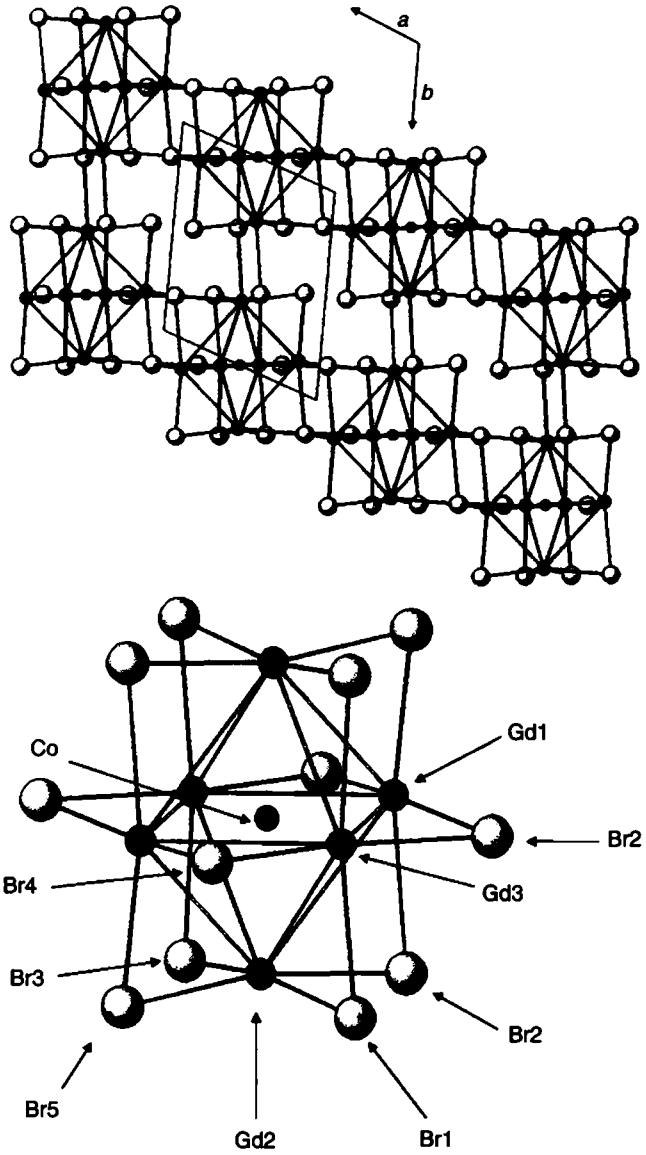
Crystal structure of hexagadolinium cobalt decabromide, Gd_6CoBr_{10}, *a Y_6RuI_{10}-type structure*

C. Lefevre*, C. Hoch, R. Eger and A. Simon

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

Received December 14, 2004, accepted and available on-line January 10, 2005; CSD no. 409809



Abstract

$Br_{10}CoGd_6$, triclinic, $P\bar{1}$ (no. 2), $a = 7.3051(8)$ Å, $b = 9.040(1)$ Å, $c = 9.090(1)$ Å, $\alpha = 108.868(1)°$, $\beta = 97.260(1)°$, $\gamma = 106.299(1)°$, $V = 529.4$ Å^3, $Z = 1$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.096$, $T = 293$ K.

Source of material

Gd_6CoBr_{10} formed in a reaction of $GdBr_3$, Gd and Co in a molar ratio 2:2:1. The mixture was sealed in a tantalum capsule under argon and heated at 1173 K for 10 days. Three different phases were obtained, which were analyzed through SEM as Gd_2Co_2Br, $GdCo_3$ and Gd_6CoBr_{10}. The new compound Gd_6CoBr_{10} forms thin dark silvery platelet-like crystals.

Discussion

Gd_6CoBr_{10} (figure, top) is isostructural to Y_6RuI_{10} [1]. This structure has been observed for several compounds, Y_6MI_{10} (M = Co, Ni, Rh, Os, Ir, Pt) and Pr_6MI_{10} (M = Co, Ru, Os) [2,3]. It can be described as a chain of distorted cuboctahedral clusters Gd_6Br_{12} (figure, bottom) in which the cobalt atom occupies the center of the distorted Gd_6 octahedron ($d_{Co—Gd1} = 2.6833$ Å, $d_{Co—Gd2} = 2.6142$ Å and $d_{Co—Gd3} = 2.6313$ Å). Each cuboctahedron is connected to others via halogen atoms Br2 and Br4 resulting in a cluster chain $^1_\infty[Gd_6CoBr_8Br_{4/2}]$ oriented along the a-axis (figure, top). The distance between two chains is equal to 2.572 Å.

Table 1. Data collection and handling.

Crystal:	dark silvery platelet, size 0.06 × 0.12 × 0.18 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	203.80 cm^{-1}
Diffractometer, scan mode:	IPDS I, φ
$2\theta_{max}$:	42°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8780, 2215
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2041
$N(param)_{refined}$:	80
Programs:	SHELX-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)	2*i*	−0.13224(5)	0.14171(5)	0.68380(5)	0.0166(2)	0.0216(2)	0.0182(2)	0.0070(2)	0.0047(2)	0.0084(2)
Gd(2)	2*i*	0.47492(5)	0.29765(5)	0.59422(5)	0.0194(2)	0.0205(2)	0.0211(3)	0.0082(2)	0.0061(2)	0.0098(2)
Gd(3)	2*i*	0.37701(5)	−0.04370(4)	0.74777(5)	0.0183(2)	0.0201(2)	0.0183(2)	0.0077(2)	0.0049(2)	0.0086(2)

* Correspondence author (e-mail: c.lefevre@fkf.mpg.de)

Table 2. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	2*i*	0.2990(1)	0.2685(1)	0.8595(1)	0.0234(4)	0.0231(4)	0.0203(4)	0.0092(3)	0.0067(3)	0.0065(3)
Br(2)	2*i*	–0.0505(1)	–0.1816(1)	0.5867(1)	0.0185(4)	0.0236(4)	0.0231(5)	0.0073(3)	0.0049(3)	0.0102(3)
Br(3)	2*i*	0.5890(2)	0.3709(1)	0.3225(1)	0.0499(6)	0.0245(4)	0.0311(5)	0.0197(4)	0.0199(4)	0.0159(4)
Br(4)	2*i*	–0.2362(1)	0.0877(1)	0.9640(1)	0.0239(4)	0.0479(6)	0.0204(5)	0.0044(4)	0.0038(3)	0.0169(4)
Br(5)	2*i*	–0.1334(1)	0.4693(1)	0.7789(1)	0.0281(5)	0.0211(4)	0.0408(6)	0.0062(3)	–0.0035(4)	0.0037(4)
Co	1*f*	½	0	½	0.0151(7)	0.0158(6)	0.0143(7)	0.0064(5)	0.0040(5)	0.0071(5)

References

1. Hughbanks, T.; Corbett, J. D.: Encapsulation of Heavy Transition Metals in Iodide Clusters. Synthesis, Structure and Bonding of the Unusual Cluster Phase $Y_6I_{10}Ru$. Inorg. Chem. **28** (1989) 631-635.
2. Payne, M. W.; Corbett, J. D.: Encapsulation of the Platinum Metals within Cluster Iodides of Rare Earth Elements. Inorg. Chem. **29** (1990) 2246-2251.
3. Llusar, R.; Corbett, J. D.: Reduced Praseodymium Cluster Bromides Stabilized by Transition Metals. Inorg. Chem. **33** (1994) 849-853.
4. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
5. Dowty, E.: ATOMS for Windows and Macintosh. Version 5.0. Shape Software, Kingsport, Tennessee, USA 1999.