	132	147
0	5	15	-501	539
0	5	17	-184	178
0	5	19	87	123
0	5	21	124	162
0	5	23	74	81
0	5	25	103	115
0	5	27	-213	232
0	5	29	37	55
0	5	31	44	46
0	5	33	202	186
0	5	35	-86	62
0	6	0	-254	270
0	6	4	-48	57
0	6	6	262	259
0	6	8	149	149
0	6	12	111	172
0	6	16	50	57
0	6	18	247	255
0	6	20	-105	121
0	6	24	-158	190
0	6	28	34	47
0	6	30	221	164
0	6	32	122	80
0	7	1	135	157
0	7	3	82	80
0	7	5	-187	180
0	7	7	83	106
0	7	9	-264	362
0	7	13	33	54
0	7	15	293	400
0	7	19	119	124
0	7	23	-170	210
0	7	25	31	42
0	7	27	99	97
0	7	29	-135	75
0	8	0	689	815
0	8	4	111	126
0	8	8	-62	83
0	8	12	367	470
0	8	16	51	62
0	8	20	112	96
0	8	24	472	202
0	9	1	39	45
0	9	3	-145	180
0	9	5	-45	56
0	9	7	130	129
0	9	9	281	307
0	9	11	-119	105
0	9	13	107	91
0	9	15	-300	255
1	0	35	59	51
1	1	2	-244	173
1	1	6	-343	350
1	1	10	-35	35
1	1	14	173	156
1	1	18	205	226
1	1	22	43	50
1	1	26	-186	211
1	1	30	-140	164
1	1	34	68	76
1	1	38	108	95
1	2	1	97	81
1	2	3	697	501
1	2	5	-93	94
1	2	7	115	115
1	2	9	176	212
1	2	11	-191	177
1	2	13	-20	44
1	2	15	242	263
1	2	17	167	161
1	2	21	371	333
1	2	23	60	72
1	2	27	395	418
1	2	29	-84	109
1	2	33	83	72
1	2	35	-143	128
1	2	37	60	61
1	2	39	152	138
1	3	2	114	88
1	3	4	133	105
1	3	6	272	297
1	3	8	-130	125
1	3	10	120	123
1	3	14	-210	180
1	3	16	102	104
1	3	18	-209	227
1	3	20	-95	107
1	3	22	35	46
1	3	24	8	64
1	3	26	134	148
1	3	28	63	78
1	3	30	99	139
1	3	32	-63	75
1	3	38	-125	85
1	4	1	-42	44
1	4	3	202	182
1	4	5	84	74
1	4	7	-85	79
1	4	9	479	427
1	4	11	127	123
1	4	13	97	98
1	4	15	483	437
1	4	17	-122	118
1	4	21	99	113
1	4	23	-115	132
1	4	25	89	88
1	4	27	180	210
1	4	29	92	99
1	4	33	202	175
1	4	35	66	58
1	5	2	-216	146
1	5	4	94	96
1	5	6	-226	207
1	5	8	-92	101
1	5	10	44	74
1	5	14	72	33
1	5	16	76	110
1	5	18	125	177
1	5	20	-73	83
1	5	22	91	103
1	5	26	-179	165
1	5	28	55	77
1	5	30	-135	133
1	5	32	-51	55
1	5	34	101	84
1	6	1	87	80
1	6	3	369	323
1	6	5	-47	55
1	6	7	78	89
1	6	9	75	103
1	6	11	-85	105
1	6	15	110	161
1	6	17	113	122
1	6	21	244	255
1	6	23	74	80
1	6	27	258	297
1	6	29	-57	60
1	7	4	134	142
1	7	6	149	206
1	7	8	-132	[illegible]
1	7	10	112	148
1	7	12	6	59
1	7	14	-166	176
1	7	16	114	131
1	7	18	-149	188
1	7	20	-110	121
1	7	22	67	81
1	7	24	6	39
1	7	26	67	61
1	7	28	86	55
1	8	3	70	93
1	8	5	59	69
1	8	9	243	225
1	8	11	109	103
1	8	13	81	81
1	8	15	249	296
1	8	17	-66	66
1	8	23	-43	41
1	9	2	-152	135
1	9	4	85	92
1	9	6	-129	130
1	9	8	-34	85
1	9	10	58	61
2	0	40	43	35
2	1	19	23	39
2	2	0	1077	785
2	2	4	-93	87
2	2	8	169	140
2	2	12	1400	972
2	2	16	110	107
2	2	20	-203	168
2	2	24	612	706
2	2	28	113	117
2	2	32	113	115
2	2	36	553	457
2	3	1	166	127
2	3	3	-695	526
2	3	5	-201	145
2	3	7	27	39
2	3	9	204	202
2	3	11	89	94
2	3	13	56	74
2	3	15	-267	249
2	3	17	62	80
2	3	19	79	91
2	3	21	360	459
2	3	23	-113	136
2	3	25	77	80
2	3	27	-401	415
2	3	29	-131	130
2	3	31	59	78
2	3	33	85	95
2	3	35	92	83
2	3	37	96	78
2	4	0	216	230
2	4	4	113	110
2	4	6	338	290
2	4	8	-133	122
2	4	12	-229	251
2	4	16	287	279
2	4	20	158	173
2	4	24	119	187
2	4	30	252	213
2	4	32	-116	106
2	4	36	-65	84
2	5	3	407	383
2	5	7	169	155
2	5	9	-85	82
2	5	11	-185	165
2	5	13	68	90
2	5	15	129	144
2	5	17	-187	193
2	5	19	96	133
2	5	21	-267	283
2	5	27	281	315
2	5	31	68	67
2	5	35	-147	15
2	6	0	570	568
2	6	8	132	135
2	6	12	833	750
2	6	16	97	119
2	6	20	-122	145
2	6	24	390	468
2	6	28	98	99
2	7	1	141	154
2	7	3	-405	473
2	7	5	-173	173
2	7	7	73	107
2	7	9	144	192
2	7	13	77	92
2	7	15	-190	237
2	7	19	100	112
2	7	21	258	283
2	7	23	-115	113
2	7	25	89	78
2	7	27	-293	246
2	8	0	69	146
2	8	4	91	113
2	8	6	201	162
2	8	8	-55	65
2	8	12	-187	205
2	8	16	192	132
2	8	20	122	104
2	9	1	27	51
2	9	3	222	184
2	9	5	-50	65
2	9	7	134	125
2	9	9	-48	45
2	9	11	-132	104
2	9	13	70	57
3	3	6	224	222
3	3	10	184	160
3	3	14	-239	199
3	3	18	-213	261
3	3	22	98	143
3	3	26	89	111
3	3	30	64	109
3	3	34	44	56
3	4	1	-105	107
3	4	3	126	130
3	4	5	173	145
3	4	7	30	55
3	4	9	382	367
3	4	11	49	41
3	4	15	338	409
3	4	17	-38	52
3	4	19	83	55
3	4	21	71	52
3	4	23	-156	171
3	4	27	132	168
3	4	29	132	128
3	4	31	81	88
3	4	33	185	136
3	5	2	-133	118
3	5	4	173	139
3	5	6	-193	202
3	5	8	-171	166
3	5	14	109	133
3	5	16	143	169
3	5	18	137	197
3	5	20	-139	151
3	5	24	9	52
3	5	26	-135	144
3	5	28	105	98
3	5	30	-122	114
3	5	32	-97	85
3	6	1	132	121
3	6	3	374	388
3	6	5	-118	115
3	6	9	103	135
3	6	11	-28	49
3	6	13	58	62
3	6	15	144	208
3	6	17	51	52
3	6	19	-46	50
3	6	21	243	286
3	6	23	111	117
3	6	25	69	84
3	6	27	266	251
3	6	29	-92	71
3	7	4	56	93
3	7	6	133	173
3	7	8	-55	64
3	7	10	160	164
3	7	14	-191	177
3	7	16	48	66
3	7	18	-154	186
3	7	20	-46	65
3	7	22	109	99
3	7	26	36	41
3	8	1	-34	53
3	8	5	113	104
3	8	7	28	41
3	8	9	207	184
3	8	11	62	71
3	8	13	36	53
3	8	15	208	200
3	8	17	-16	20
3	8	19	64	55
3	9	2	-106	95
3	9	4	130	111
3	9	6	-116	111
3	9	8	-128	96
3	9	10	16	24
4	4	0	1047	823
4	4	4	128	113
4	4	8	-113	123
4	4	12	580	663
4	4	16	49	63
4	4	20	127	147
4	4	24	673	739
4	4	28	67	89
4	4	32	-117	92
4	5	3	-180	195
4	5	7	137	150
4	5	9	377	484
4	5	11	-143	160
4	5	13	122	142
4	5	15	-399	500
4	5	17	-152	164
4	5	19	69	94
4	5	21	96	120
4	5	23	48	60
4	5	25	96	102
4	5	27	-166	166
4	5	31	33	28
4	6	0	-189	232
4	6	4	-53	65
4	6	6	227	209
4	6	8	115	131
4	6	12	118	196
4	6	18	217	203
4	6	20	-99	117
4	6	24	-121	151
4	7	1	105	113
4	7	5	-163	157
4	7	7	75	77
4	7	9	-237	233
4	7	13	21	32
4	7	15	240	227
4	7	19	107	86
4	7	23	-136	97
4	8	0	569	640
4	8	4	105	92
4	8	8	-45	61
4	8	12	298	298
4	8	16	52	49
5	0	5	-23	52
5	4	29	35	28
5	5	2	-208	196
5	5	6	-176	215
5	5	10	86	105
5	5	18	85	146
5	5	22	121	136
5	5	26	-173	135
5	6	3	261	261
5	6	7	127	135
5	6	11	-108	139
5	6	15	66	70
5	6	17	143	134
5	6	19	78	86
5	6	21	189	167
5	7	2	53	69
5	7	4	160	148
5	7	6	126	154
5	7	8	-158	139
5	7	10	54	61
5	7	14	-104	102
5	7	16	139	108
5	7	18	-108	100
5	7	20	-133	72
5	8	1	42	33
5	8	3	76	74
5	8	7	-75	70
5	8	9	213	164
5	8	11	122	68
6	6	0	356	389
6	6	8	117	117
6	6	12	566	548
6	6	16	87	93
6	6	20	-76	59
6	7	1	125	97
6	7	3	-274	276
6	7	5	-121	111
6	7	7	45	59
6	7	9	85	108
6	7	15	-114	41

gram (*b*)] In2 atoms are linked both to S2 and S3, and the tetrahedral sites above the layer are vacant, each S2 atom being associated with a vacant site. The absence of the tetrahedral bond causes a shortening of the octahedral bonds between S2 and the In2 atoms in the layer and the In1 atom in the first layer. These contractions are accomplished mainly by the large shifts of S2 towards In1, and In2 towards S2 atoms. An S3 atom, being linked octahedrally with three In2 atoms, two in the layer and one in the layer above [diagram (*c*)], is displaced outwards almost parallel to the tetrahedral bond by the shifts of the In2 atoms. The movements of the S3 atoms, in turn, displace the In3 atom towards the layer. Finally, the same pattern of movement is seen in the next layer [diagram (*c*)] the displacements now being caused by vacant tetrahedral sites lying below the layer.

The bond lengths of In1–S, In2–S octahedra and In3–S, V–S tetrahedra are given in Table 3. Although the In2–S octahedron is considerably distorted, the average S–S distance is of the same order of magnitude, 3·70 Å compared with 3·72 Å, as that of the In1–S

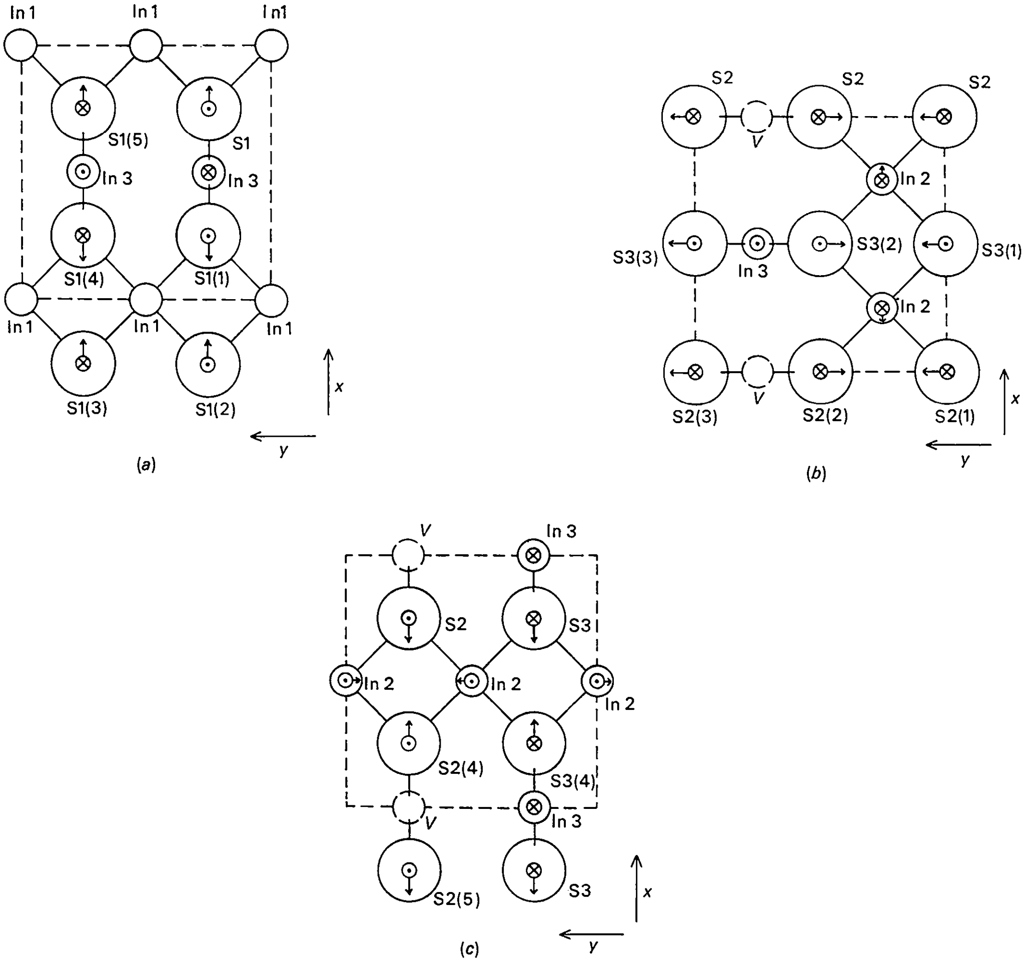

Fig. 1. Atomic displacements from idealized position. Shifts parallel to Z are represented by ⊙ in direction of Z increasing and ⊗ in direction of Z decreasing. The magnitudes of the shifts (in Å) are:

	Parallel to X (or Y)	Parallel to Z
In1	0	0
In2	0·14	0·03
In3	0	0·12
S1	0·03	0·02
S2	0·06	0·16
S3	0·18	0·12

(*a*) Layer of atoms in unit cell at height $z=0$ with tetrahedrally coordinated In 3 atoms at $z=c/24$ and $z=-c/24$. (*b*) Layer of atoms in unit cell at height $z=c/12$ with tetrahedrally coordinated In3 atom $z=c/24$ and vacant tetrahedral sites, V, at $z=c/8$. (*c*) Layer of atoms in unit cell at height $z=c/6$ with tetrahedrally coordinated In3 atoms at $z=5c/24$ and vacant tetrahedral sites, V, at $z=c/8$.

octahedron, and both these values are significantly less than 3·81 Å, the ideal S–S distance. On the other hand, all the S–S distances in both types of tetrahedron are greater than 3·81 Å, the average values being 4·01 Å for an In3–S tetrahedron and 4·04 Å for a vacant tetrahedron.

Table 3. *Bond lengths*

Standard deviation in each bond length = 0·01 Å

		Å
In1–S Octahedron		
	In–S1(1), In–S1(2)	2·68
	In–S2(2)	2·54
	S1(1)–S1(2)	3·76
	S1(1)–S1(4)	3·81
	S1(1)–S2(2), S1(2)–S2(2)	3·64
	S1(3)–S2(2), S1(4)–S2(2)	3·74
In2–S Octahedron		
	In–S2(1), In–S2(2)	2·56
	In–S3(1), In–S3(2)	2·68
	In–S3(4)	2·63
	In–S1(1)	2·65
	S1(1)–S2(1), S1(1)–S2(2)	3·64
	S1(1)–S3(1), S1(1)–S3(2)	3·81
	S2(1)–S3(1), S2(2)–S3(2)	3·82
	S2(1)–S2(2)	3·68
	S3(1)–S3(2)	3·45
	S2(1)–S3(4), S2(2)–S3(4)	3·90
	S3(1)–S3(4), S3(2)–S3(4)	3·47
In3–S Tetrahedron		
	In–S1(4), In–S1(5)	2·44
	In–S3(2), In–S3(3)	2·48
	S1(4)–S1(5)	3·86
	S1(4)–S3(2), S1(4)–S3(3) S1(5)–S3(2), S1(5)–S3(3)	4·01
	S3(2)–S3(3)	4·17
Vacant tetrahedron		
	S2(1)–S2(3), S2(4)–S2(5)	3·94
	S2(2)–S2(4), S2(2)–S2(5) S2(3)–S2(4), S2(3)–S2(5)	4·10

See Fig. 1 for location of atoms.

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Oxygen Coordinates of Compounds with Garnet Structure*

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By full-matrix least-squares refinement, the O parameters of one natural and twelve synthetic garnets $M_5R_3O_{12}$ were determined, with M and R as follows:

M:	Al	Ga	Fe ....
R:	Lu Yb Y Gd	Lu Yb Y	Lu Yb Y Dy Sm .

The refinement was based on those Bragg reflections to which only the oxygen ions contribute. The integrated X-ray intensities were counted after elimination of Renninger effects. The resulting O parameters are interpreted by polar coordinates which indicate size, shape and orientation of the oxygen octahedra and are closely associated with the effects of shortened shared edges on the shape of the other polyhedra. The cell edges a are studied as functions of the rare-earth atomic numbers. The crystal field effects on a, shown by Espinosa on iron garnets with non-spherical ions R, appear also in the other two series. For spherical R, the increments Δa associated with changes in M and R are independent of each other. Such additivity of a is destroyed in $Al_5Gd_3O_{12}$ by the resistance of the large rare-earth ions to the small lattice. These effects are demonstrated also on selected interionic distances and angles.

Introduction

As Menzer (1928) has found, the garnet structure belongs to the space group $Ia3d(O_h^{10})$ with cations in 16(a), 24(c) and 24(d) positions,* defined by fixed fractions of the cubic cell edge a. The 96(h) positions of the anions (oxygen in most garnets) depend on three variable structure parameters x, y, z which, in general, differ with composition.

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* Portions of this work were presented at the Pittsburgh Diffraction Conference, Pittsburgh, Pennsylvania, on November 7, 1962.

* Nomenclature of *International Tables for X-Ray Crystallography* (1952).