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Cerium cadmium diantimonide, $CeCd_{0.660}Sb_2$

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(Ce–Sb) = 0.0003 Å
Disorder in main residue
R factor = 0.018
wR factor = 0.045
Data-to-parameter ratio = 21.6

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

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Cerium cadmium diantimonide, $CeCd_{0.660\,(4)}Sb_2$, adopts the $HfCuSi_2$-type structure and is confirmed to have defects in the Cd site. Layers of condensed $CdSb_{4/4}$ tetrahedra and square nets of Sb atoms are separated by Ce atoms.

Comment

A large number of ternary rare-earth transition-metal antimonides, (RE)$M_{1-x}Sb_2$, adopt a simple layered tetragonal structure (Pearson symbol *tP*8). The structure type has been given various names, but it will be referred to here as the $HfCuSi_2$-type. The phase forms with the lighter RE elements and many transition metals (M = Mn, Fe, Co, Ni, Pd, Cu, Ag, Au, Zn and Cd; Pankevich *et al.*, 1983; Cordier *et al.*, 1985; Leithe-Jasper & Rogl, 1994; Sologub *et al.*, 1994; Brylak *et al.*, 1995; Sologub, Hiebl *et al.*, 1995; Sologub, Noël *et al.*, 1995; Wollesen *et al.*, 1996; Zeng *et al.*, 2002). Some of these compounds are fully stoichiometric, whereas others exhibit partial occupancy of the transition-metal site. The emerging interest in these compounds stems from their magnetic and other physical properties (Houshiar *et al.*, 1995; André *et al.*, 1997; Muro *et al.*, 1997; Kolenda *et al.*, 2001). The (RE)$Cd_{1-x}Sb_2$ series (RE = La, Ce, Pr, Nd and Sm) has been reported previously, with partial occupancy being demon-

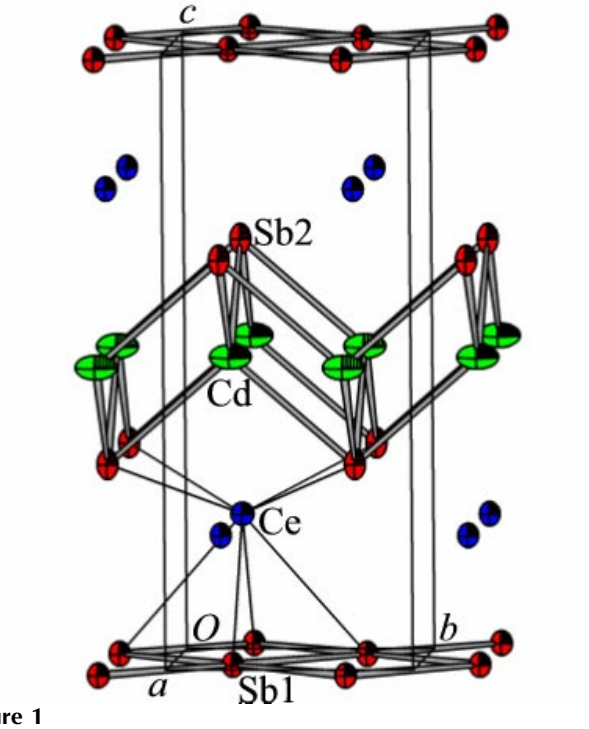

Figure 1
$CeCd_{0.66}Sb_2$ viewed approximately down the a axis. Displacement ellipsoids are drawn at the 75% probability level. Colour key: Ce blue, Cd green, Sb red.

strated for the La member [$LaCd_{0.700\ (5)}Sb_2$] by single-crystal X-ray diffraction (Sologub, Hiebl *et al.*, 1995; Wollesen *et al.*, 1996). The structure of $CeCd_{0.660\ (4)}Sb_2$ is presented here. The cell parameters are close to those previously reported from refinements of powder data [a = 4.3751 (7) Å and c = 10.900 (2) Å (Sologub, Hiebl *et al.*, 1995), or a = 4.3761 (9) Å and c = 10.912 (4) Å (Wollesen *et al.*, 1996)].

Fig. 1 shows the structure of $CeCd_{0.660\ (4)}Sb_2$ projected along the a axis. It consists of layers of condensed $CdSb_{4/4}$ tetrahedra [Cd—Sb2 = 2.9013 (4) Å] alternating with square Sb nets [Sb1—Sb1 = 3.0963 (2) Å]. The Ce atoms lie between these layers and nets, and are coordinated by Sb atoms in a square antiprismatic geometry [Ce—Sb2 = 3.2752 (3) Å and Ce—Sb1 = 3.3095 (4) Å]. The Cd atoms also form a square net similar to the Sb1 net, but the Cd—Cd distance [3.0963 (2) Å] is probably too long to be significant. A simple bonding analysis with the assumptions of one-electron Sb1—Sb1 bonds, trivalent Ce and divalent Cd yields the idealized formulation $(Ce^{3+})(Cd^{2+})_{0.5}(Sb1)^{1-}(Sb2)^{3-}$. Mixed-valent Ce is unlikely because the cell parameters do not deviate from the monotonic decrease observed in the series $(RE)Cd_{1-x}Sb_2$ (Sologub, Hiebl *et al.*, 1995; Wollesen *et al.*, 1996). The actual refined composition, $CeCd_{0.660\ (4)}Sb_2$, can be rationalized if the excess electrons provided by additional Cd atoms are accommodated in Sb—Sb non-bonding or weakly antibonding states within the Sb1 square net (Mills *et al.*, 2002).

Experimental

The starting materials were Ce chips (Alfa, 99.9%), Cd powder (Cerac, 99.999%) and Sb powder (Cerac, 99.995%). Ce, Cd and Sb were reacted in a 1:2:2 molar ratio in an evacuated fused-silica tube. The tube was heated at 1173 K for 2 d, cooled to 873 K over a period of 2 d, kept at that temperature for 2 d and then cooled to room temperature over a period of 1 d. The product contained, among other phases, silver plate-shaped crystals, which were found by semiquantitative energy-dispersive X-ray analysis to have a composition (wt%) of 32 (3)% Ce, 11 (3)% Cd and 57 (3)% Sb, in fair agreement with the expected values of 31% Ce, 16% Cd and 53% Sb.

Crystal data

$CeCd_{0.66}Sb_2$
M_r = 457.81
Tetragonal, $P4/nmm$
a = 4.3788 (3) Å
c = 10.9062 (8) Å
V = 209.11 (3) Å^3
Z = 2
D_x = 7.271 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3037 reflections
θ = 4.7–33.1°
μ = 26.55 mm^{-1}
T = 295 (2) K
Plate, silver
0.13 × 0.11 × 0.04 mm

Data collection

Bruker Platform/SMART 1000 CCD diffractometer
ω scans
Absorption correction: numerical (*SHELXTL*; Sheldrick, 1997)
T_{min} = 0.062, T_{max} = 0.325
3517 measured reflections
281 independent reflections
278 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 33.1°
$h = -6 \rightarrow 6$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.045
S = 1.20
281 reflections
13 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 1.0041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −1.49 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0049 (7)

Table 1
Selected interatomic distances (Å).

Ce—Sb2^{i}	3.2752 (3)	Cd—Sb2	2.9013 (4)
Ce—Sb1	3.3095 (4)	Cd—Cd^{ii}	3.0963 (2)
Ce—Cd	3.6908 (4)	Sb1—Sb1^{iii}	3.0963 (2)

Symmetry codes: (i) $-x, -y, 1-z$; (ii) $1-x, -y, 1-z$; (iii) $1-x, -y, -z$.

The maximum peak and deepest hole are located 0.70 Å from Ce and 1.08 Å from Sb2, respectively.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *SHELXTL*.

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