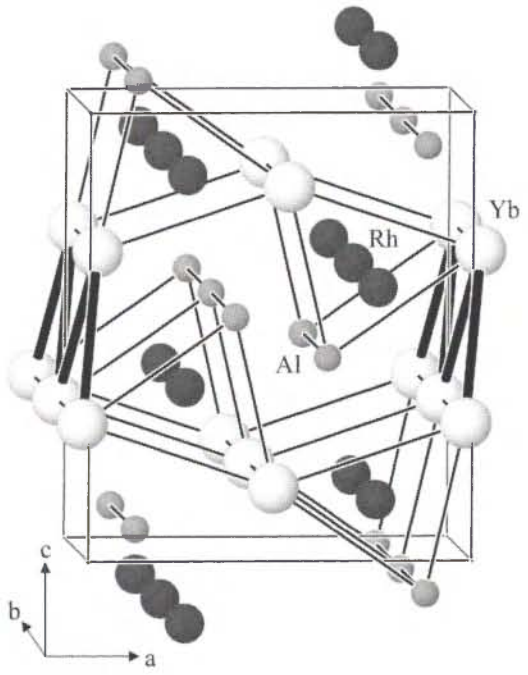
Crystal structure of ytterbium-rhodium-aluminium [1:1:1], YbRhAl

R. H. Cardoso Gil*, O. Trovarelli, Ch. Geibel and Yu. Grin

Max-Planck-Institut für Chemische Physik fester Stoffe, Bayreuther Str. 40, D-01187 Dresden, Germany

Received May 21, 1999, transferred to 2nd update of database ICSD in 1999, CSD-No. 409429



Abstract

AlRhYb, orthorhombic, *Pnma* (No. 62), $a = 6.763(1)$ Å, $b = 4.134(1)$ Å, $c = 7.906(2)$ Å, $V = 221.0$ Å^3, $Z = 4$, $R_{gt}(F) = 0.016$, $wR(F) = 0.036$, $T = 293$ K.

Source of material

Samples of YbRhAl were synthesized from stoichiometric amounts of pure constituents (4N-Yb Ames, 3N-Rh Hereaus, 5N-Al Johnson-Matthey) in tantalum crucibles sealed under purified (6N) Ar atmosphere and heated at 1773 K for a few minutes. An excess of 2 at.% Yb was added in order to compensate possible loses due to its high vapor pressure. No structural modification was observed after annealing at 973 K for 120 h, as observed in another LnTAl (Ln = rare-earth, T = transition metal) compounds [1].

Discussion

The new compound YbRhAl crystallizes in the orthorhombic TiNiSi structure type, an ordered version of the Co_2Si type. The title compound is one of the missing members of the previous reported LnRhAl series (Ln = Pr, Nd, Gd, Ho, and Tm), which crystallize in the TiNiSi-type structure as well [2]. The structure of YbRhAl features the trigonal prismatic coordination of Rh (2Al + 4Yb). Remarkable is the shortest Yb–Yb distance d(Yb–Yb) = 352.0 pm, which occurs between the Yb atoms belonging to neighbouring chains of trigonal prisms. In other homologous, e.g. YbNiSn [3], the shortest Yb–Yb distance occurs between Yb atoms belonging to the same chain.

Table 1. Data collection and handling.

Crystal:	silver metallic plate, size 0.05 × 0.15 × 0.15 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	264.50 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 280 exposures, $\Delta\varphi = 1°$
$2\theta_{max}$:	55.26°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5149, 516
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 496
$N(param)_{refined}$:	20
Programs:	SHELXL-97 [4], ATOMS [5]

References

1. Hulliger, F.: On the new rare-earth palladium aluminides LnPdAl. J. Alloys Comp. **218** (1995) 44.
2. Schwer, H.; Hulliger, F.: On the new rare-earth compounds LnRhAl. J. Alloys Comp. **259** (1997) 249.
3. Bonville, P.; Bellot, P.; Hodges, J. A.; Imbert, P.; Jéhanno, G.; Le Bras, G.; Hammann, J.; Leylekian, L.; Chevrier, G.; Thuéri, P.; D'Onofrio, L.; Hamzic, A.; Barthélémy, A.: YbNiSn, a ferromagnetic Kondo lattice. Physica B **182** (1992) 105.
4. Sheldrick, G. M.: SHELXL-97, a program for refining crystal structures. University of Göttingen, Germany 1997.
5. Dowty, E.: Atoms 4.1, A Complete Program for Displaying Atomic Structures. By Shape software, 521 Hidden Valley Road, Kingsport, TN 37663, USA 1998.

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}
Yb	4c	0.03427(2)	1/4	0.67825(2)	0.0052(1)	0.00574(9)	0.0051(1)	0	–0.00030(4)	0
Rh	4c	0.26470(5)	1/4	0.37582(4)	0.0060(1)	0.0055(1)	0.0060(2)	0	–0.00044(9)	0
Al	4c	0.1368(2)	1/4	0.0592(2)	0.0050(4)	0.0031(4)	0.0042(5)	0	0.0001(4)	0

* Correspondence author (e-mail: cardoso@cpfs.mpg.de)