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Abstract

Gd2Sc3Ge4 adopts the orthorhombic Pu5Rh4-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.

Keywords

single-crystal x-ray study, T=298 K, mean average (Ge-Sc) = 0.003 A, disorder in main residue, R factor=0.031, wR factor=0.066, data-to-parameter ratio=19.6

Disciplines

Materials Chemistry | Other Chemistry | Physical Chemistry

Comments

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Gadolinium scandium germanide, $Gd_2Sc_3Ge_4$

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ(Ge–Sc) = 0.003 Å; disorder in main residue; R factor = 0.031; wR factor = 0.066; data-to-parameter ratio = 19.6.

$Gd_2Sc_3Ge_4$ adopts the orthorhombic Pu_5Rh_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_5Rh_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

$Gd_2Sc_3Ge_4$	a = 7.2445 (13) Å
M_r = 739.74	b = 14.101 (3) Å
Orthorhombic, $Pnma$	c = 7.4930 (14) Å
V = 765.4 (2) Å^3	μ = 34.91 mm^{-1}
Z = 4	T = 298 K
Mo $K\alpha$ radiation	0.06 × 0.05 × 0.01 mm

Data collection

Bruker SMART CCD area-detector diffractometer	6182 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	958 independent reflections
T_{min} = 0.127, T_{max} = 0.705	816 reflections with $I > 2s(I)$
	R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031	49 parameters
$wR(F^2)$ = 0.066	$\Delta\rho_{max}$ = 2.20 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −1.44 e Å^{-3}
958 reflections	

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2062).

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supplementary materials

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Gadolinium scandium germanide, $Gd_2Sc_3Ge_4$

S. Misra and **G. J. Miller**

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. $Gd_2Sc_3Ge_4$ crystallizes in the orthorhombic Pu_5Rh_4-type structure (Cromer, 1977). Two 3^2434 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 $Gd_5Ga_2Ge_2$ [2.741 (1) Å; Gd_5Si_4-type (Holtzberg *et al.*, 1967)] and $Gd_5Ga_{0.7}Ge_{3.3}$ [3.461 (5) Å; Sm_5Ge_4-type (Smith *et al.*, 1967)] (Mozharivskyj *et al.*, 2003).

Experimental

$Gd_2Sc_3Ge_4$ 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. %.

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).

Figures

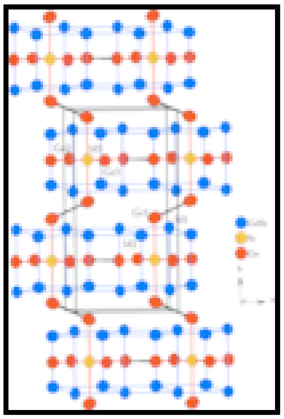

Fig. 1. View of $Gd_2Sc_3Ge_4$ along [001], with displacement ellipsoids drawn at the 99 % probability level.

Diadolinium triscandium tetragermanide

Crystal data

$Gd_2Sc_3Ge_4$

$M_r = 739.74$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 7.2445\ (13)$ Å

$b = 14.101\ (3)$ Å

$c = 7.4930\ (14)$ Å

$V = 765.4\ (2)$ Å^3

$Z = 4$

$F_{000} = 1276$

$D_x = 6.419$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 6182 reflections

$\theta = 3.1$–$27.8°$

$\mu = 34.91$ mm^{-1}

$T = 298$ K

Plate, grey

0.06 × 0.05 × 0.01 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2002)

$T_{min} = 0.127$, $T_{max} = 0.705$

6182 measured reflections

958 independent reflections

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

$R_{int} = 0.070$

$\theta_{max} = 28.2°$

$\theta_{min} = 2.9°$

$h = -9 \rightarrow 9$

$k = -17 \rightarrow 18$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0171P)^2 + 3.8343P]$

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

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, °)

Gd1—Ge3$^{\rm i}$	2.9452 (9)	Sc3—Gd2$^{\rm xiv}$	3.268 (2)
Gd1—Ge1$^{\rm ii}$	2.9605 (10)	Sc3—Sc2$^{\rm xii}$	3.283 (2)
Gd1—Ge1	3.1097 (10)	Sc3—Gd2$^{\rm iii}$	3.283 (2)
Gd1—Ge3$^{\rm iii}$	3.1101 (10)	Ge1—Sc2$^{\rm i}$	2.8070 (16)
Gd1—Ge2$^{\rm iv}$	3.1478 (10)	Ge1—Gd2$^{\rm i}$	2.8070 (16)
Gd1—Ge1$^{\rm v}$	3.1519 (10)	Ge1—Sc2$^{\rm xv}$	2.8759 (17)
Gd1—Ge1$^{\rm i}$	3.1861 (10)	Ge1—Gd2$^{\rm xv}$	2.8759 (17)
Gd1—Sc3$^{\rm i}$	3.4681 (17)	Ge1—Ge1$^{\rm v}$	2.8907 (17)
Gd1—Sc3$^{\rm iii}$	3.4877 (17)	Ge1—Gd1$^{\rm xvi}$	2.9605 (10)
Gd1—Sc2$^{\rm i}$	3.5083 (15)	Ge1—Sc1$^{\rm xvi}$	2.9605 (10)
Gd1—Gd2$^{\rm i}$	3.5083 (15)	Ge1—Sc3$^{\rm iii}$	2.9614 (10)
Gd1—Gd2$^{\rm vi}$	3.5762 (15)	Ge2—Ge3$^{\rm vi}$	2.7572 (17)
Gd2—Ge1	2.7421 (15)	Ge2—Sc2$^{\rm xiv}$	2.7668 (16)
Gd2—Ge2$^{\rm vii}$	2.7668 (16)	Ge2—Gd2$^{\rm xiv}$	2.7668 (16)
Gd2—Ge1$^{\rm viii}$	2.8070 (16)	Ge2—Sc2$^{\rm xiii}$	2.7668 (16)
Gd2—Ge2$^{\rm iii}$	2.8234 (17)	Ge2—Gd2$^{\rm xiii}$	2.7668 (16)
Gd2—Ge1$^{\rm ix}$	2.8759 (17)	Ge2—Sc3$^{\rm xvi}$	2.800 (2)
Gd2—Ge3$^{\rm x}$	2.9010 (16)	Ge2—Sc2$^{\rm xii}$	2.8234 (17)
Gd2—Sc3$^{\rm vii}$	3.268 (2)	Ge2—Gd2$^{\rm xii}$	2.8234 (17)
Gd2—Sc3$^{\rm iii}$	3.283 (2)	Ge2—Gd2$^{\rm iii}$	2.8234 (17)
Gd2—Gd1$^{\rm viii}$	3.5083 (15)	Ge2—Sc2$^{\rm iii}$	2.8234 (17)
Gd2—Sc1$^{\rm viii}$	3.5083 (15)	Ge2—Sc1$^{\rm iv}$	3.1478 (10)
Gd2—Sc2$^{\rm xi}$	3.552 (3)	Ge3—Ge2$^{\rm xvii}$	2.7572 (17)
Gd2—Gd2$^{\rm xi}$	3.552 (3)	Ge3—Sc3$^{\rm xv}$	2.864 (2)
Sc3—Ge2$^{\rm ii}$	2.800 (2)	Ge3—Sc2$^{\rm xviii}$	2.9010 (16)
Sc3—Ge3$^{\rm ix}$	2.864 (2)	Ge3—Gd2$^{\rm xviii}$	2.9010 (16)
Sc3—Ge3	2.878 (2)	Ge3—Sc2$^{\rm x}$	2.9010 (16)
Sc3—Ge1$^{\rm xii}$	2.9614 (10)	Ge3—Gd2$^{\rm x}$	2.9010 (16)
Sc3—Ge1$^{\rm iii}$	2.9614 (10)	Ge3—Gd1$^{\rm xix}$	2.9452 (9)
Sc3—Ge2	2.977 (2)	Ge3—Sc1$^{\rm xix}$	2.9452 (9)
Sc3—Sc2$^{\rm xiii}$	3.268 (2)	Ge3—Gd1$^{\rm viii}$	2.9452 (9)
Sc3—Gd2$^{\rm xiii}$	3.268 (2)	Ge3—Sc1$^{\rm viii}$	2.9452 (9)
Sc3—Sc2$^{\rm xiv}$	3.268 (2)	Ge3—Gd1$^{\rm iii}$	3.1101 (10)
Ge3$^{\rm i}$—Gd1—Ge1$^{\rm ii}$	94.17 (3)	Ge3$^{\rm ix}$—Sc3—Gd2$^{\rm iii}$	127.47 (6)
Ge3$^{\rm i}$—Gd1—Ge1	87.88 (3)	Ge3—Sc3—Gd2$^{\rm iii}$	126.76 (6)
Ge1$^{\rm ii}$—Gd1—Ge1	137.90 (3)	Ge1$^{\rm xii}$—Sc3—Gd2$^{\rm iii}$	117.23 (7)
Ge3$^{\rm i}$—Gd1—Ge3$^{\rm iii}$	82.64 (2)	Ge1$^{\rm iii}$—Sc3—Gd2$^{\rm iii}$	51.79 (3)
Ge1$^{\rm ii}$—Gd1—Ge3$^{\rm iii}$	133.89 (3)	Ge2—Sc3—Gd2$^{\rm iii}$	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)
Ge1^{iii}—Sc3—Sc2^{xiii}	54.72 (4)	Sc3—Ge3—Sc1^{xix}	73.09 (4)
Ge2—Sc3—Sc2^{xiii}	52.35 (4)	Sc2^{xviii}—Ge3—Sc1^{xix}	83.28 (3)
Ge2^{ii}—Sc3—Gd2^{xiii}	124.88 (6)	Gd2^{xviii}—Ge3—Sc1^{xix}	83.28 (3)
Ge3^{ix}—Sc3—Gd2^{xiii}	56.01 (5)	Sc2^{x}—Ge3—Sc1^{xix}	141.76 (5)
Ge3—Sc3—Gd2^{xiii}	127.54 (6)	Gd2^{x}—Ge3—Sc1^{xix}	141.76 (5)
Ge1^{xii}—Sc3—Gd2^{xiii}	120.23 (7)	Gd1^{xix}—Ge3—Sc1^{xix}	0.000 (17)
Ge1^{iii}—Sc3—Gd2^{xiii}	54.72 (4)	Ge2^{xvii}—Ge3—Gd1^{viii}	132.513 (19)
Ge2—Sc3—Gd2^{xiii}	52.35 (4)	Sc3^{xv}—Ge3—Gd1^{viii}	73.78 (4)
Sc2^{xiii}—Sc3—Gd2^{xiii}	0.00 (3)	Sc3—Ge3—Gd1^{viii}	73.09 (4)
Ge2^{ii}—Sc3—Sc2^{xiv}	124.88 (6)	Sc2^{xviii}—Ge3—Gd1^{viii}	141.76 (5)
Ge3^{ix}—Sc3—Sc2^{xiv}	56.01 (5)	Gd2^{xviii}—Ge3—Gd1^{viii}	141.76 (5)
Ge3—Sc3—Sc2^{xiv}	127.54 (6)	Sc2^{x}—Ge3—Gd1^{viii}	83.28 (3)
Ge1^{xii}—Sc3—Sc2^{xiv}	54.72 (4)	Gd2^{x}—Ge3—Gd1^{viii}	83.28 (3)
Ge1^{iii}—Sc3—Sc2^{xiv}	120.23 (7)	Gd1^{xix}—Ge3—Gd1^{viii}	94.96 (4)
Ge2—Sc3—Sc2^{xiv}	52.35 (4)	Sc1^{xix}—Ge3—Gd1^{viii}	94.96 (4)
Sc2^{xiii}—Sc3—Sc2^{xiv}	65.84 (6)	Ge2^{xvii}—Ge3—Sc1^{viii}	132.513 (19)
Gd2^{xiii}—Sc3—Sc2^{xiv}	65.84 (6)	Sc3^{xv}—Ge3—Sc1^{viii}	73.78 (4)
Ge2^{ii}—Sc3—Gd2^{xiv}	124.88 (6)	Sc3—Ge3—Sc1^{viii}	73.09 (4)

Ge3^{ix}—Sc3—Gd2^{xiv}	56.01 (5)	Sc2^{xviii}—Ge3—Sc1^{viii}	141.76 (5)
Ge3—Sc3—Gd2^{xiv}	127.54 (6)	Gd2^{xviii}—Ge3—Sc1^{viii}	141.76 (5)
Ge1^{xii}—Sc3—Gd2^{xiv}	54.72 (4)	Sc2^{x}—Ge3—Sc1^{viii}	83.28 (3)
Ge1^{iii}—Sc3—Gd2^{xiv}	120.23 (7)	Gd2^{x}—Ge3—Sc1^{viii}	83.28 (3)
Ge2—Sc3—Gd2^{xiv}	52.35 (4)	Gd1^{xix}—Ge3—Sc1^{viii}	94.96 (4)
Sc2^{xiii}—Sc3—Gd2^{xiv}	65.84 (6)	Sc1^{xix}—Ge3—Sc1^{viii}	94.96 (4)
Gd2^{xiii}—Sc3—Gd2^{xiv}	65.84 (6)	Gd1^{viii}—Ge3—Sc1^{viii}	0.000 (17)
Sc2^{xiv}—Sc3—Gd2^{xiv}	0.00 (3)	Ge2^{xvii}—Ge3—Gd1^{iii}	64.56 (3)
Ge2^{ii}—Sc3—Sc2^{xii}	53.40 (4)	Sc3^{xv}—Ge3—Gd1^{iii}	134.19 (2)
Ge3^{ix}—Sc3—Sc2^{xii}	127.47 (6)	Sc3—Ge3—Gd1^{iii}	71.12 (4)
Ge3—Sc3—Sc2^{xii}	126.76 (6)	Sc2^{xviii}—Ge3—Gd1^{iii}	124.12 (5)
Ge1^{xii}—Sc3—Sc2^{xii}	51.79 (3)	Gd2^{xviii}—Ge3—Gd1^{iii}	124.12 (5)
Ge1^{iii}—Sc3—Sc2^{xii}	117.23 (7)	Sc2^{x}—Ge3—Gd1^{iii}	72.92 (3)
Ge2—Sc3—Sc2^{xii}	53.35 (4)	Gd2^{x}—Ge3—Gd1^{iii}	72.92 (3)
Sc2^{xiii}—Sc3—Sc2^{xii}	105.69 (6)	Gd1^{xix}—Ge3—Gd1^{iii}	144.10 (4)
Gd2^{xiii}—Sc3—Sc2^{xii}	105.69 (6)	Sc1^{xix}—Ge3—Gd1^{iii}	144.10 (4)
Sc2^{xiv}—Sc3—Sc2^{xii}	71.49 (4)	Gd1^{viii}—Ge3—Gd1^{iii}	77.357 (18)
Gd2^{xiv}—Sc3—Sc2^{xii}	71.49 (4)	Sc1^{viii}—Ge3—Gd1^{iii}	77.357 (18)
Ge2^{ii}—Sc3—Gd2^{iii}	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.

Fig. 1