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The intermetallic compound BaAgBi

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Ag–Ba) = 0.0004 Å
R factor = 0.038
wR factor = 0.102
Data-to-parameter ratio = 16.6

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

Barium silver bismuth is isostructural with ZrBeSi. The Ag and Bi atoms form planar honeycomb layers with an Ag—Bi distance of 2.8534 (4) Å. The displacement parameters of Ag and Bi show a strong anisotropy.

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Comment

During studies on the ternary barium–silver–bismuth system, the intermetallic compound BaAgBi was obtained as a side product. Previously, this compound was prepared by stoichiometric reaction of the elements and characterized by X-ray powder diffraction (Merlo *et al.*, 1990).

BaAgBi is isostructural with ZrBeSi (Vogel & Schuster, 1980). The Ag and Bi atoms form planar hexagonal sheets like graphite, with Ag and Bi alternating in the layer. The Ba atoms lie between two layers and are positioned over the centers of the hexagonal rings. The shortest interatomic distance, Ag—Bi, is 2.8534 (4) Å, and each Ba atom is surrounded by six Au and six Sb atoms at distances of 3.6533 (4) Å. The displacement parameters of the Ag and Bi atoms display a strong anisotropy; the U_{11} values of the Ag and Bi atoms are 0.0120 (11) and 0.0066 (7) Å^2 while the U_{33} values are 0.0231 (18) and 0.0140 (10) Å^2, respectively. This anisotropy also appears in several ZrBeSi-type compounds, such as EuZnGe (Pöttgen, 1995), CaCuBi (Merlo *et al.*, 1990), and EuAgAs (Tomuschat & Schuster, 1981), suggesting the possibility of interlayer interactions.

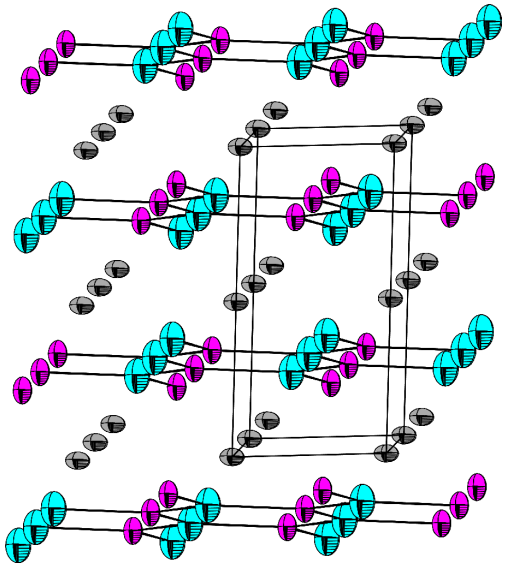

Figure 1
The layer structure of BaAgBi along the z axis. Displacement ellipsoids are drawn at the 99% probability level. Key: Ba grey, Ag blue, Bi red.

Experimental

BaAgBi was obtained as a by-product when Ba [rod, Alfa–Aesar (99.99%)], Ag [powder, −100 mesh, Alfa–Aesar (99.999%)], and Bi [powder, −100 mesh, Alfa–Aesar (99.999%)] were loaded into a tantalum tube (Nobel-Met. Ltd, >99.85%, 0.375 in. OD) in a 1:1:2 molar ratio in an Ar-filled glovebox. The tube was sealed in an arc-melter under argon, placed in a fused-silica jacket, and heated at 973 K for 3 days. 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 glovebox, grey irregular-shaped crystals of BaAgBi were found in the product. Single crystals were mounted in 0.3 mm thin-walled capillaries for diffraction experiments.

Crystal data

AgBaBi
M_r = 454.19
Hexagonal, $P6_3/mmc$
a = 4.9423 (7) Å
c = 9.1251 (18) Å
V = 193.03 (5) Å^3
Z = 2
D_x = 7.814 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 27 reflections
θ = 6.5–14.4°
μ = 60.31 mm^{-1}
T = 293 (2) K
Irregular, grey
0.09 × 0.03 × 0.03 mm

Data collection

Rigaku AFC-6R diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.132, T_{max} = 0.164
133 measured reflections
133 independent reflections
89 reflections with $I > 2\sigma(I)$
θ_{max} = 30.0°
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 3$
$l = 0 \rightarrow 12$
3 standard reflections
every 100 reflections
intensity decay: 0.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.16
133 reflections
8 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 2.2564P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.76 e Å^{-3}
$\Delta\rho_{min}$ = −3.98 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.011 (2)

Table 1
Selected geometric parameters (Å, °).

Ba—Bi^{i}	3.6533 (4)	Ag—Bi^{ii}	2.8534 (4)
Ba—Ag	3.6533 (4)		
Bi^{ii}—Ag—Bi^{iii}	120	Ag^{ii}—Bi—Ag^{iii}	120

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 2-y, 1-z$; (iii) $-x, 1-y, 1-z$.

Based on the observed systematic absences, space groups $P\bar{3}1c$, $P31c$, $P6_3mc$, $P6_3/mmc$, and $P\bar{6}2c$ are allowed. Space group $P6_3/mmc$ was initially selected and confirmed by comparing the refinement results with those of the other four space groups. The Ba, Ag, and Bi atoms were readily located from the E map, and refined with anisotropic displacement parameters. The reflection $\bar{1}24$ was omitted from the refinement because of possible interference from the beam stop of the X-ray diffractometer. The largest residuals in the final difference map were 2.76 e Å^{-3} at a distance of 0.74 Å from Bi, and −3.98e Å^{-3} at a distance of 0.92 Å from Bi.

Data collection: *TEXSAN* (Molecular Structure Corporation, 1990); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; 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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