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Ytterbium sesquiselenide Yb_2Se_3

Abdeljalil Assoud and Holger Kleinke*

Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

Correspondence e-mail: kleinke@uwaterloo.ca

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(Yb–Se) = 0.001 Å
R factor = 0.033
wR factor = 0.074
Data-to-parameter ratio = 45.3

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

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Ytterbium selenide, Yb_2Se_3, was prepared by reacting the elements at 1173 K in an evacuated silica tube in an Sn flux. The ytterbium sesquiselenide crystallizes in the orthorhombic space group *Fddd*, adopting the Sc_2S_3 structure type. Its structure consists of edge-sharing (slightly distorted) $YbSe_6$ octahedra, and may be regarded as a defect NaCl structure.

Comment

The sesquichalcogenides of the rare earth elements adopt different structure types. While the La–Gd chalcogenides crystallize in defect variants of the Th_3P_4 type (Mauricot *et al.*, 1995), Yb_2S_3 adopts the α-Al_2O_3 structure (El Fadli *et al.*, 1994). Based on powder diffractograms, the Sc, Y and Dy–Yb selenides (Dismukes & White, 1965; Flahaut *et al.*, 1965) were reported to form the Sc_2S_3 structure (Tremblet *et al.*, 1963). The cell dimensions for Yb_2Se_3 (orthorhombic system) were determined by Dismukes & White (1965) to be a = 11.274 Å, b = 8.021 Å, c = 23.98 Å and V = 2168.5 Å, and by Flahaut *et al.* (1965) to be a = 11.27 Å, b = 8.02 Å, c = 23.96 Å and V = 2165.6 Å. The atomic positions of Yb_2Se_3 were not refined in either case; Flahaut *et al.* (1965) merely extrapolated them from the ideal NaCl structure type. Our single-crystal structure study on Yb_2Se_3 confirms the suggested Sc_2S_3 type, and delivers crystallographic details with high precision. It is evident that the shifts from the NaCl structure are significant; *e.g.* the x parameters of Se1 and Se2 are not 3/8 = 0.375, but 0.37062 (10) for Se1 and 0.38115 (7) for Se2. This is reflected in deviations from the ideal Se—Yb—Se bond angles of up to 4.5° and Yb—Se bond lengths varying from 2.7943 (6) to 2.8184 (6) Å (Yb1) and from 2.7967 (6) to 2.8188 (3) Å (Yb2).

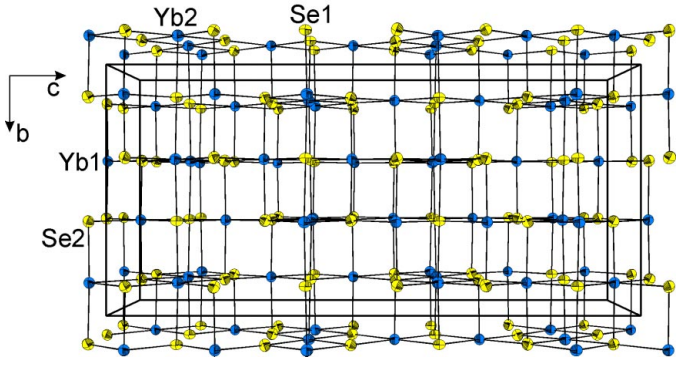

Figure 1
A projection of Yb_2Se_3 along the a axis. Displacement ellipsoids are drawn at the 99.9% probability level. Colour code: blue Yb and yellow Se.

Experimental

Yb_2Se_3 was obtained from a reaction of elemental ytterbium and selenium in a tin flux. The mixture was annealed at 1173 K over a period of 4 d, and then slowly cooled (3 K h^{-1}) to room temperature. Yb_2Se_3 crystallized in the form of black block-shaped crystals.

Crystal data

Yb_2Se_3
M_r = 582.96
Orthorhombic, *Fddd*
a = 8.0183 (7) Å
b = 11.272 (1) Å
c = 23.961 (2) Å
V = 2165.7 (3) Å^3
Z = 16
D_x = 7.152 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5337 reflections
θ = 3.2–35.0°
μ = 54.32 mm^{-1}
T = 298 (2) K
Block, black
0.01 × 0.01 × 0.01 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.487, T_{max} = 0.581
5337 measured reflections
1179 independent reflections
937 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 35.0°
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -32 \rightarrow 38$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.074
S = 1.12
1179 reflections
26 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.70 e Å^{-3}
$\Delta\rho_{min}$ = −3.52 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.000397 (11)

Table 1
Selected geometric parameters (Å).

Yb1—Se2^{i}	2.7943 (6)	Yb2—Se2	2.7967 (6)
Yb1—Se2^{ii}	2.7943 (6)	Yb2—Se2^{iii}	2.7967 (6)
Yb1—Se1	2.8095 (6)	Yb2—Se2^{vi}	2.8086 (7)
Yb1—Se1^{iii}	2.8095 (6)	Yb2—Se2^{vii}	2.8086 (7)
Yb1—Se2^{iv}	2.8184 (6)	Yb2—Se1^{i}	2.8188 (3)
Yb1—Se2^{v}	2.8184 (6)	Yb2—Se1^{ii}	2.8188 (2)

Symmetry codes: (i) $\frac{1}{2}-x, -y, \frac{1}{2}-z$; (ii) $x-\frac{1}{4}, \frac{1}{4}+y, \frac{1}{2}-z$; (iii) $\frac{1}{4}-x, \frac{1}{4}-y, z$; (iv) $x-\frac{1}{2}, y, z-\frac{1}{2}$; (v) $\frac{3}{4}-x, \frac{1}{4}-y, z-\frac{1}{2}$; (vi) $x-\frac{1}{2}, \frac{1}{4}-y, \frac{3}{4}-z$; (vii) $\frac{3}{4}-x, y, \frac{3}{4}-z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *SHELXL*97.

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