inorganic compounds

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.127$, $T_{max} = 0.705$

6182 measured reflections

958 independent reflections

816 reflections with $I > 2s(I)$

$R_{int} = 0.070$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.066$

$S = 1.05$

958 reflections

49 parameters

$\Delta\rho_{max} = 2.20$ e Å^{-3}

$\Delta\rho_{min} = -1.44$ e Å^{-3}

Gadolinium scandium germanide, Gd$_2$Sc$_3$Ge$_4$

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Gd$_2$Sc$_3$Ge$_4$ adopts the orthorhombic Pu$_5$Rh$_4$-type structure. The crystal structure contains six sites in the asymmetric unit: two sites are statistically occupied by rare-earth atoms with Gd:Sc ratios of 0.967 (4):0.033 (4) and 0.031 (3):0.969 (3), one site (.*m*. symmetry) is occupied by Sc atoms, and three distinct sites (two of which with .*m*. symmetry) are occupied by Ge atoms. The rare-earth atoms form two-dimensional slabs with Ge atoms occupying the trigonal-prismatic voids.

Related literature

The title compound adopts the Pu$_5$Rh$_4$-type structure (Cromer, 1977). For Ge$\cdots$Ge distances, see: Mozharivskyj *et al.* (2003); Holtzberg *et al.* (1967); Smith *et al.* (1967). For atomic radii. see: Shannon (1976). For the Hamilton significance test, see: Hamilton (1965). For a mixed rare-earth system, see: Misra & Miller (2008).

Experimental

Crystal data

Gd$_2$Sc$_3$Ge$_4$

$M_r = 739.74$

Orthorhombic, *Pnma*

$a = 7.2445$ (13) Å

$b = 14.101$ (3) Å

$c = 7.4930$ (14) Å

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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supporting information

Gadolinium scandium germanide, Gd$_2$Sc$_3$Ge$_4$

Sumohan Misra and Gordon J. Miller

S1. Comment

Continuing our efforts in mixed rare-earth systems bearing the formula $(R_{1-x}R'_x)_5T_4$, where T = Si, Ge, Ga, Sn, we have studied the effect of substitution of Gd by nonmagnetic Sc. Gd$_2$Sc$_3$Ge$_4$ crystallizes in the orthorhombic Pu$_5$Rh$_4$-type structure (Cromer, 1977). Two 3^{2}434 nets built up of Gd and Sc atoms are placed over one another to form two-dimensional slabs with additional Sc atoms in pseudo-cubic coordination and Ge atoms in trigonal prismatic voids (Fig. 1).

The two metal sites situated at the edges of the cube (M1 and M2) exhibit mixed site occupancies, with Gd (the larger atom; Shannon, 1976) having a preference for the M1 site and Sc (the smaller atom; Shannon, 1976) having a preference for the M2 site. The M3 site is completely occupied by Sc atom. This disordered model which introduces two additional refinement parameters yields a statistically significant improvement over various ordered models, at the 0.5% significance level according to a Hamilton's significance test on the crystallographic R factor (Hamilton, 1965).

The Ge1–Ge1 distances are intermediate between those in Gd$_5$Ga$_2$Ge$_2$ [2.741 (1) Å; Gd$_5$Si$_4$-type (Holtzberg *et al.*, 1967)] and Gd$_5$Ga$_{0.7}$Ge$_{3.3}$ [3.461 (5) Å; Sm$_5$Ge$_4$-type (Smith *et al.*, 1967)] (Mozharivskyj *et al.*, 2003).

S2. Experimental

Gd$_2$Sc$_3$Ge$_4$ was prepared by arc-melting pieces of the constituent elements (Gd, 99.99 wt. %, Materials Preparation Center, Ames Laboratory; Sc, 99.99 wt. %, Materials Preparation Center, Ames Laboratory; Ge, 99.9999 wt. %, Alfa Aesar) in an argon atmosphere on a water-cooled copper hearth. The ingot had a total weight of ca. 0.8 g and was remelted six times with the button being turned over after each melting to ensure homogeneity. Weight losses during melting were less than 0.1 wt. %.

S3. Refinement

A disordered model works best compared to an ordered model and this has been confirmed by a Hamilton's significance test on the crystallographic R factor. We formulated four hypotheses to be tested: (A) M1 site is all Gd, M2 site is all Sc; (B) M1 site is all Gd, M2 site is mixed with Gd and Sc; (C) M1 site is mixed with Gd and Sc, M1 site is all Sc; and (D) both M1 and M2 sites are mixed with Gd and Sc. The number of parameters refined in the four cases were m_A = 47, m_B = 48, m_C = 48, and m_D = 49. There were 958 reflections. The R factors achieved were R_A = 0.0333, R_B = 0.0318, R_C = 0.0326, and R_D = 0.0313. We could reject hypotheses (A), (B), and (C) at the 0.5% level of significance corresponding to hypothesis (D).
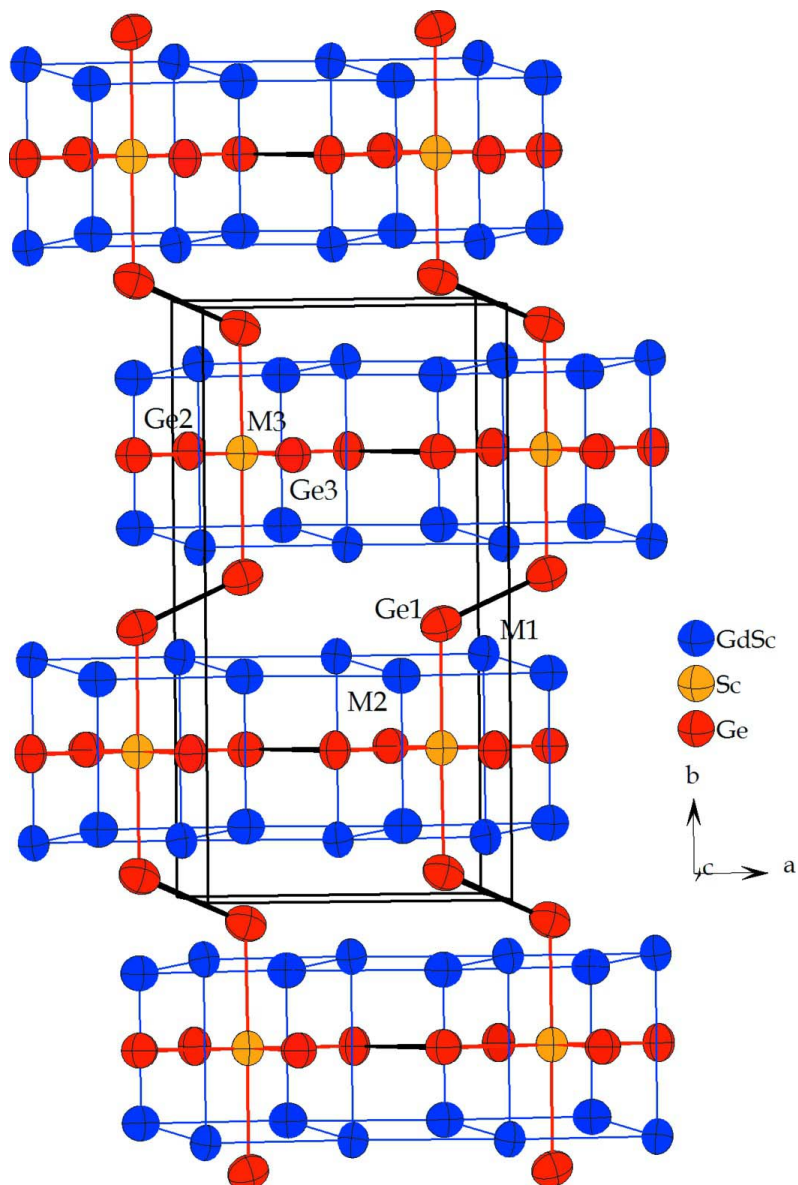
Figure 1

View of $Gd_2Sc_3Ge_4$ along [001], with displacement ellipsoids drawn at the 99 % probability level.

Diadolinium triscandium tetragermanide

Crystal data

$Gd_2Sc_3Ge_4$	$F(000) = 1276$
$M_r = 739.74$	$D_x = 6.419$ Mg m^{-3}
Orthorhombic, *Pnma*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2n	Cell parameters from 6182 reflections
$a = 7.2445$ (13) Å	$\theta = 3.1–27.8°$
$b = 14.101$ (3) Å	$\mu = 34.91$ mm^{-1}
$c = 7.4930$ (14) Å	$T = 298$ K
$V = 765.4$ (2) Å^3	Plate, grey
$Z = 4$	$0.06 \times 0.05 \times 0.01$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	6182 measured reflections
Radiation source: fine-focus sealed tube	958 independent reflections
Graphite monochromator	816 reflections with $I > 2s(I)$
φ and ω scans	$R_{int} = 0.070$
Absorption correction: multi-scan ($SADABS$; Bruker, 2002)	$\theta_{max} = 28.2°$, $\theta_{min} = 2.9°$
$T_{min} = 0.127$, $T_{max} = 0.705$	$h = -9 \rightarrow 9$
	$k = -17 \rightarrow 18$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.0171P)^2 + 3.8343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.066$	
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
958 reflections	$\Delta\rho_{max} = 2.20$ e Å^{-3}
49 parameters	$\Delta\rho_{min} = -1.44$ e Å^{-3}
0 restraints	Extinction correction: $SHELXL97$ (Bruker, 2002), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00245 (16)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Gd1	0.99788 (5)	0.40395 (3)	0.17641 (5)	0.00746 (16)	0.967 (4)
Sc1	0.99788 (5)	0.40395 (3)	0.17641 (5)	0.00746 (16)	0.033 (4)
Gd2	0.6602 (2)	0.37594 (9)	0.83229 (17)	0.0081 (5)	0.031 (3)
Sc2	0.6602 (2)	0.37594 (9)	0.83229 (17)	0.0081 (5)	0.969 (3)
Sc3	0.1761 (3)	0.7500	0.5005 (3)	0.0072 (4)	
Ge1	0.82216 (12)	0.45888 (6)	0.54068 (11)	0.0091 (2)	
Ge2	0.03997 (16)	0.7500	0.12561 (16)	0.0081 (3)	
Ge3	0.30680 (16)	0.7500	0.86322 (15)	0.0081 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.0064 (2)	0.0085 (2)	0.0074 (2)	0.00025 (14)	0.00024 (15)	0.00013 (15)
Sc1	0.0064 (2)	0.0085 (2)	0.0074 (2)	0.00025 (14)	0.00024 (15)	0.00013 (15)
Gd2	0.0095 (8)	0.0083 (7)	0.0065 (8)	0.0000 (5)	0.0006 (5)	0.0001 (5)
Sc2	0.0095 (8)	0.0083 (7)	0.0065 (8)	0.0000 (5)	0.0006 (5)	0.0001 (5)

Sc3	0.0067 (10)	0.0079 (10)	0.0072 (10)	0.000	0.0000 (8)	0.000
Ge1	0.0113 (5)	0.0086 (4)	0.0073 (4)	0.0011 (3)	−0.0009 (3)	0.0008 (3)
Ge2	0.0068 (6)	0.0098 (6)	0.0077 (6)	0.000	0.0012 (5)	0.000
Ge3	0.0085 (6)	0.0082 (6)	0.0077 (6)	0.000	−0.0008 (5)	0.000

Geometric parameters (Å, º)

Gd1—Ge3[i]	2.9452 (9)	Sc3—Gd2[xiv]	3.268 (2)
Gd1—Ge1[ii]	2.9605 (10)	Sc3—Sc2[xii]	3.283 (2)
Gd1—Ge1	3.1097 (10)	Sc3—Gd2[iii]	3.283 (2)
Gd1—Ge3[iii]	3.1101 (10)	Ge1—Sc2[i]	2.8070 (16)
Gd1—Ge2[iv]	3.1478 (10)	Ge1—Gd2[i]	2.8070 (16)
Gd1—Ge1[v]	3.1519 (10)	Ge1—Sc2[xv]	2.8759 (17)
Gd1—Ge1[i]	3.1861 (10)	Ge1—Gd2[xv]	2.8759 (17)
Gd1—Sc3[i]	3.4681 (17)	Ge1—Ge1[v]	2.8907 (17)
Gd1—Sc3[iii]	3.4877 (17)	Ge1—Gd1[xvi]	2.9605 (10)
Gd1—Sc2[i]	3.5083 (15)	Ge1—Sc1[xvi]	2.9605 (10)
Gd1—Gd2[i]	3.5083 (15)	Ge1—Sc3[iii]	2.9614 (10)
Gd1—Gd2[vi]	3.5762 (15)	Ge2—Ge3[vi]	2.7572 (17)
Gd2—Ge1	2.7421 (15)	Ge2—Sc2[xiv]	2.7668 (16)
Gd2—Ge2[vii]	2.7668 (16)	Ge2—Gd2[xiv]	2.7668 (16)
Gd2—Ge1[viii]	2.8070 (16)	Ge2—Sc2[xiii]	2.7668 (16)
Gd2—Ge2[iii]	2.8234 (17)	Ge2—Gd2[xiii]	2.7668 (16)
Gd2—Ge1[ix]	2.8759 (17)	Ge2—Sc3[xvi]	2.800 (2)
Gd2—Ge3[x]	2.9010 (16)	Ge2—Sc2[xii]	2.8234 (17)
Gd2—Sc3[vii]	3.268 (2)	Ge2—Gd2[xii]	2.8234 (17)
Gd2—Sc3[iii]	3.283 (2)	Ge2—Gd2[iii]	2.8234 (17)
Gd2—Gd1[viii]	3.5083 (15)	Ge2—Sc2[iii]	2.8234 (17)
Gd2—Sc1[viii]	3.5083 (15)	Ge2—Sc1[iv]	3.1478 (10)
Gd2—Sc2[xi]	3.552 (3)	Ge3—Ge2[xvii]	2.7572 (17)
Gd2—Gd2[xi]	3.552 (3)	Ge3—Sc3[xv]	2.864 (2)
Sc3—Ge2[ii]	2.800 (2)	Ge3—Sc2[xviii]	2.9010 (16)
Sc3—Ge3[ix]	2.864 (2)	Ge3—Gd2[xviii]	2.9010 (16)
Sc3—Ge3	2.878 (2)	Ge3—Sc2[x]	2.9010 (16)
Sc3—Ge1[xii]	2.9614 (10)	Ge3—Gd2[x]	2.9010 (16)
Sc3—Ge1[iii]	2.9614 (10)	Ge3—Gd1[xix]	2.9452 (9)
Sc3—Ge2	2.977 (2)	Ge3—Sc1[xix]	2.9452 (9)
Sc3—Sc2[xiii]	3.268 (2)	Ge3—Gd1[viii]	2.9452 (9)
Sc3—Gd2[xiii]	3.268 (2)	Ge3—Sc1[viii]	2.9452 (9)
Sc3—Sc2[xiv]	3.268 (2)	Ge3—Gd1[iii]	3.1101 (10)
Ge3[i]—Gd1—Ge1[ii]	94.17 (3)	Ge3[ix]—Sc3—Gd2[iii]	127.47 (6)
Ge3[i]—Gd1—Ge1	87.88 (3)	Ge3—Sc3—Gd2[iii]	126.76 (6)
Ge1[ii]—Gd1—Ge1	137.90 (3)	Ge1[xii]—Sc3—Gd2[iii]	117.23 (7)
Ge3[i]—Gd1—Ge3[iii]	82.64 (2)	Ge1[iii]—Sc3—Gd2[iii]	51.79 (3)
Ge1[ii]—Gd1—Ge3[iii]	133.89 (3)	Ge2—Sc3—Gd2[iii]	53.35 (4)
Ge1—Gd1—Ge3[iii]	88.12 (3)	Sc2[xiii]—Sc3—Gd2[iii]	71.49 (4)
Ge3[i]—Gd1—Ge2[iv]	82.83 (3)	Gd2[xiii]—Sc3—Gd2[iii]	71.49 (4)

Ge1^{ii}—Gd1—Ge2^{iv}	81.64 (3)	Sc2^{xiv}—Sc3—Gd2^{iii}	105.69 (6)
Ge1—Gd1—Ge2^{iv}	140.09 (3)	Gd2^{xiv}—Sc3—Gd2^{iii}	105.69 (6)
Ge3^{iii}—Gd1—Ge2^{iv}	52.28 (3)	Sc2^{xii}—Sc3—Gd2^{iii}	65.50 (6)
Ge3^{i}—Gd1—Ge1^{v}	86.21 (3)	Gd2—Ge1—Sc2^{i}	144.75 (4)
Ge1^{ii}—Gd1—Ge1^{v}	83.153 (17)	Gd2—Ge1—Gd2^{i}	144.75 (4)
Ge1—Gd1—Ge1^{v}	54.98 (3)	Sc2^{i}—Ge1—Gd2^{i}	0.00 (5)
Ge3^{iii}—Gd1—Ge1^{v}	141.82 (3)	Gd2—Ge1—Sc2^{xv}	85.83 (4)
Ge2^{iv}—Gd1—Ge1^{v}	160.52 (3)	Sc2^{i}—Ge1—Sc2^{xv}	118.86 (4)
Ge3^{i}—Gd1—Ge1^{i}	161.59 (3)	Gd2^{i}—Ge1—Sc2^{xv}	118.86 (4)
Ge1^{ii}—Gd1—Ge1^{i}	104.08 (3)	Gd2—Ge1—Gd2^{xv}	85.83 (4)
Ge1—Gd1—Ge1^{i}	80.275 (17)	Sc2^{i}—Ge1—Gd2^{xv}	118.86 (4)
Ge3^{iii}—Gd1—Ge1^{i}	82.92 (3)	Gd2^{i}—Ge1—Gd2^{xv}	118.86 (4)
Ge2^{iv}—Gd1—Ge1^{i}	97.23 (3)	Sc2^{xv}—Ge1—Gd2^{xv}	0.00 (7)
Ge1^{v}—Gd1—Ge1^{i}	98.23 (3)	Gd2—Ge1—Ge1^{v}	136.10 (5)
Ge3^{i}—Gd1—Sc3^{i}	52.57 (4)	Sc2^{i}—Ge1—Ge1^{v}	60.61 (4)
Ge1^{ii}—Gd1—Sc3^{i}	54.16 (3)	Gd2^{i}—Ge1—Ge1^{v}	60.61 (4)
Ge1—Gd1—Sc3^{i}	140.20 (4)	Sc2^{xv}—Ge1—Ge1^{v}	58.26 (4)
Ge3^{iii}—Gd1—Sc3^{i}	90.58 (3)	Gd2^{xv}—Ge1—Ge1^{v}	58.26 (4)
Ge2^{iv}—Gd1—Sc3^{i}	49.79 (4)	Gd2—Ge1—Gd1^{xvi}	89.24 (4)
Ge1^{v}—Gd1—Sc3^{i}	110.99 (4)	Sc2^{i}—Ge1—Gd1^{xvi}	86.99 (4)
Ge1^{i}—Gd1—Sc3^{i}	138.95 (4)	Gd2^{i}—Ge1—Gd1^{xvi}	86.99 (4)
Ge3^{i}—Gd1—Sc3^{iii}	52.04 (4)	Sc2^{xv}—Ge1—Gd1^{xvi}	138.69 (4)
Ge1^{ii}—Gd1—Sc3^{iii}	146.21 (4)	Gd2^{xv}—Ge1—Gd1^{xvi}	138.69 (4)
Ge1—Gd1—Sc3^{iii}	52.97 (3)	Ge1^{v}—Ge1—Gd1^{xvi}	134.14 (5)
Ge3^{iii}—Gd1—Sc3^{iii}	51.34 (4)	Gd2—Ge1—Sc1^{xvi}	89.24 (4)
Ge2^{iv}—Gd1—Sc3^{iii}	92.20 (3)	Sc2^{i}—Ge1—Sc1^{xvi}	86.99 (4)
Ge1^{v}—Gd1—Sc3^{iii}	93.70 (4)	Gd2^{i}—Ge1—Sc1^{xvi}	86.99 (4)
Ge1^{i}—Gd1—Sc3^{iii}	109.66 (4)	Sc2^{xv}—Ge1—Sc1^{xvi}	138.69 (4)
Sc3^{i}—Gd1—Sc3^{iii}	96.92 (4)	Gd2^{xv}—Ge1—Sc1^{xvi}	138.69 (4)
Ge3^{i}—Gd1—Sc2^{i}	130.59 (3)	Ge1^{v}—Ge1—Sc1^{xvi}	134.14 (5)
Ge1^{ii}—Gd1—Sc2^{i}	102.15 (3)	Gd1^{xvi}—Ge1—Sc1^{xvi}	0.000 (17)
Ge1—Gd1—Sc2^{i}	49.75 (3)	Gd2—Ge1—Sc3^{iii}	70.16 (5)
Ge3^{iii}—Gd1—Sc2^{i}	114.68 (3)	Sc2^{i}—Ge1—Sc3^{iii}	140.10 (6)
Ge2^{iv}—Gd1—Sc2^{i}	145.18 (3)	Gd2^{i}—Ge1—Sc3^{iii}	140.10 (6)
Ge1^{v}—Gd1—Sc2^{i}	50.82 (3)	Sc2^{xv}—Ge1—Sc3^{iii}	68.07 (5)
Ge1^{i}—Gd1—Sc2^{i}	48.06 (3)	Gd2^{xv}—Ge1—Sc3^{iii}	68.07 (5)
Sc3^{i}—Gd1—Sc2^{i}	154.50 (3)	Ge1^{v}—Ge1—Sc3^{iii}	111.92 (6)
Sc3^{iii}—Gd1—Sc2^{i}	101.62 (3)	Gd1^{xvi}—Ge1—Sc3^{iii}	71.70 (5)
Ge3^{i}—Gd1—Gd2^{i}	130.59 (3)	Sc1^{xvi}—Ge1—Sc3^{iii}	71.70 (5)
Ge1^{ii}—Gd1—Gd2^{i}	102.15 (3)	Gd2—Ge1—Gd1	140.21 (4)
Ge1—Gd1—Gd2^{i}	49.75 (3)	Sc2^{i}—Ge1—Gd1	72.53 (3)
Ge3^{iii}—Gd1—Gd2^{i}	114.68 (3)	Gd2^{i}—Ge1—Gd1	72.53 (3)
Ge2^{iv}—Gd1—Gd2^{i}	145.18 (3)	Sc2^{xv}—Ge1—Gd1	80.83 (4)
Ge1^{v}—Gd1—Gd2^{i}	50.82 (3)	Gd2^{xv}—Ge1—Gd1	80.83 (4)
Ge1^{i}—Gd1—Gd2^{i}	48.06 (3)	Ge1^{v}—Ge1—Gd1	63.25 (3)
Sc3^{i}—Gd1—Gd2^{i}	154.50 (3)	Gd1^{xvi}—Ge1—Gd1	77.14 (2)
Sc3^{iii}—Gd1—Gd2^{i}	101.62 (3)	Sc1^{xvi}—Ge1—Gd1	77.14 (2)
Sc2^{i}—Gd1—Gd2^{i}	0.00 (4)	Sc3^{iii}—Ge1—Gd1	70.08 (4)

Ge3[i]—Gd1—Gd2[vi]	126.15 (3)	Ge3[vi]—Ge2—Sc2[xiv]	140.05 (3)
Ge1[ii]—Gd1—Gd2[vi]	100.11 (3)	Ge3[vi]—Ge2—Gd2[xiv]	140.05 (3)
Ge1—Gd1—Gd2[vi]	112.35 (3)	Sc2[xiv]—Ge2—Gd2[xiv]	0.00 (5)
Ge3[iii]—Gd1—Gd2[vi]	50.84 (3)	Ge3[vi]—Ge2—Sc2[xiii]	140.05 (3)
Ge2[iv]—Gd1—Gd2[vi]	49.15 (3)	Sc2[xiv]—Ge2—Sc2[xiii]	79.86 (7)
Ge1[v]—Gd1—Gd2[vi]	146.68 (3)	Gd2[xiv]—Ge2—Sc2[xiii]	79.86 (7)
Ge1[i]—Gd1—Gd2[vi]	48.63 (3)	Ge3[vi]—Ge2—Gd2[xiii]	140.05 (3)
Sc3[i]—Gd1—Gd2[vi]	97.04 (4)	Sc2[xiv]—Ge2—Gd2[xiii]	79.86 (7)
Sc3[iii]—Gd1—Gd2[vi]	100.63 (4)	Gd2[xiv]—Ge2—Gd2[xiii]	79.86 (7)
Sc2[i]—Gd1—Gd2[vi]	96.57 (3)	Sc2[xiii]—Ge2—Gd2[xiii]	0.00 (5)
Gd2[i]—Gd1—Gd2[vi]	96.57 (3)	Ge3[vi]—Ge2—Sc3[xvi]	114.80 (6)
Ge1—Gd2—Ge2[vii]	92.98 (5)	Sc2[xiv]—Ge2—Sc3[xvi]	72.27 (5)
Ge1—Gd2—Ge1[viii]	94.01 (4)	Gd2[xiv]—Ge2—Sc3[xvi]	72.27 (5)
Ge2[vii]—Gd2—Ge1[viii]	150.21 (6)	Sc2[xiii]—Ge2—Sc3[xvi]	72.27 (5)
Ge1—Gd2—Ge2[iii]	91.61 (5)	Gd2[xiii]—Ge2—Sc3[xvi]	72.27 (5)
Ge2[vii]—Gd2—Ge2[iii]	93.56 (4)	Ge3[vi]—Ge2—Sc2[xii]	62.63 (4)
Ge1[viii]—Gd2—Ge2[iii]	115.13 (5)	Sc2[xiv]—Ge2—Sc2[xii]	86.39 (4)
Ge1—Gd2—Ge1[ix]	117.05 (5)	Gd2[xiv]—Ge2—Sc2[xii]	86.39 (4)
Ge2[vii]—Gd2—Ge1[ix]	90.00 (5)	Sc2[xiii]—Ge2—Sc2[xii]	138.11 (5)
Ge1[viii]—Gd2—Ge1[ix]	61.14 (4)	Gd2[xiii]—Ge2—Sc2[xii]	138.11 (5)
Ge2[iii]—Gd2—Ge1[ix]	150.92 (6)	Sc3[xvi]—Ge2—Sc2[xii]	139.64 (4)
Ge1—Gd2—Ge3[x]	148.48 (6)	Ge3[vi]—Ge2—Gd2[xii]	62.63 (4)
Ge2[vii]—Gd2—Ge3[x]	95.19 (5)	Sc2[xiv]—Ge2—Gd2[xii]	86.39 (4)
Ge1[viii]—Gd2—Ge3[x]	93.83 (5)	Gd2[xiv]—Ge2—Gd2[xii]	86.39 (4)
Ge2[iii]—Gd2—Ge3[x]	57.57 (4)	Sc2[xiii]—Ge2—Gd2[xii]	138.11 (5)
Ge1[ix]—Gd2—Ge3[x]	93.37 (5)	Gd2[xiii]—Ge2—Gd2[xii]	138.11 (5)
Ge1—Gd2—Sc3[vii]	149.10 (6)	Sc3[xvi]—Ge2—Gd2[xii]	139.64 (4)
Ge2[vii]—Gd2—Sc3[vii]	58.41 (5)	Sc2[xii]—Ge2—Gd2[xii]	0.00 (7)
Ge1[viii]—Gd2—Sc3[vii]	105.69 (5)	Ge3[vi]—Ge2—Gd2[iii]	62.63 (4)
Ge2[iii]—Gd2—Sc3[vii]	100.88 (5)	Sc2[xiv]—Ge2—Gd2[iii]	138.11 (5)
Ge1[ix]—Gd2—Sc3[vii]	57.21 (4)	Gd2[xiv]—Ge2—Gd2[iii]	138.11 (5)
Ge3[x]—Gd2—Sc3[vii]	54.94 (5)	Sc2[xiii]—Ge2—Gd2[iii]	86.39 (4)
Ge1—Gd2—Sc3[iii]	58.06 (4)	Gd2[xiii]—Ge2—Gd2[iii]	86.39 (4)
Ge2[vii]—Gd2—Sc3[iii]	54.33 (5)	Sc3[xvi]—Ge2—Gd2[iii]	139.64 (4)
Ge1[viii]—Gd2—Sc3[iii]	148.75 (6)	Sc2[xii]—Ge2—Gd2[iii]	77.95 (6)
Ge2[iii]—Gd2—Sc3[iii]	57.77 (5)	Gd2[xii]—Ge2—Gd2[iii]	77.95 (6)
Ge1[ix]—Gd2—Sc3[iii]	141.16 (6)	Ge3[vi]—Ge2—Sc2[iii]	62.63 (4)
Ge3[x]—Gd2—Sc3[iii]	103.67 (5)	Sc2[xiv]—Ge2—Sc2[iii]	138.11 (5)
Sc3[vii]—Gd2—Sc3[iii]	105.56 (5)	Gd2[xiv]—Ge2—Sc2[iii]	138.11 (5)
Ge1—Gd2—Gd1[viii]	59.81 (3)	Sc2[xiii]—Ge2—Sc2[iii]	86.39 (4)
Ge2[vii]—Gd2—Gd1[viii]	102.14 (4)	Gd2[xiii]—Ge2—Sc2[iii]	86.39 (4)
Ge1[viii]—Gd2—Gd1[viii]	57.73 (3)	Sc3[xvi]—Ge2—Sc2[iii]	139.64 (4)
Ge2[iii]—Gd2—Gd1[viii]	147.65 (5)	Sc2[xii]—Ge2—Sc2[iii]	77.95 (6)
Ge1[ix]—Gd2—Gd1[viii]	58.16 (3)	Gd2[xii]—Ge2—Sc2[iii]	77.95 (6)
Ge3[x]—Gd2—Gd1[viii]	146.13 (5)	Gd2[iii]—Ge2—Sc2[iii]	0.00 (7)
Sc3[vii]—Gd2—Gd1[viii]	111.45 (5)	Ge3[vi]—Ge2—Sc3	116.13 (6)
Sc3[iii]—Gd2—Gd1[viii]	110.10 (4)	Sc2[xiv]—Ge2—Sc3	69.24 (5)
Ge1—Gd2—Sc1[viii]	59.81 (3)	Gd2[xiv]—Ge2—Sc3	69.24 (5)

Ge2[vii]—Gd2—Sc1[viii]	102.14 (4)	Sc2[xiii]—Ge2—Sc3	69.24 (5)
Ge1[viii]—Gd2—Sc1[viii]	57.73 (3)	Gd2[xiii]—Ge2—Sc3	69.24 (5)
Ge2[iii]—Gd2—Sc1[viii]	147.65 (5)	Sc3[xvi]—Ge2—Sc3	129.07 (7)
Ge1[ix]—Gd2—Sc1[viii]	58.16 (3)	Sc2[xii]—Ge2—Sc3	68.88 (5)
Ge3[x]—Gd2—Sc1[viii]	146.13 (5)	Gd2[xii]—Ge2—Sc3	68.88 (5)
Sc3[vii]—Gd2—Sc1[viii]	111.45 (5)	Gd2[iii]—Ge2—Sc3	68.88 (5)
Sc3[iii]—Gd2—Sc1[viii]	110.10 (4)	Sc2[iii]—Ge2—Sc3	68.88 (5)
Gd1[viii]—Gd2—Sc1[viii]	0.000 (12)	Ge3[vi]—Ge2—Sc1[iv]	63.16 (3)
Ge1—Gd2—Sc2[xi]	115.24 (3)	Sc2[xiv]—Ge2—Sc1[iv]	143.07 (5)
Ge2[vii]—Gd2—Sc2[xi]	50.07 (3)	Gd2[xiv]—Ge2—Sc1[iv]	143.07 (5)
Ge1[viii]—Gd2—Sc2[xi]	146.07 (3)	Sc2[xiii]—Ge2—Sc1[iv]	85.07 (3)
Ge2[iii]—Gd2—Sc2[xi]	51.02 (3)	Gd2[xiii]—Ge2—Sc1[iv]	85.07 (3)
Ge1[ix]—Gd2—Sc2[xi]	113.99 (3)	Sc3[xvi]—Ge2—Sc1[iv]	71.06 (4)
Ge3[x]—Gd2—Sc2[xi]	52.25 (3)	Sc2[xii]—Ge2—Sc1[iv]	125.53 (5)
Sc3[vii]—Gd2—Sc2[xi]	57.08 (3)	Gd2[xii]—Ge2—Sc1[iv]	125.53 (5)
Sc3[iii]—Gd2—Sc2[xi]	57.25 (3)	Gd2[iii]—Ge2—Sc1[iv]	73.36 (3)
Gd1[viii]—Gd2—Sc2[xi]	152.21 (2)	Sc2[iii]—Ge2—Sc1[iv]	73.36 (3)
Sc1[viii]—Gd2—Sc2[xi]	152.21 (2)	Sc3—Ge2—Sc1[iv]	135.00 (2)
Ge1—Gd2—Gd2[xi]	115.24 (3)	Ge2[xvii]—Ge3—Sc3[xv]	113.62 (6)
Ge2[vii]—Gd2—Gd2[xi]	50.07 (3)	Ge2[xvii]—Ge3—Sc3	116.29 (7)
Ge1[viii]—Gd2—Gd2[xi]	146.07 (3)	Sc3[xv]—Ge3—Sc3	130.10 (7)
Ge2[iii]—Gd2—Gd2[xi]	51.02 (3)	Ge2[xvii]—Ge3—Sc2[xviii]	59.80 (4)
Ge1[ix]—Gd2—Gd2[xi]	113.99 (3)	Sc3[xv]—Ge3—Sc2[xviii]	69.05 (5)
Ge3[x]—Gd2—Gd2[xi]	52.25 (3)	Sc3—Ge3—Sc2[xviii]	140.34 (4)
Sc3[vii]—Gd2—Gd2[xi]	57.08 (3)	Ge2[xvii]—Ge3—Gd2[xviii]	59.80 (4)
Sc3[iii]—Gd2—Gd2[xi]	57.25 (3)	Sc3[xv]—Ge3—Gd2[xviii]	69.05 (5)
Gd1[viii]—Gd2—Gd2[xi]	152.21 (2)	Sc3—Ge3—Gd2[xviii]	140.34 (4)
Sc1[viii]—Gd2—Gd2[xi]	152.21 (2)	Sc2[xviii]—Ge3—Gd2[xviii]	0.00 (3)
Sc2[xi]—Gd2—Gd2[xi]	0.00 (6)	Ge2[xvii]—Ge3—Sc2[x]	59.80 (4)
Ge2[ii]—Sc3—Ge3[ix]	178.82 (9)	Sc3[xv]—Ge3—Sc2[x]	69.05 (5)
Ge2[ii]—Sc3—Ge3	90.52 (7)	Sc3—Ge3—Sc2[x]	140.34 (4)
Ge3[ix]—Sc3—Ge3	88.30 (6)	Sc2[xviii]—Ge3—Sc2[x]	75.49 (6)
Ge2[ii]—Sc3—Ge1[xii]	87.76 (4)	Gd2[xviii]—Ge3—Sc2[x]	75.49 (6)
Ge3[ix]—Sc3—Ge1[xii]	92.35 (4)	Ge2[xvii]—Ge3—Gd2[x]	59.80 (4)
Ge3—Sc3—Ge1[xii]	95.56 (4)	Sc3[xv]—Ge3—Gd2[x]	69.05 (5)
Ge2[ii]—Sc3—Ge1[iii]	87.76 (4)	Sc3—Ge3—Gd2[x]	140.34 (4)
Ge3[ix]—Sc3—Ge1[iii]	92.35 (4)	Sc2[xviii]—Ge3—Gd2[x]	75.49 (6)
Ge3—Sc3—Ge1[iii]	95.56 (4)	Gd2[xviii]—Ge3—Gd2[x]	75.49 (6)
Ge1[xii]—Sc3—Ge1[iii]	168.04 (8)	Sc2[x]—Ge3—Gd2[x]	0.00 (4)
Ge2[ii]—Sc3—Ge2	89.64 (6)	Ge2[xvii]—Ge3—Gd1[xix]	132.513 (19)
Ge3[ix]—Sc3—Ge2	91.54 (7)	Sc3[xv]—Ge3—Gd1[xix]	73.78 (4)
Ge3—Sc3—Ge2	179.85 (9)	Sc3—Ge3—Gd1[xix]	73.09 (4)
Ge1[xii]—Sc3—Ge2	84.44 (4)	Sc2[xviii]—Ge3—Gd1[xix]	83.28 (3)
Ge1[iii]—Sc3—Ge2	84.44 (4)	Gd2[xviii]—Ge3—Gd1[xix]	83.28 (3)
Ge2[ii]—Sc3—Sc2[xiii]	124.88 (6)	Sc2[x]—Ge3—Gd1[xix]	141.76 (5)
Ge3[ix]—Sc3—Sc2[xiii]	56.01 (5)	Gd2[x]—Ge3—Gd1[xix]	141.76 (5)
Ge3—Sc3—Sc2[xiii]	127.54 (6)	Ge2[xvii]—Ge3—Sc1[xix]	132.513 (19)
Ge1[xii]—Sc3—Sc2[xiii]	120.23 (7)	Sc3[xv]—Ge3—Sc1[xix]	73.78 (4)

Ge1ⁱⁱⁱ—Sc3—Sc2ˣⁱⁱⁱ	54.72 (4)	Sc3—Ge3—Sc1ˣⁱˣ	73.09 (4)
Ge2—Sc3—Sc2ˣⁱⁱⁱ	52.35 (4)	Sc2ˣᵛⁱⁱⁱ—Ge3—Sc1ˣⁱˣ	83.28 (3)
Ge2ⁱⁱ—Sc3—Gd2ˣⁱⁱⁱ	124.88 (6)	Gd2ˣᵛⁱⁱⁱ—Ge3—Sc1ˣⁱˣ	83.28 (3)
Ge3ⁱˣ—Sc3—Gd2ˣⁱⁱⁱ	56.01 (5)	Sc2ˣ—Ge3—Sc1ˣⁱˣ	141.76 (5)
Ge3—Sc3—Gd2ˣⁱⁱⁱ	127.54 (6)	Gd2ˣ—Ge3—Sc1ˣⁱˣ	141.76 (5)
Ge1ˣⁱⁱ—Sc3—Gd2ˣⁱⁱⁱ	120.23 (7)	Gd1ˣⁱˣ—Ge3—Sc1ˣⁱˣ	0.000 (17)
Ge1ⁱⁱⁱ—Sc3—Gd2ˣⁱⁱⁱ	54.72 (4)	Ge2ˣᵛⁱⁱ—Ge3—Gd1ᵛⁱⁱⁱ	132.513 (19)
Ge2—Sc3—Gd2ˣⁱⁱⁱ	52.35 (4)	Sc3ˣᵛ—Ge3—Gd1ᵛⁱⁱⁱ	73.78 (4)
Sc2ˣⁱⁱⁱ—Sc3—Gd2ˣⁱⁱⁱ	0.00 (3)	Sc3—Ge3—Gd1ᵛⁱⁱⁱ	73.09 (4)
Ge2ⁱⁱ—Sc3—Sc2ˣⁱᵛ	124.88 (6)	Sc2ˣᵛⁱⁱⁱ—Ge3—Gd1ᵛⁱⁱⁱ	141.76 (5)
Ge3ⁱˣ—Sc3—Sc2ˣⁱᵛ	56.01 (5)	Gd2ˣᵛⁱⁱⁱ—Ge3—Gd1ᵛⁱⁱⁱ	141.76 (5)
Ge3—Sc3—Sc2ˣⁱᵛ	127.54 (6)	Sc2ˣ—Ge3—Gd1ᵛⁱⁱⁱ	83.28 (3)
Ge1ˣⁱⁱ—Sc3—Sc2ˣⁱᵛ	54.72 (4)	Gd2ˣ—Ge3—Gd1ᵛⁱⁱⁱ	83.28 (3)
Ge1ⁱⁱⁱ—Sc3—Sc2ˣⁱᵛ	120.23 (7)	Gd1ˣⁱˣ—Ge3—Gd1ᵛⁱⁱⁱ	94.96 (4)
Ge2—Sc3—Sc2ˣⁱᵛ	52.35 (4)	Sc1ˣⁱˣ—Ge3—Gd1ᵛⁱⁱⁱ	94.96 (4)
Sc2ˣⁱⁱⁱ—Sc3—Sc2ˣⁱᵛ	65.84 (6)	Ge2ˣᵛⁱⁱ—Ge3—Sc1ᵛⁱⁱⁱ	132.513 (19)
Gd2ˣⁱⁱⁱ—Sc3—Sc2ˣⁱᵛ	65.84 (6)	Sc3ˣᵛ—Ge3—Sc1ᵛⁱⁱⁱ	73.78 (4)
Ge2ⁱⁱ—Sc3—Gd2ˣⁱᵛ	124.88 (6)	Sc3—Ge3—Sc1ᵛⁱⁱⁱ	73.09 (4)
Ge3ⁱˣ—Sc3—Gd2ˣⁱᵛ	56.01 (5)	Sc2ˣᵛⁱⁱⁱ—Ge3—Sc1ᵛⁱⁱⁱ	141.76 (5)
Ge3—Sc3—Gd2ˣⁱᵛ	127.54 (6)	Gd2ˣᵛⁱⁱⁱ—Ge3—Sc1ᵛⁱⁱⁱ	141.76 (5)
Ge1ˣⁱⁱ—Sc3—Gd2ˣⁱᵛ	54.72 (4)	Sc2ˣ—Ge3—Sc1ᵛⁱⁱⁱ	83.28 (3)
Ge1ⁱⁱⁱ—Sc3—Gd2ˣⁱᵛ	120.23 (7)	Gd2ˣ—Ge3—Sc1ᵛⁱⁱⁱ	83.28 (3)
Ge2—Sc3—Gd2ˣⁱᵛ	52.35 (4)	Gd1ˣⁱˣ—Ge3—Sc1ᵛⁱⁱⁱ	94.96 (4)
Sc2ˣⁱⁱⁱ—Sc3—Gd2ˣⁱᵛ	65.84 (6)	Sc1ˣⁱˣ—Ge3—Sc1ᵛⁱⁱⁱ	94.96 (4)
Gd2ˣⁱⁱⁱ—Sc3—Gd2ˣⁱᵛ	65.84 (6)	Gd1ᵛⁱⁱⁱ—Ge3—Sc1ᵛⁱⁱⁱ	0.000 (17)
Sc2ˣⁱᵛ—Sc3—Gd2ˣⁱᵛ	0.00 (3)	Ge2ˣᵛⁱⁱ—Ge3—Gd1ⁱⁱⁱ	64.56 (3)
Ge2ⁱⁱ—Sc3—Sc2ˣⁱⁱ	53.40 (4)	Sc3ˣᵛ—Ge3—Gd1ⁱⁱⁱ	134.19 (2)
Ge3ⁱˣ—Sc3—Sc2ˣⁱⁱ	127.47 (6)	Sc3—Ge3—Gd1ⁱⁱⁱ	71.12 (4)
Ge3—Sc3—Sc2ˣⁱⁱ	126.76 (6)	Sc2ˣᵛⁱⁱⁱ—Ge3—Gd1ⁱⁱⁱ	124.12 (5)
Ge1ˣⁱⁱ—Sc3—Sc2ˣⁱⁱ	51.79 (3)	Gd2ˣᵛⁱⁱⁱ—Ge3—Gd1ⁱⁱⁱ	124.12 (5)
Ge1ⁱⁱⁱ—Sc3—Sc2ˣⁱⁱ	117.23 (7)	Sc2ˣ—Ge3—Gd1ⁱⁱⁱ	72.92 (3)
Ge2—Sc3—Sc2ˣⁱⁱ	53.35 (4)	Gd2ˣ—Ge3—Gd1ⁱⁱⁱ	72.92 (3)
Sc2ˣⁱⁱⁱ—Sc3—Sc2ˣⁱⁱ	105.69 (6)	Gd1ˣⁱˣ—Ge3—Gd1ⁱⁱⁱ	144.10 (4)
Gd2ˣⁱⁱⁱ—Sc3—Sc2ˣⁱⁱ	105.69 (6)	Sc1ˣⁱˣ—Ge3—Gd1ⁱⁱⁱ	144.10 (4)
Sc2ˣⁱᵛ—Sc3—Sc2ˣⁱⁱ	71.49 (4)	Gd1ᵛⁱⁱⁱ—Ge3—Gd1ⁱⁱⁱ	77.357 (18)
Gd2ˣⁱᵛ—Sc3—Sc2ˣⁱⁱ	71.49 (4)	Sc1ᵛⁱⁱⁱ—Ge3—Gd1ⁱⁱⁱ	77.357 (18)
Ge2ⁱⁱ—Sc3—Gd2ⁱⁱⁱ	53.40 (4)		

Symmetry codes: (i) −x+3/2, −y+1, z−1/2; (ii) x+1/2, y, −z+1/2; (iii) −x+1, −y+1, −z+1; (iv) −x+1, −y+1, −z; (v) −x+2, −y+1, −z+1; (vi) x, y, z−1; (vii) −x+1/2, −y+1, z+1/2; (viii) −x+3/2, −y+1, z+1/2; (ix) x−1/2, y, −z+3/2; (x) −x+1, −y+1, −z+2; (xi) x, −y+1/2, z; (xii) −x+1, y+1/2, −z+1; (xiii) −x+1/2, −y+1, z−1/2; (xiv) −x+1/2, y+1/2, z−1/2; (xv) x+1/2, y, −z+3/2; (xvi) x−1/2, y, −z+1/2; (xvii) x, y, z+1; (xviii) −x+1, y+1/2, −z+2; (xix) −x+3/2, y+1/2, z+1/2.