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Rubidium Indium Antimonide, $Rb_2In_2Sb_3$

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Abstract

The structure of dirubidium diindium triantimonide, a layered material isotypic with $A_2In_2Sb_3$ (A = Na, K, Cs), is reported.

Comment

The title compound, $Rb_2In_2Sb_3$, has been structurally characterized and shown to contain discrete layers of $InSb_4$ tetrahedra separated by rubidium. These tetrahedra are connected *via* common corners, edges and short Sb—Sb distances. All distances and angles are as expected [In—Sb distances are in the range 2.8075 (10)–2.9646 (10) Å] and correspond well with the previously reported isotypic structures [*cf.* In—Sb distances in the range 2.804 (4)–2.962 (4) Å for $Cs_2In_2Sb_3$] (Cordier & Ochmann, 1991; Blase, Cordier, Poth & Weil, 1995).

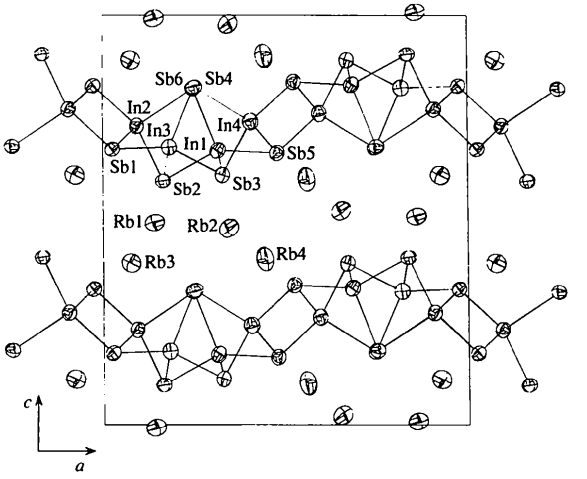

Fig. 1. *ORTEP* (Johnson, 1965) representation of the layered structure of $Rb_2In_2Sb_3$ showing the In_2Sb_3 layers separated by rubidium (90% probability level).

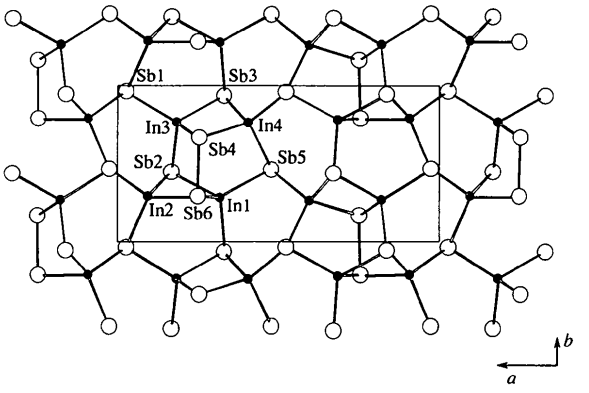

Fig. 2. Cross-section of the In_2Sb_3 layer showing corner- and edge-sharing connections of $InSb_4$ tetrahedra and the short Sb—Sb distances.

Experimental

$Rb_2In_2Sb_3$ was prepared by direct combination of the elements. A dry quartz tube was charged with Rb (0.26 g, 3 mmol), In (0.23 g, 2 mmol) and Sb (0.36 g, 3 mmol). The tube was evacuated for 1.5 h at 5×10^{-3} Torr (1 Torr = 133.322 Pa) and sealed under vacuum. The sample was heated at 873 K in an automatic control furnace for 10 h and then cooled to ambient temperature over a 96 h period.

Crystal data

$Rb_2In_2Sb_3$ — Ag $K\alpha$ radiation
M_r = 765.83 — λ = 0.56086 Å

Monoclinic
$P2_1/c$
a = 15.555 (2) Å
b = 7.5692 (6) Å
c = 17.362 (7) Å
β = 90.598 (14)°
V = 2044.0 (9) Å^3
Z = 8
D_x = 4.977 Mg m^{-3}
D_m not measured

Cell parameters from 26 reflections
θ = 1.8–8.5°
μ = 11.538 mm^{-1}
T = 293 (2) K
Rectangular block
0.26 × 0.18 × 0.08 mm
Dark grey metallic

Data collection

Siemens $P4$ four-circle diffractometer
Bisecting ω scans
Absorption correction: numeric
T_{min} = 0.152, T_{max} = 0.409
10 021 measured reflections
8167 independent reflections

R_{int} = 0.0559
θ_{max} = 26°
$h = -1 \rightarrow 24$
$k = -1 \rightarrow 11$
$l = -27 \rightarrow 27$
3 standard reflections monitored every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.0388
$wR(F^2)$ = 0.0732
S = 0.699
8167 reflections
127 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0093P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 1.679 e Å^{-3}
$\Delta\rho_{min}$ = −1.625 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Rb1	0.85862 (6)	0.02746 (14)	0.00788 (5)	0.0281 (2)
Rb2	0.34667 (6)	0.45606 (15)	0.97831 (6)	0.0298 (2)
Rb3	0.07657 (6)	0.4674 (2)	0.89068 (5)	0.0310 (2)
Rb4	0.55711 (6)	0.0548 (2)	0.09933 (6)	0.0367 (3)
In1	0.31611 (4)	0.72107 (9)	0.16956 (4)	0.01758 (14)
In2	0.90699 (4)	0.21146 (9)	0.27031 (4)	0.01658 (13)
In3	0.18136 (4)	0.23595 (9)	0.17727 (4)	0.01747 (14)
In4	0.40668 (4)	0.23851 (9)	0.24018 (4)	0.01798 (14)
Sb1	0.97431 (4)	0.53666 (9)	0.32768 (3)	0.01620 (12)
Sb2	0.16409 (4)	0.55444 (9)	0.09520 (3)	0.01652 (13)
Sb3	0.32931 (4)	1.06473 (8)	0.10988 (4)	0.01645 (13)
Sb4	0.25209 (4)	0.16508 (8)	0.82458 (4)	0.01753 (13)
Sb5	0.47704 (4)	0.53923 (9)	0.16277 (4)	0.01711 (13)
Sb6	0.24813 (4)	0.78693 (9)	0.82086 (4)	0.01772 (13)

Table 2. *Selected geometric parameters (Å, °)*

In1—Sb3	2.8083 (10)	In3—Sb1^{iii}	2.8534 (9)
In1—Sb6^{i}	2.8425 (14)	In3—Sb4^{v}	2.8730 (13)
In1—Sb5	2.8602 (9)	In3—Sb3^{vi}	2.8983 (9)
In1—Sb2	2.9638 (10)	In4—Sb5	2.8663 (10)
In2—Sb1^{ii}	2.8494 (10)	In4—Sb3^{vi}	2.8704 (12)
In2—Sb1	2.8506 (10)	In4—Sb5^{iii}	2.8847 (10)
In2—Sb2^{iii}	2.8532 (12)	In4—Sb4^{v}	2.9215 (10)
In2—Sb6^{iv}	2.8720 (10)	Sb4—Sb6^{vi}	2.8637 (9)
In3—Sb2	2.8118 (10)		

Symmetry codes: (i) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (ii) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $1-x, 1-y, 1-z$; (v) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (vi) $x, y-1, z$.

Data collection: Siemens $P4$ diffractometer software. Cell refinement: *XSCANS* (Siemens, 1994). Data reduction: *XSCANS*. Program(s) used to refine structure: *SHELXTL/PC* (Sheldrick, 1995).

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Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1152). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Triclinic $Fe_3Al_2Si_3$ and Orthorhombic $Fe_3Al_2Si_4$ with New Structure Types

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Abstract

The title compounds, dialuminium triiron trisilicide and dialuminium triiron tetrasilicide, crystallize with new structure types. The coordination polyhedra in $Fe_3Al_2Si_3$ derive from icosahedra and those in $Fe_3Al_2Si_4$ from hexagonal cuboctahedra.

Comment

The ternary system Fe–Al–Si contains numerous ternary compounds. Six crystallize with known structures: