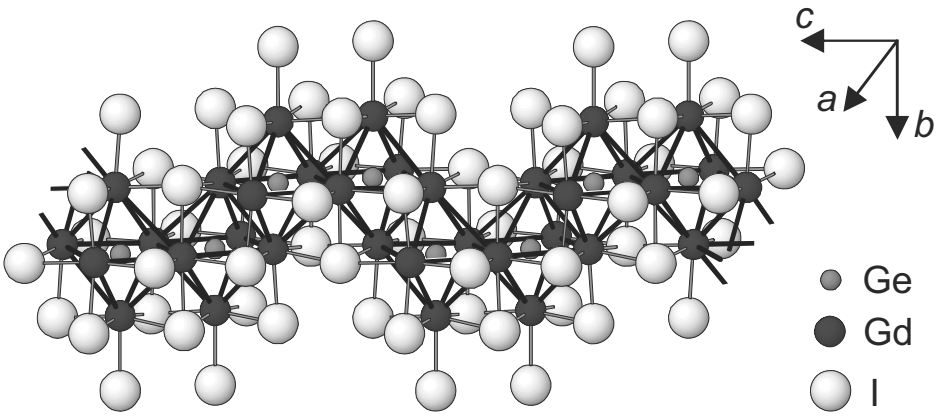
Crystal structure of tetragadolinium hexaiodide monogermanide, Gd_4I_6Ge

M. Lukachuk*, Hj. Mattausch and A. Simon

Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Received February 3, 2006, accepted and available on-line March 2, 2006; CSD no. 409864



Abstract

Gd_4GeI_6, monoclinic, $C12/c1$ (no. 15), a = 19.315(2) Å, b = 12.101(1) Å, c = 13.531(1) Å, β = 97.545(8)°, V = 3135.2 Å^3, Z = 8, $R_{gt}(F)$ = 0.057, $wR_{ref}(F^2)$ = 0.094, T = 293 K.

Source of material

The compound was synthesized by heating stoichiometric amounts of GdI_3, Gd and Ge under Ar atmosphere in sealed Ta capsules at 1000 °C for 6 days.

Discussion

Gd_4I_6Ge is isotypic with Y_4Br_6B [1] and Tb_4Br_6B [2]. In the crystal structure octahedra of Gd atoms are centered by Ge atoms. Two Gd_6Ge octahedra are connected via a common edge and form octahedron pairs which are further linked to zig-zag chains parallel [001]. The I atoms coordinate all free edges of the octhahedra chains and interconnect these three-dimensionally. The Gd—Gd distances range from 3.822(3) Å to 4.193(2) Å, Gd—I distances – from 3.013(3) Å to 3.240(2) Å, Gd—Ge distances – from 2.797(3) Å to 2.867(3) Å. Relatively long Gd—Gd distances are the result of the distortion of the Gd_6Ge octahedra due to the packing effect.

Table 1. Data collection and handling.

Crystal:	black needle, size 0.04 × 0.06 × 0.10 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	303.55 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS II, ω
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10929, 3050
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1696
$N(param)_{refined}$:	101
Programs:	SHELXS-97 [3], SHELXL-97 [4], ATOMS [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd(1)	8*f*	0.03520(7)	0.14552(9)	0.1065(1)	0.0115(4)	0.0093(6)	0.0121(6)	–0.0002(5)	0.0022(4)	0.0009(5)
Gd(2)	8*f*	0.03168(7)	0.6133(1)	0.09351(9)	0.0120(5)	0.0094(5)	0.0108(7)	0.0007(5)	0.0005(5)	–0.0001(5)
Gd(3)	8*f*	0.83124(5)	0.6217(1)	0.95326(8)	0.0103(5)	0.0120(5)	0.0109(5)	–0.0003(5)	0.0032(4)	–0.0003(5)
Gd(4)	8*f*	0.90360(6)	0.6223(1)	0.68636(9)	0.0112(5)	0.0112(5)	0.0095(5)	–0.0017(5)	0.0012(4)	–0.0010(5)
I(1)	8*f*	0.88974(9)	0.1178(2)	0.1771(2)	0.0134(7)	0.0131(7)	0.0140(8)	–0.0008(8)	0.0013(6)	–0.0019(8)
I(2)	8*f*	0.88802(8)	0.6404(1)	0.1831(1)	0.0117(7)	0.0117(8)	0.0083(8)	0.0011(6)	0.0006(6)	–0.0017(7)
I(3)	8*f*	0.81855(9)	0.3657(2)	0.9673(1)	0.0135(7)	0.0079(7)	0.0134(8)	–0.0028(7)	0.0004(6)	–0.0002(7)
I(4)	8*f*	0.8186(1)	0.8759(2)	0.9647(2)	0.0125(7)	0.0127(6)	0.0255(9)	0.0021(7)	0.0103(6)	–0.0001(8)
I(5)	8*f*	0.9621(1)	0.1222(2)	0.8911(2)	0.0260(7)	0.0106(6)	0.0138(7)	–0.0036(9)	–0.0027(6)	0.0008(9)
I(6)	8*f*	0.7482(1)	0.8804(2)	0.2539(2)	0.0112(6)	0.0274(9)	0.0130(8)	–0.0006(7)	0.0011(5)	0.0002(7)
Ge	8*f*	0.9656(1)	0.6234(2)	0.8921(2)	0.0064(8)	0.0013(8)	0.0040(9)	0.000(1)	0.0007(7)	0.001(1)

* Correspondence author (e-mail: m.lukachuk@fkf.mpg.de)

References

1. Mattausch, Hj.; Simon, A.: Crystal structure of tetrayttrium hexabromide monoboride, Y_4Br_6B. Z. Kristallogr. NCS **212** (1997) 99.
2. Mattausch, Hj.; Oeckler, O.; Simon, A.: Crystal structure of tetraterbium hexabromide monoboride, Tb_4Br_6B. Z. Kristallogr. NCS **215** (2000) 199.
3. Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
4. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
5. Dowty, E.: ATOMS. A Complete Program for Displaying Atomic Structures. Version 5.0. Shape Software, Kingsport, Tennessee, USA 1999.