Crystal structure of tetragadolinium monosilicide hexabromide, Gd_4SiBr_6

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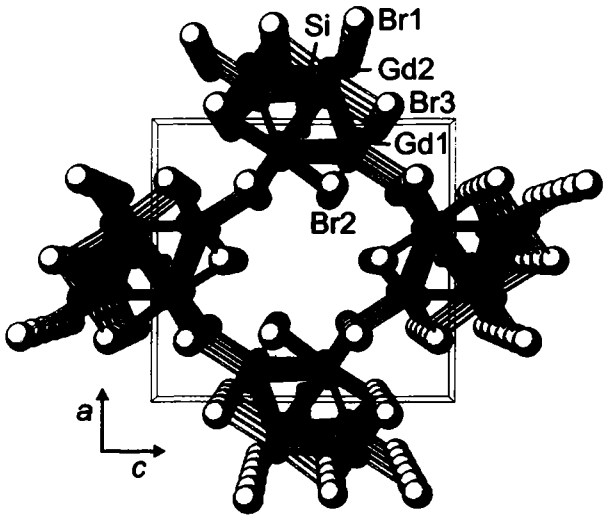
Received July 11, 2005, accepted and available on-line September 6, 2005; CSD no. 409839



Abstract

Br_6Gd_4Si, orthorhombic, *Pbam* (no. 55), $a = 13.172(2)$ Å, $b = 13.982(1)$ Å, $c = 4.083(1)$ Å, $V = 752.0$ Å^3, $Z = 2$, $R_{gt}(F) = 0.026$, $wR_{ref}(F^2) = 0.061$, $T = 293$ K.

Source of material

Gd_4SiBr_6 is prepared by heating stoichiometric amounts of $GdBr_3$, Gd and Si under Ar atmosphere in sealed Ta capsules at 900 °C for 4 days.

Discussion

Gd_4SiBr_6 is isotypic with Tb_4SiBr_6, Gd_4CBr_6 and Sc_4CCl_6 [1-3]. In the crystal structure octahedra of Gd atoms are centered by Si atoms. The [$SiGd_6$] octahedra are connected via opposite edges to chains. In terms of condensed clusters [4,5] the crystal structure is to be described as $Gd_2Gd_{4/2}SiBr(i)_4Br(a\text{-}a)_{4/2}$. The Gd—Gd distances range from 3.922(1) Å – 4.083(4) Å, Gd—Br from 2.911(1) Å – 2.981(1) Å, Gd—Si from 2.741(1) Å – 2.807(1) Å. As expected from the lanthanide contraction all distances are 0.03 Å – 0.04 Å larger as in Tb_4Br_6Si.

Table 1. Data collection and handling.

Crystal:	blue-black needle, size 0.04 × 0.05 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	333.82 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1132, 1132
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 968
$N(param)_{refined}$:	36
Programs:	SHELXL-97 [6], ATOMS [7]

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)	4*h*	0.11866(3)	0.33891(2)	½	0.0212(2)	0.0200(2)	0.0180(2)	0.0044(1)	0	0
Gd(2)	4*g*	0.12027(3)	0.57837(2)	0	0.0176(2)	0.0194(2)	0.0155(2)	–0.0018(1)	0	0
Br(1)	4*h*	0.24129(7)	0.16104(6)	½	0.0333(4)	0.0349(4)	0.0206(4)	0.0176(3)	0	0
Br(2)	4*g*	0.25763(6)	0.40890(5)	0	0.0211(3)	0.0281(3)	0.0223(4)	0.0025(3)	0	0
Br(3)	4*g*	–0.00025(6)	0.24117(5)	0	0.0269(3)	0.0210(3)	0.0221(3)	–0.0007(3)	0	0
Si(1)	2*d*	0	½	½	0.016(1)	0.016(1)	0.016(1)	0.0005(9)	0	0

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