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The intermetallic compound $Gd_6Ta_4Al_{43}$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Al–Al) = 0.002 Å
R factor = 0.019
wR factor = 0.043
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Gadolinium tantalum aluminium, $Gd_6Ta_4Al_{43}$, adopts the $Ho_6Mo_4Al_{43}$ structure type, with 12-fold coordination around the Gd and twofold coordination around the Ta and Al atoms.

Comment

Compounds with the $Ho_6Mo_4Al_{43}$ structure type are good candidates for studying magnetic anisotropic effects because of their hexagonal symmetry and the presence of only one rare-earth site. To investigate this anisotropy, the availability of good-quality single crystals is important. Single crystals of $Gd_6Ta_4Al_{43}$ were prepared using the metallic solution growth method (Canfield & Fisk, 1992). Previously, this compound was prepared by annealing a pressed pellet of the elements with atomic ratio R:Ta:Al = 6:4:48 (Wolff *et al.*, 2001).

$Gd_6Ta_4Al_{43}$ belongs to a large family of isotypic aluminides, $R_6T_4Al_{43}$ (R = rare-earth element; T = Ti, V, Nb, Ta, Cr, Mo, W) (Niemann & Jeitschko, 1995). Single-crystal refinement has been reported for $Ho_6Mo_4Al_{43}$ (Niemann & Jeitschko, 1994), $Dy_6Ti_4Al_{43}$ (Niemann & Jeitschko, 1995) and $Ca_6W_4Al_{43}$ (Thiede *et al.*, 1998), as well as $Yb_6V_4Al_{43}$ and $Yb_6Ta_4Al_{43}$ (Wolff *et al.*, 2001). Other isotypic compounds deviating from the ideal composition have also been reported: $Yb_6Cr_{4+x}Al_{43-x}$ (x = 1.76; Yanson, Manyako, Bodak, Zarechnyuk *et al.*, 1994), $Ho_6Mo_{4+x}Al_{43-x}$ (x = 0.11) and $Yb_6Cr_{4+x}Al_{43-x}$ (x = 1.15; Niemann & Jeitschko, 1994), $Y_6Cr_{4+x}Al_{43-x}$ (x = 2.57; Černý *et al.*, 1995), along with $Tb_6Cr_{4+x}Al_{43-x}$ (x = 1.6), $Ho_6Cr_{4+x}Al_{43-x}$ (x = 1.6), $Er_6Cr_{4+x}Al_{43-x}$ (x = 1.96) and $Lu_6Cr_{4+x}Al_{43-x}$ (x = 2.76) (Yanson, Manyako, Bodak, Černý *et al.*, 1994). The lattice parameters previously refined from powder data for $Gd_6Ta_4Al_{43}$ [a = 11.099 (2) Å and c = 17.896 (4) Å; Niemann & Jeitschko, 1995] differ only slightly from those presented here. There was no evidence of deviation from the ideal composition in the present structure refinement.

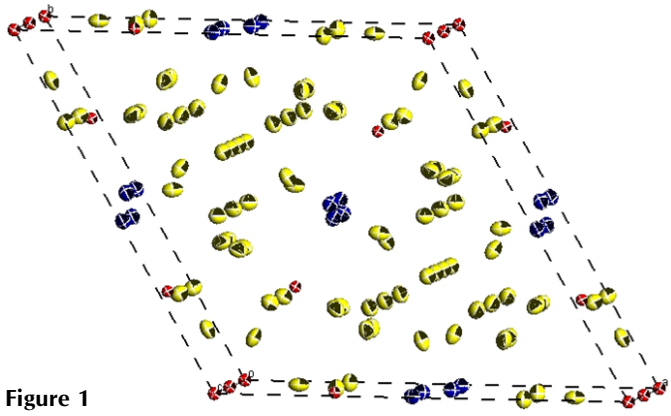

Figure 1
Displacement ellipsoids drawn at the 90% probability level (Sheldrick, 2001). Key: Gd, blue; Ta, red; Al, yellow.

Fig. 1 shows the hexagonal unit cell of $Gd_6Ta_4Al_{43}$. Each Gd atom is coordinated by 17 atoms (one Gd, one Ta, and 15 Al atoms). The Gd—Al distances range from 3.0681 (14) to 3.4178 (5) Å, and the Gd—Gd and Gd—Ta distances are 3.489 (2) and 3.533 (6) Å, respectively. The remaining atoms are 12-coordinate: distorted icosahedra around Ta1, Al4, Al5, and Al6; regular icosahedron around Ta2; and distorted bicapped pentagonal prisms around Al1, Al2, Al3, and Al7. The short Gd—Gd distances suggest the formation of pairs that extend quasi-infinitely in the *c* direction. The distance between these pairs is significantly larger at 5.513 (2) Å, beyond the expected metal–metal bonding distance for Gd. Magnetic measurements on powder samples for many members of the $R_6T_4Al_{43}$ family have been reported (Wolff *et al.*, 2001). Powder samples of $Gd_6Ta_4Al_{43}$ exhibit ferro- or meta-magnetic behavior; magnetic measurements on single crystals are envisaged.

Experimental

The elements Gd (99.999%; Ames Laboratory), Ta (99.999%; Ames Laboratory), and Al (99.98%; Alfa) were combined in the atomic ratio $Gd_6Ta_4Al_{100}$ in a 2 ml alumina crucible. The crucible was placed into a fused silica tube and a second crucible, filled with SiO_2 wool, was placed inverted on top of the first. The tube was sealed under 1/5 atm Ar and placed into a box furnace. The mixture was heated to 1463 K in 3 h, kept at 1463 K for 2 h, and then cooled to 1173 K over 64 h. The reaction vessel was removed from the furnace at 1173 K, and the excess liquid was immediately decanted to isolate hexagonal prisms of the title compound.

Crystal data

$Gd_6Ta_4Al_{43}$
M_r = 2827.44
Hexagonal, $P6_3/mcm$
a = 11.1047 (16) Å
c = 17.885 (4) Å
V = 1910.0 (5) Å^3
Z = 2
D_x = 4.916 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12079 reflections
θ = 4.6–56.5°
μ = 22.66 mm^{-1}
T = 293 (2) K
Prism, silver
0.19 × 0.09 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.099, T_{max} = 0.322
11039 measured reflections
873 independent reflections
859 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.2°
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 10$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.043
S = 1.34
873 reflections
53 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0157P)^2 + 8.7197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00078 (5)

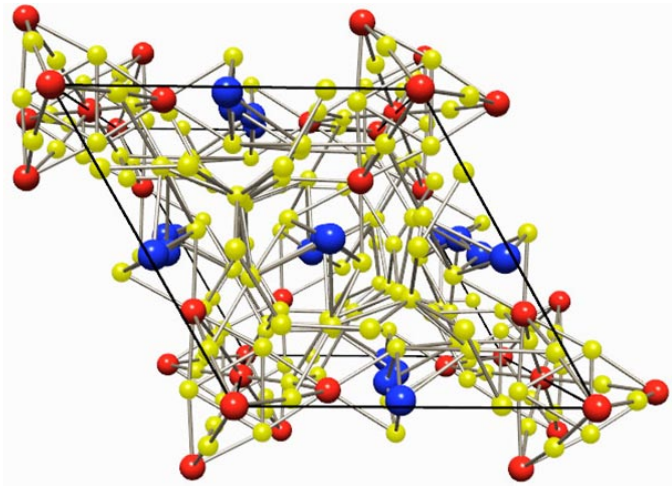

Figure 2
Packing diagram of $Gd_6Ta_4Al_{43}$, viewed along the *c* axis. Key: Gd, blue; Ta, red; Al, yellow.

The highest peak in the difference density map is 0.77 Å from Ta1.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *Balls and Sticks* (Kang & Ozawa, 2003); software used to prepare material for publication: *SHELXTL*.

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