trigonal configurations SGa_3 and $SMgGa_2$ and irregular tetrahedral arrangements SMg_2Ga_2 and SMg_3Ga.

Comparison of Fig. 1 of this paper with Fig. 2 of Goodyear & Steigmann's publication on the structure of α-Ga_2S_3 demonstrates that the stacking of sulphur atoms is similar in the two compounds. In α-Ga_2S_3 the third layer of sulphur atoms is identical with the first one, giving rise to a wurtzite type lattice with four cation vacancies per cell. In $MgGa_2S_4$ double the number of sulphur layers is required to define the period in the direction [100]. Starting with the slab of octahedra at $x=0$, $y=0$ one notices the following arrangement of atom layers parallel to (100):

$$x = -\tfrac{1}{8},\ 0,\ \tfrac{1}{8},\ 0{\cdot}3,\ \tfrac{3}{8},\ \tfrac{5}{8},\ 0{\cdot}7,\ \tfrac{7}{8},\ 1,\ \tfrac{9}{8}$$
$$\mathrm{S\ Mg\ S\ Ga\ S\ S\ Ga\ S\ Mg\ S}$$

Three filled double layers of anions are succeeded by an empty double layer. The mutual distance in the empty double layer (3·3 Å) is larger than in the filled layers (3·0 Å), an effect which can be readily explained in terms of attractive and repulsive electrostatic forces. The same type of empty and filled layers also occurs in $MgAl_2S_4$ and $MnAl_2S_4$. In this structure, however, the stacking sequence is not disrupted in directions perpendicular to the layers, explaining why these compounds have rhombohedral (hexagonal) symmetry. The C centring in $MgGa_2S_4$ destroys this hexagonal layer symmetry. Why gallium causes this less symmetric coordination in this class of compounds is not clear and will be an object of further investigations.

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The Crystal Structure of $Ho_{11}Ge_{10}$*

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The crystal structure of a compound in the holmium–germanium system near 1:1 stoichiometry has been determined by single-crystal X-ray diffraction techniques. The composition established is $Ho_{11}Ge_{10}$. The unit cell is body-centered tetragonal, and contains four $Ho_{11}Ge_{10}$ units. Lattice constants are $a=10{\cdot}79$, $c=16{\cdot}23$ Å; the calculated density is 8·93 $g.cm^{-3}$. The space group as deduced from the structure analysis is $I4/mmm$.

Germanium atoms in the structure are of three types: (1) isolated atoms; (2) pairs of atoms (bond lengths 2·54 and 2·96 Å); and (3) a square cluster of four atoms (bond length 2·58 Å). Infinite chains of Ge atoms found in CrB-type HoGe do not occur in $Ho_{11}Ge_{10}$. Coordination numbers of Ge atoms are either 8 or 9; of Ho, 15–17.

Introduction

During a recent investigation of rare-earth monogermanide compounds (Tharp, Smith & Johnson, 1966), three different structure-types were encountered. Two of these, FeB- and CrB-types, were similar to phases observed in the rare-earth monosilicide series (Gladyshevskii & Kripyakevich, 1964). The third, a complex, body-centered tetragonal phase of unknown structure-type, occurred for the eight rare-earth elements, gadolinium through lutetium. This phase was consistently obtained from preparations whose initial composition was equiatomic; however, composition of the crystals was not definitely established as 1:1. The

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present crystal-structure analysis of the holmium compound shows the stoichiometry to be $Ho_{11}Ge_{10}$. Quite unexpectedly, the crystal structure of this tetragonal compound bears little resemblance to FeB- and CrB-types.

Experimental

The holmium compound was prepared by conventional arc-melting techniques as previously described (Tharp, Smith & Johnson, 1966). Single crystals, obtained by crushing the arc-melted buttons, were typically in the form of small, square pyramids. Weissenberg and precession photographs showed a body-centered tetragonal unit cell. The diffraction symmetry was $4/mmm$, and there were no other systematic extinctions other than the body-centered condition: hkl missing for $h+k+l=2n+1$. Possible space groups are: $I4/mmm$, $I4mm$, $I422$, $I\bar{4}m2$ or $I\bar{4}2m$. Of these, the first named is centrosymmetric; the others are all non-centrosymmetric. Lattice constants determined from the photographs with Cu $K\alpha$ radiation ($\lambda=1{\cdot}5418$ Å) are $a=10{\cdot}79$, $c=16{\cdot}23$ Å (probable errors are estimated to be 0·5%).

Intensities were measured on a General Electric XRD-5 diffractometer equipped with a single-crystal orienter and a scintillation counter. The radiation employed was Zr-filtered Mo $K\alpha$, and the crystalline specimen was a somewhat irregular fragment approximately $0{\cdot}10\times0{\cdot}12\times0{\cdot}15$ mm in size. The adverse effects of absorption were partially offset by: (*a*) applying a φ-dependent correction measured at three different 2θ values, and (*b*) selecting from among the equivalent reflections the one whose φ-dependent correction was smallest. Lorentz–polarization factors were applied through the aid of the IBM-7094 program of Larson, Cromer & Roof (1964).

Determination of the structure

For several of the rare-earth metals, we had observed the tetragonal phase and a CrB-type phase to occur in the same preparation. Various pieces of indirect evidence suggested that the tetragonal phase might be a high-temperature 1:1 modification, quenched in during the generally rapid cooling. CrB-type HoGe has a unit-cell volume of 177 Å^3, and the unit cell contains four HoGe units. Comparison of these figures with the unit-cell volume (1890 Å^3) of the tetragonal compound indicated approximately 43 HoGe units per unit cell. (An even number is, however, required.)

An $N(z)$ curve (Howells, Phillips & Rogers, 1950) lay closer to the curve for a centrosymmetric structure, and in interpreting the Patterson function, the centrosymmetric space group, $I4/mmm$, was the first to be considered. This space group has 32-fold general positions and various special positions which are 16-, 8-, 4- and 2-fold (*International Tables for X-ray Crystallography*, 1952). By examining possible inter- and intra-atomic vectors and aided also by packing considerations, we were able to place one Ho in a 16(n), $0,x,z$ position, ($x\sim0{\cdot}25$, $z\sim0{\cdot}19$) and another in an 8(h), $x,x,0$ position ($x\sim0{\cdot}18$). There also appeared to be a Ho atom in a 4(e), $0,0,z$ position ($z\sim0{\cdot}34$); however, to be on the safe side this was put in as a Ge atom in the initial structure factor calculation. Refinement of the scale factor only resulted in an R index of 54% at this stage. An electron-density synthesis displayed several additional atoms which were included in further structure-factor calculations. Successive electron-density syntheses and least-squares refinements of parameters thus led to the placing of 44 Ho and 40 Ge within the unit cell. During this process, the R index decreased steadily to about 10%. There appeared no reason at any point to consider the non-centrosymmetric space groups.

Final refinement of the 21 variable parameters was carried out by the full-matrix least-squares program of Gantzel, Sparks & Trueblood (ACA Program no. 319, unpublished) to an R index of 7·6% (all reflections). Changes in the parameters in the last cycle were in all cases $<0{\cdot}001$ times the e.s.d.'s. The resulting parameter values are listed in Table 1. The refinement was based on $|F_o|$, the following weighting scheme (Smith, Johnson & Nordine, 1965) being employed: $w=F_o^{1/4}$ for $F_o<A$; $w=A^{5/4}F_o^{-1}$ for $F_o>A$. On the scale of the structure factor data in Table 2, $A=326$. The scattering factors for Ho were Hartree–Fock–Slater values given by Hanson, Herman, Lea & Skillman (1964); the scattering factors for Ge were those listed in *International Tables for X-ray Crystallography* (1962). A difference Fourier synthesis prepared with the final parameters displayed little detail of significance; the largest peak

Table 1. *Final parameters*

e.s.d.'s are given in parentheses.

	Wyckoff notation	$10^4\,x$	$10^4\,y$	$10^4\,z$	B
Ho(1)	(n)	0	2518 (4)	1897 (2)	0·8 (0·1) Å^2
Ho(2)	(h)	1786 (4)	1786 (4)	0	1·0 (0·1)
Ho(3)	(e)	0	0	3394 (5)	1·0 (0·2)
Ho(4)	(n)	0	3241 (4)	3975 (2)	0·9 (0·3)
Ge(1)	(i)	3630 (12)	0	0	0·9 (0·3)
Ge(2)	(e)	0	0	1129 (11)	0·8 (0·4)
Ge(3)	(h)	3803 (9)	3803 (9)	0	1·0 (0·3)
Ge(4)	(d)	0	$\frac{1}{2}$	$\frac{1}{4}$	0·4 (0·3)
Ge(5)	(m)	2097 (6)	2097 (6)	3186 (5)	0·8 (0·2)

was 1·1 e.Å^{-3}. Temperature parameters obtained in the refinement appear to be reasonable, and thus there is little evidence of partial occupancy or substitutional disorder between Ho and Ge. Consideration of the various interatomic distances makes the latter possibility unlikely in any event.

Discussion of the structure

Our structure determination shows the composition of this body-centered tetragonal phase to be $Ho_{11}Ge_{10}$. Thus, the compound is not actually 1:1 in stoichiometry, but is instead slightly rich in holmium. The calculated density for $Ho_{11}Ge_{10}$ is essentially the same as for CrB-type HoGe, 8·93 *versus* 8·92 g.cm^{-3}.

A notable feature, compared with the CrB-type monogermanide, is the relatively large number of crystallographically different atoms and the variety of structural roles which these atoms assume. Of the 84 atoms within the unit cell, the 44 Ho atoms are situated in four different crystallographic sites; the 40 Ge atoms are in five crystallographic sites. These Ge atoms can be classified into three types: (1) isolated atoms [Ge(2) and Ge(4)]; (2) pairs of atoms (Ge(1)–Ge(1), Ge(5)–Ge(5); bond lengths = 2·96 and 2·54 Å, respectively); and (3) a square cluster of four atoms (Ge(3) atoms; bond length = 2·58 Å). This latter arrangement is not known in any other germanide or silicide. We note further that the infinite chains of Ge atoms found in CrB-type HoGe are not present in $Ho_{11}Ge_{10}$. There are no other Ge–Ge bonds in $Ho_{11}Ge_{10}$, and thus bonding between Ge atoms is confined to self-bonding, *i.e.* bonding between crystallographically equivalent atoms.

Ho(1), Ho(2) and Ho(4) also use self-bonding to form planar four-clusters, although in the case of Ho(4) the cluster is a rectangle rather than a square. Of special interest is the exceptionally short bond length on two sides of the rectangle. This distance of 3·33 Å is 6% shorter than twice the metallic radius of Ho, and is one of the shortest Ho–Ho distances known. Evidently Ho(4) also exhibits a tendency toward pair formation. Ho(3) forms no self-bonds.

The description of the structure is facilitated by examining first the coordination polyhedra (C.P.'s) which occur along the *c* axis, *i.e.* the C.P.'s of Ge(2) and Ho(3). Ge(2) is bonded to four Ho(1) and four Ho(2) which outline a square antiprism [Fig. 1(*a*)]. Ho(3) is bonded to 16 atoms [4 Ho(1), 4 Ho(4), 4 Ge(3) and 4 Ge(5)]. Like the square antiprism and cuboctahedron, the C.P. of Ho(3) can be considered as based on the stacking of squares, each successive square being rotated in its plane by 45° from the previous square. The resulting polyhedron, illustrated in Fig. 1(*b*), has 16 triangular faces, 4 rhombus-shaped faces and 2 square faces; squares of Ho and Ge alternate along the fourfold axis. The stacking sequence of these two types of polyhedra along the *c* axis is shown in Fig. 2. A body-centering condition produces four other stacks which surround the one passing through the origin. Within these stacks the sequence of C.P.'s is, of course, shifted by *c*/2 relative to that shown in Fig. 2.

Connections between stacks are provided by Ho(2)–Ge(3) bonds along [110] directions at levels of $Z=0$ and $\frac{1}{2}$. The observed Ho(2)–Ge(3) bond length of 3·08 Å is only slightly smaller than the sum of atomic radii of Ge (= 1·37 Å) and Ho (= 1·77 Å) [values from the compilation of Teatum, Gschneidner & Waber (1959)]. In fact, values of the lattice constants along *a* can be predicted to an accuracy of about 1% for the $R_{11}Ge_{10}$ series by assuming that it is the contacts among and between Ho(2) [R(2) in the general case] and Ge(3)

Table 2. *Observed and calculated structure factors*

```
H,K= 0, 0
L FOB FCA
 2  10   4
 4  86 -22
 6 514 584
 8  96  39
10 831 965
12 409 434
14 328-341

H,K= 0, 1
L FOB FCA
 1  24 -24
 3  18  17
 5 225 254
 7  81 -93
 9  59  52
11  56  66
13 141-150
15 213 222

H,K= 0, 2
L FOB FCA
 0  54  40
 2  51 -40
 4 214-212
 6 250-263
 8 155 163
10 134-137
12  48 -24
14  54 -63

H,K= 0, 3
L FOB FCA
 1 304-304
 3 176-167
 5 584 612
 7 138-145
 9 358-366
11  44 -33
13 192-192

H,K= 0, 4
L FOB FCA
 0 663 778
 2 560-579
 4 319-317
 6 160 131
 8 443-448
10 250 228
12  66 -19
14 414-428

H,K= 0, 5
L FOB FCA
 1 240 233
 3 393 379
 5 302 293
 7 156 153
 9 348 357
11 160 171
13  69  67

H,K= 0, 6
L FOB FCA
 0 668 758
 2 250 242
 4 145-145
 6 104 -39
 8 354 367
10 383 373
12 261 249

H,K= 0, 7
L FOB FCA
 1  55 -45
 3 241-233
 5 333 336
 7 147-147
 9 169-170
11 114 120

H,K= 0, 8
L FOB FCA
 0 431 426
 2 247-261
 4  48 -49
 6 146 133
 8 188-186

H,K= 0, 9
L FOB FCA
 1 343-362
 3  31 -14
 5 121 121
 7 146-157

H,K= 0,10
L FOB FCA
 0 430 416
 2  28 -23
 4 107-109

H,K= 1, 1
L FOB FCA
 0  73 -59
 2  39 -21
 4  45  28
 6 301 319
 8  83 -87
10 125-134
12  32  18
14 128 136

H,K= 1, 2
L FOB FCA
 1  25  -5
 3  68  59
 5 559-597
 7 114-107
 9 205 236
11  65 -75
13 101-107
15 216-228

H,K= 1, 3
L FOB FCA
 0  78  72
 2  87 -69
 4 416-391
 6 107-100
 8  79 -72
10  14 -15
12  63 -77
14 113-117

H,K= 1, 4
L FOB FCA
 1 157 149
 3 186-171
 5  96 -80
 7 198-193
 9 171 175
11 161 166
13 268-281

H,K= 1, 5
L FOB FCA
 0 127-107
 2  85 -72
 4  51  43
 6 324 304
 8 138-132
10 180-171
12  27   7

H,K= 1, 6
L FOB FCA
 1  84 -86
 3 362 343
 5  88 -75
 7 121 113
 9 142 138
11 118-118

H,K= 1, 7
L FOB FCA
 0 110 -75
 2  49 -34
 4  93 -71
 6 116 113
 8  66 -67
10 109-106

H,K= 1, 8
L FOB FCA
 1 109 110
 3 266-269
 5 197-190
 7 242-238
 9 111 111

H,K= 1, 9
L FOB FCA
 0  94 105
 2  16 -11
 4 180-190
 6  16  20

H,K= 1,10
L FOB FCA
 1  67 -68
 3 119 134

H,K= 2, 2
L FOB FCA
 0 334-288
 2 141 134
 4 200 182
 6 144 138
 8 275 278
10 435-458
12 195 207
14 192 200

H,K= 2, 3
L FOB FCA
 1  55 -47
 3 648 596
 5 132-120
 7 212 209
 9 305 304
11 145-144
13 222 229

H,K= 2, 4
L FOB FCA
 0 106-106
 2 133-112
 4 100  77
 6  87  62
 8  41  34
10 259-263
12  16  18
14  86  85

H,K= 2, 5
L FOB FCA
 1  98  96
 3  63 -51
 5 504-459
 7 113 -97
 9 203 196
11  47  44
13 143-142

H,K= 2, 6
L FOB FCA
 0 211-217
 2 122 113
 4 209-212
 6 331-314
 8 307 301
10 313-319
12  58  59

H,K= 2, 7
L FOB FCA
 1  76 -76
 3 245 240
 5 483-457
 7  35 -24
 9 257 253
11 173-172

H,K= 2, 8
L FOB FCA
 0  90  90
 2  54 -48
 4 247 242
 6 329 320
 8  15  14

H,K= 2, 9
L FOB FCA
 1  16 -12
 3 172 184
 5  36 -35
 7  77  79

H,K= 2,10
L FOB FCA
 0 341-333
 2 116 129

H,K= 3, 3
L FOB FCA
 0 687 979
 2 396 384
 4 227-202
 6 225 202
 8 304 303
10 596 591
12 300 285
14 104 -96

H,K= 3, 4
L FOB FCA
 1  70 -45
 3 164-145
 5 332 286
 7 144-137
 9 100 -83
11  91  90
13 206-209

H,K= 3, 5
L FOB FCA
 0  20 -23
 2  57  52
 4 233-210
 6  70 -60
 8  51  44
10  42 -36
12  53 -56

H,K= 3, 6
L FOB FCA
 1 456-474
 3 259 232
 5  91  -4
 7  36 -12
 9 213-203
11 397-386

H,K= 3, 7
L FOB FCA
 0 305 313
 2  62 -57
 4 295-277
 6  64  57
 8 101 -91
10 138 134

H,K= 3, 8
L FOB FCA
 1 215 235
 3 200 183
 5 301 293
 7  97 103

H,K= 3, 9
L FOB FCA
 0 314 344
 2 220 220
 4 198-213
 6  57 -69

H,K= 4, 4
L FOB FCA
 0 542 528
 2 411-414
 4  91  62
 6 420 379
 8 378-347
10 119 108
12  55  40

H,K= 4, 5
L FOB FCA
 1  43  42
 3 201-191
 5 237-258
 7 279-248
 9 159 148
11  61  56

H,K= 4, 6
L FOB FCA
 0 244 232
 2 109 -75
 4 199-174
 6 106 -93
 8  89  56
10  31  -8

H,K= 4, 7
L FOB FCA
 1  93 100
 3 218-217
 5  56  68
 7 171-161
 9  32  33

H,K= 4, 8
L FOB FCA
 0 199 204
 2 320-334
 4  79  83
 6 250 255

H,K= 4, 9
L FOB FCA
 1  17  -8
 3  56  52

H,K= 5, 5
L FOB FCA
 0 163 139
 2  42  46
 4 251 235
 6 496 536
 8  67 -57
10  55 -23

H,K= 5, 6
L FOB FCA
 1  41  27
 3 348 346
 5  70 -48
 7 165 152
 9 227 206

H,K= 5, 7
L FOB FCA
 0 225-226
 2  15   6
 4  32 -31
 6  27  38
 8  19 -10

H,K= 5, 8
L FOB FCA
 1 202 218
 3 195-206
 5 116-108

H,K= 5, 9
L FOB FCA
 0  20  31
 2 112-131

H,K= 6, 6
L FOB FCA
 0 308 280
 2 368 391
 4 144-144
 6 232-222
 8 591 545

H,K= 6, 7
L FOB FCA
 1 153-169
 3 196 207
 5  65 -71
 7  31  33

H,K= 6, 8
L FOB FCA
 0  73  61
 2 113-132
 4 119-124

H,K= 7, 7
L FOB FCA
 0 140 123
 2 114-127
 4 119-124
```

which determine the length of a. The derived expression is $a_{\text{calc}} = 2(1+\sqrt{2}/2)(r_{\text{R}}+r_{\text{Ge}})$ where r_{R} = the radius of the rare-earth metal. In the present case of $\text{Ho}_{11}\text{Ge}_{10}$, $a_{\text{calc}} = 10{\cdot}72$ Å, compared with $a_{\text{obs}} = 10{\cdot}79$ Å. There are several Ho–Ge distances (see below) which are shorter than Ho(2)–Ge(3) and which should also be instrumental in governing the size of a. Thus, while the good agreement may be fortuitous the relationship could have predictive value if and when compounds of this composition are found in other systems.

The remaining Ge atoms are accommodated in holes which exist in the framework. A Ge(1)–Ge(1) dumbbell is situated along the a axis at $\frac{1}{2},0,0$; a Ge(5)–Ge(5) dumbbell in the 110 plane and centered at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; and an isolated Ge(4) atom at the special position $0,\frac{1}{2},\frac{1}{4}$. These atoms (and those in equivalent positions) serve also to 'cement' the individual stacks together. In particular, Ge(4) is coordinated to eight Ho atoms, two each from four different stacks; the bond lengths are: Ge(4)–4 Ho(1), 2·85 Å; Ge(4)–4 Ho(4), 3·06 Å. The C.P. for Ge(4), illustrated in Fig. 1(*c*), is the familar bisphenoidal configuration seen in a number of eight-coordinate, inorganic complexes (Hoard & Silverton, 1963). Ge(1) and Ge(5) are both coordinated to eight Ho atoms, as well as to the other Ge atom in the dumbbell. The eight Ho neighbors surrounding Ge(1) are at distances ranging from 2·77 to 3·31 Å; those surrounding Ge(5), 2·88 to 3·40 Å. The C.P.'s for these atoms can be regarded as distortions from either a square antiprism + 1 configuration or a trigonal prism + 3 configuration. (These latter two arrangements do not themselves differ greatly from one another.)

Each Ge(3) in the square of four Ge(3) atoms is coordinated to seven Ho and two Ge atoms, figures which are identical with those for Ge in CrB-type HoGe. The Ge(3)–Ho bond lengths range from 3·05 to 3·18 Å. The C.P. for each individual Ge(3) of the cluster approximates a square antiprism + 1 configuration, the extra atom lying outside a square face.

Holmium atoms in the cluster-of-fours have C.P.'s which are less well-defined. Coordination numbers of 15, 17 and 15 for Ho(1), Ho(2) and Ho(4), respectively, are somewhat larger than the coordination of 13 for Ho in HoGe. Each Ho atom in each cluster is coordinated to seven Ge atoms, as is Ho in HoGe. Thus, the larger coordination numbers result from an increased number of Ho–Ho interactions. The various Ho–Ge and Ho–Ho bond distances range from 2·77 to 3·40 Å and 3·33 to 3·85 Å, respectively. A summary of interatomic distances is given in Table 3.

From the foregoing we conclude that $\text{Ho}_{11}\text{Ge}_{10}$ is a discrete compound, close to but not encompassing a composition of 1:1. We presume also that the same is true of the other rare-earth metals forming this tetragonal phase. It is not at present clear, however, why this phase is found only for the heavier rare-earth metals.

Table 3. *Interatomic distances in* $\text{Ho}_{11}\text{Ge}_{10}$

e.s.d.'s include only uncertainties in positional parameters.

Atom 1	Atom 2	Distance (Å)	e.s.d. (Å)
Ho(1)	Ge(4)	2·852	0·004
	Ge(2)	2·989	0·009
	2 Ge(5)	3·114	0·007
	2 Ge(5)	3·163	0·007
	Ge(1)	3·305	0·006
	Ho(4)	3·461	0·005
	2 Ho(4)	3·575	0·004
	Ho(3)	3·643	0·007
	2 Ho(2)	3·717	0·003
	2 Ho(1)	3·842	0·006
Ho(2)	2 Ge(1)	2·770	0·009
	Ge(3)	3·078	0·014
	2 Ge(2)	3·284	0·011
	2 Ge(5)	3·402	0·009
	4 Ho(1)	3·717	0·003
	4 Ho(4)	3·847	0·004
	2 Ho(2)	3·854	0·006
Ge(1)	2 Ho(2)	2·770	0·009
	4 Ho(4)	2·925	0·007
	Ge(1)	2·957	0·026
	2 Ho(1)	3·305	0·006
Ge(5)	Ge(5)	2·543	0·016
	2 Ho(4)	2·878	0·005
	2 Ho(1)	3·114	0·007
	2 Ho(1)	3·163	0·007
	Ho(3)	3·218	0·009
	Ho(2)	3·402	0·009
Ho(3)	4 Ge(3)	3·184	0·010
	4 Ge(5)	3·218	0·009
	4 Ho(4)	3·623	0·004
	4 Ho(1)	3·643	0·007
Ho(4)	2 Ge(5)	2·878	0·005
	2 Ge(1)	2·925	0·007
	2 Ge(3)	3·050	0·004
	Ge(4)	3·055	0·004
	Ho(4)	3·327	0·007
	Ho(1)	3·461	0·005
	2 Ho(1)	3·575	0·004
	Ho(3)	3·623	0·004
	Ho(4)	3·795	0·008
	2 Ho(2)	3·847	0·004
Ge(2)	4 Ho(1)	2·989	0·009
	4 Ho(2)	3·284	0·011
Ge(3)	2 Ge(3)	2·584	0·019
	4 Ho(4)	3·050	0·004
	Ho(2)	3·078	0·014
	2 Ho(3)	3·184	0·010
Ge(4)	4 Ho(1)	2·852	0·004
	4 Ho(4)	3·055	0·004

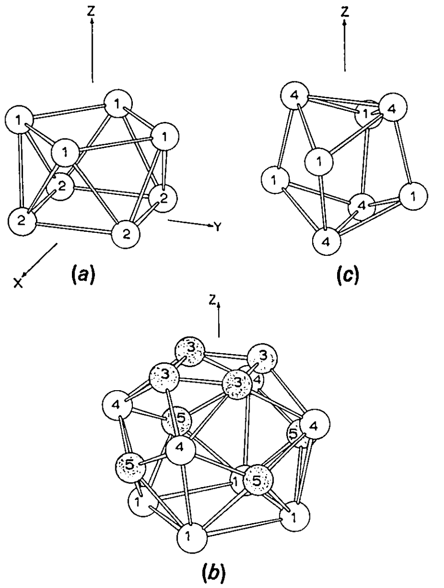

Fig. 1. Ball-and-stick drawings of coordination polyhedra for (*a*) Ge(2), (*b*) Ho(3), (*c*) Ge(4). In each case the central atom is omitted for clarity. The direction of the *Z* axis is indicated. Open circles represent Ho, shaded circles Ge. Numerals identify atoms with those in Table 1.

We are indebted to Dr A. Zalkin for furnishing copies of the several IBM-7094 programs used in the calculations. We thank Dr C. K. Johnson for supplying a copy of this ORTEP program.

Note: Bodnar & Steinfink (1967) report a body-centered tetragonal compound in the Yb–Sb system with $a = 11{\cdot}90$, $c = 17{\cdot}06$ Å, and point out the similarity of these data to those we had reported for rare-earth germanides. The composition given, Yb_5Sb_4 (55·6 at.% Yb) does not agree with that of an 11:10 compound. The experimental composition could be closely approached if one of the fourfold atoms, Ge(2) or Ge(4), were omitted in the Yb–Sb compound. This is a conceivable situation when Sb with a larger size and differing electronic configuration substitutes for Ge. Predicted values of the lattice constant are $a = 11{\cdot}37$ Å (trivalent Yb) and 12·05 Å (divalent Yb).

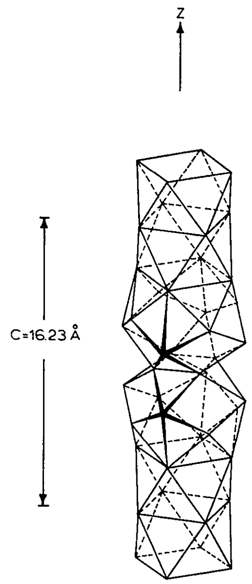

Fig. 2. Sequence of coordination polyhedra within a repeat distance along the *c* axis. Central atoms are again omitted.

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