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Gadolinium scandium germanide, Gd₂Sc₃Ge₄

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

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.

Related literature

The title compound adopts the Pu₅Rh₄-type structure (Cromer, 1977). For Ge...Ge distances, see: Mozharivskiy *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

Gd₂Sc₃Ge₄
 $M_r = 739.74$
 Orthorhombic, *Pnma*

$a = 7.2445$ (13) Å
 $b = 14.101$ (3) Å
 $c = 7.4930$ (14) Å

$V = 765.4$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 34.91$ mm⁻¹
 $T = 298$ K
 $0.06 \times 0.05 \times 0.01$ mm

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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.070$

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

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, $\text{Gd}_2\text{Sc}_3\text{Ge}_4$

S. Misra and G. J. Miller

Comment

Continuing our efforts in mixed rare-earth systems bearing the formula $(\text{R}_{1-x}\text{R}'_x)_5\text{T}_4$, where T = Si, Ge, Ga, Sn, we have studied the effect of substitution of Gd by nonmagnetic Sc. $\text{Gd}_2\text{Sc}_3\text{Ge}_4$ crystallizes in the orthorhombic Pu_5Rh_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 $\text{Gd}_5\text{Ga}_2\text{Ge}_2$ [2.741 (1) Å; Gd_5Si_4 -type (Holtzberg *et al.*, 1967)] and $\text{Gd}_5\text{Ga}_{0.7}\text{Ge}_{3.3}$ [3.461 (5) Å; Sm_5Ge_4 -type (Smith *et al.*, 1967)] (Mozharivskiy *et al.*, 2003).

Experimental

$\text{Gd}_2\text{Sc}_3\text{Ge}_4$ 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. %.

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

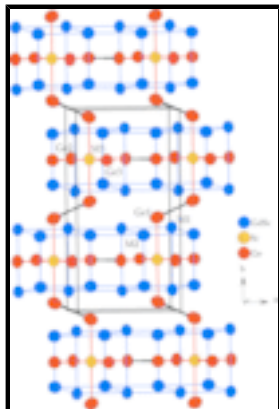


Fig. 1. View of $\text{Gd}_2\text{Sc}_3\text{Ge}_4$ along $[001]$, with displacement ellipsoids drawn at the 99 % probability level.

Diadolinium triscandium tetragermanide

Crystal data

$\text{Gd}_2\text{Sc}_3\text{Ge}_4$

$M_r = 739.74$

Orthorhombic, $Pnma$

Hall symbol: $-P\ 2ac\ 2n$

$a = 7.2445\ (13)\ \text{\AA}$

$b = 14.101\ (3)\ \text{\AA}$

$c = 7.4930\ (14)\ \text{\AA}$

$V = 765.4\ (2)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1276$

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

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6182 reflections

$\theta = 3.1\text{--}27.8^\circ$

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

$T = 298\ \text{K}$

Plate, grey

$0.06 \times 0.05 \times 0.01\ \text{mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ \text{K}$

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 $I > 2s(I)$

$R_{\text{int}} = 0.070$

$\theta_{\text{max}} = 28.2^\circ$

$\theta_{\text{min}} = 2.9^\circ$

$h = -9 \rightarrow 9$

$k = -17 \rightarrow 18$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	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 (\AA^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

supplementary materials

Geometric parameters (Å, °)

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)

supplementary materials

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)

supplementary materials

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

