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The intermetallic compound BaAuSb

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Ba–Sb) = 0.0003 Å
R factor = 0.033
wR factor = 0.082
Data-to-parameter ratio = 11.1

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

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The title compound, barium gold antimonide, BaAuSb, is isostructural with ZrBeSi, which adopts the space group $P6_3/mmc$. The Au and Sb atoms form planar honeycomb layers, with an Au—Sb distance of 2.7402 (3) Å.

Comment

During studies on the ternary barium–gold–antimony system using sealed tantalum containers for their preparation, the intermetallic compound, BaAuSb, was obtained as a side product. Previously, this compound was prepared by direct reaction with stoichiometric amounts of the components and characterized by X-ray powder diffraction (Merlo & Fornasini, 1990).

BaAuSb is isostructural with ZrBeSi, a ternary ordered variant of the binary type Ni_2In (Vogel & Schuster, 1980). Au and Sb form planar hexagonal sheets like graphite, with Au and Sb alternating in the layer. Ba atoms lie between two layers and are positioned over the centers of the hexagonal rings. The shortest interatomic distance, Au—Sb, is 2.7402 (3) Å, and each Ba atom is bonded to six Au and six Sb atoms at distances of 3.5948 (3) Å.

Experimental

The title compound was obtained as a by-product when elemental Ba [rod, Aesar (99.99%)], Au [powder, 100 mesh, Aesar (99.999%)], and Sb [powder, 100 mesh, Aesar (99.999%)] were loaded into a tantalum tube (Nobel-Met. Ltd, >99.85%, 0.375 OD) in a 1:1:2 molar ratio in an

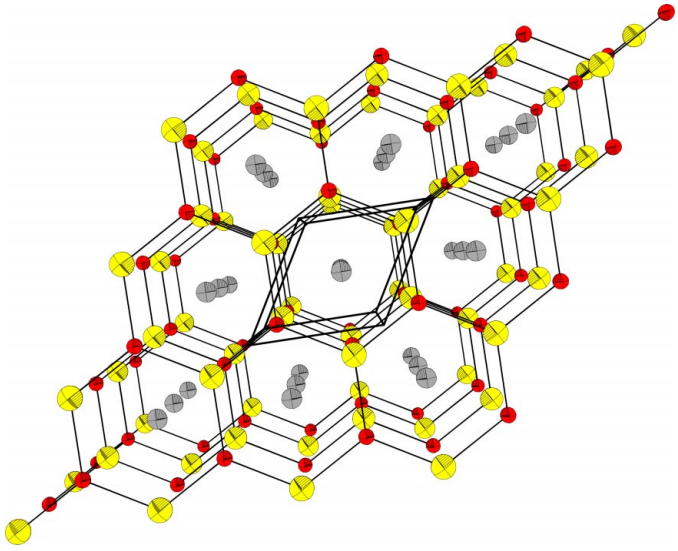

Figure 1
An (001) perspective projection of BaAuSb. Displacement ellipsoids are drawn at the 99% probability level. Key: Ba gray, Au gold and Sb red.

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Ar-filled glove-box. The tube was sealed in an arc-melter under argon, and heated to 973 K for 3 d in a fused-silica jacket. The reaction container was cooled slowly to 673 K at 10 K h^{-1}, and then quenched to room temperature. When the tantalum tube was opened in the Ar-filled glove-box, gray irregular-shaped crystals of the title compound were found in the product. Suitable single crystals were mounted in 0.3 mm thin-walled capillaries for subsequent diffraction experiments.

Crystal data

BaAuSb
M_r = 456.06
Hexagonal, $P6_3/mmc$
a = 4.7461 (6) Å
c = 9.3075 (11) Å
V = 181.57 (4) Å^3
Z = 2
D_x = 8.342 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 48 reflections
θ = 4.4–14.0°
μ = 58.13 mm^{-1}
T = 293 (2) K
Irregular, gray
0.10 × 0.05 × 0.05 mm

Data collection

Bruker $P4$ diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.030, T_{max} = 0.055
412 measured reflections
89 independent reflections
78 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 25.9°
$h = -1 \rightarrow 5$
$k = -5 \rightarrow 1$
$l = -11 \rightarrow 1$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.082
S = 1.14
89 reflections
8 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.74 e Å^{-3}
$\Delta\rho_{min}$ = −2.04 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.028 (3)

Space groups $P\bar{3}1c$, $P31c$, $P6_3mc$, $P6_3/mmc$, and $P\bar{6}2c$ were allowed based upon the observed systematic absences. Space group $P6_3/mmc$ was selected for initial refinements, and this group was confirmed by comparing the refinement results using the other four groups. Ba, Au, and Sb atoms were readily located from an E map, and refined with anisotropic displacement parameters. The largest residuals in the final difference map were 1.74 e Å^{-3} at a distance of 0.42 Å from Ba and −2.04 e %A^{-3} at a distance of 1.30 Å from the Au atom. All atoms lie in special positions with no refined coordinates.

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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