

CsYbSe₂

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Key indicators

Single-crystal X-ray study
 $T = 153$ K
Mean $\sigma(\text{Yb-Se}) = 0.001$ Å
 R factor = 0.019
 wR factor = 0.041
Data-to-parameter ratio = 17.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Caesium ytterbium diselenide, CsYbSe₂, crystallizes in space group $P6_3/mmc$ of the hexagonal system. It is isostructural with CsPrS₂, which has the β -RbScO₂ structure type. In the asymmetric unit, the site symmetries of atoms Cs, Yb and Se are $\bar{6}m2$, $\bar{3}m$ and $3m$, respectively. The structure comprises layers of edge-shared YbSe₆ octahedra perpendicular to [001], with Cs atoms between the layers in a trigonal-prismatic arrangement.

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Comment

CsYbSe₂ is a member of the large $ALnQ_2$ family (A is an alkali metal, Ln is a rare-earth metal and $Q = S, Se$ and Te) that includes over 100 compounds. Most of these adopt the trigonal α -NaFeO₂ structure, which is a rock-salt superstructure with cations ordered in alternating layers between cubic close-packed anions. Examples of the trigonal structure include NaGdS₂ (Sato *et al.*, 1984), NaLnS₂ ($Ln = Ho, Er, Tm$ and Lu ; Schleid & Lissner, 1993), NaLnS₂ ($Ln = La, Ce, Pr, Nd$ and Er ; Ballestracci & Bertaut, 1964), KLnS₂ ($Ln = La, Pr, Sm, Gd, Dy, Ho, Er$ and Yb ; Ballestracci, 1965), RbLnS₂ ($Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb$ and Lu ; Bronger *et al.*, 1996), CsLnS₂ ($Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb$ and Lu ; Bronger *et al.*, 1993), RbLnSe₂ ($Ln = La, Ce, Pr, Nd, Sm, Gd, Tb, Ho, Er$ and Lu ; Deng *et al.*, 2002), NaErSe₂ (Stöwe, 1997), KSmTe₂ (Bronger *et al.*, 1993), KErTe₂ (Keane & Ibers, 1992), KLnTe₂ ($Ln = La, Pr, Nd$ and Gd ; Stöwe *et al.*, 2003), RbLnTe₂ ($Ln = Ce$ and Nd ; Stöwe *et al.*, 2003) and CsNdTe₂ (Stöwe *et al.*, 2003). Some members of the $ALnQ_2$ family adopt the cubic rock-salt ($Fm\bar{3}m$) structure type, in which the A^+ and Ln^{3+} cations are disordered. Examples include LiLnS₂ ($Ln = Pr, Eu, Gd$ and Dy ; Ballestracci, 1965), LiLnS₂ ($Ln = Nd, Sm, Gd, Tb, Dy, Ho$ and Er ; Ohtani *et al.*, 1987), NaLnS₂ ($Ln = La, Nd$ and Pr ; Sato *et al.*, 1984), NaLnS₂ ($Ln = La, Ce, Pr$ and Nd ; Ballestracci & Bertaut, 1964) and LiLnSe₂ ($Ln = Nd, Sm, Gd, Tb, Dy, Ho$ and Er ; Ohtani *et al.*, 1987). Recently, NaPrTe₂ was found to crystallize in a new cubic $Fd\bar{3}m$ structure (Lissner & Schleid, 2003). In each of the first two structure types the A^+ and Ln^{3+} cations are octahedrally coordinated by six Q atoms. A slight distortion from octahedral towards trigonal-prismatic coord-

Yb  Se Cs

Figure 1

A view of the asymmetric unit of CsYbSe₂, with displacement ellipsoids at the 90% probability level.

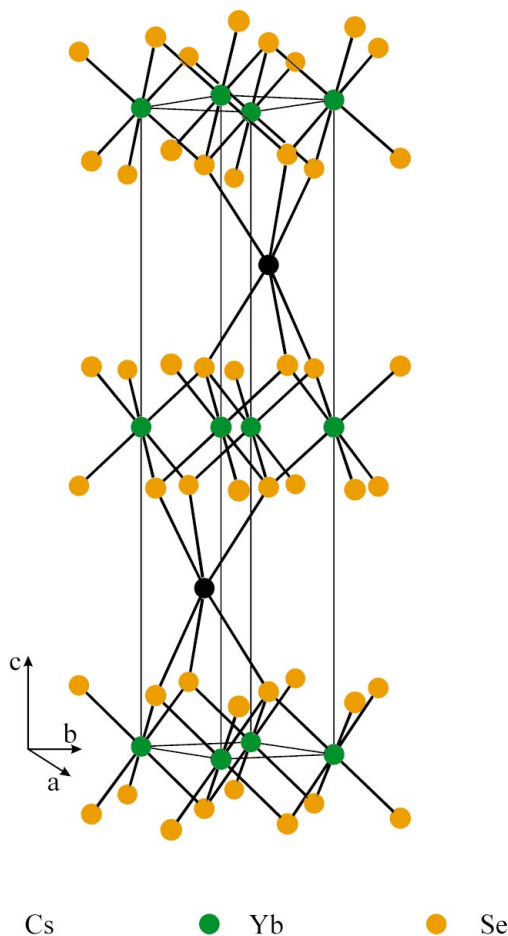


Figure 2
The crystal structure of CsYbSe₂.

ination can lead to the hexagonal β -RbScO₂ structure type. Only a few $ALnQ_2$ compounds, such as $CsLnS_2$ ($Ln = \text{Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb}$ and Lu ; Bronger *et al.*, 1993), have been found to adopt this structure.

We report here the structure of CsYbSe₂, which is a new member of the $ALnQ_2$ family. CsYbSe₂, which has the β -RbScO₂ structure type, crystallizes in space group $P6_3/mmc$ of the hexagonal system. In the asymmetric unit, the site symmetries of atoms Cs, Yb and Se are $\bar{6}m2$, $\bar{3}m$ and $3m$, respectively (Fig. 1). The structure consists of the layered packing of cations and anions (Fig. 2). Each Cs atom is surrounded by a trigonal prism of six Se atoms. The Cs–Se distance of 3.5370 (6) Å is comparable to those of 3.5926 (8)–3.8173 (8) Å in CsYbMnSe₃ (Mitchell *et al.*, 2004). Each Yb atom is surrounded by a slightly distorted octahedron of six Se atoms. The Yb–Se distance of 2.8432 (5) Å is also comparable to those of 2.8360 (5)–2.8659 (5) Å in CsYbMnSe₃ (Mitchell *et al.*, 2004).

Experimental

CsYbSe₂ was obtained as thin red plates from a solid-state reaction of Cs₂Se₃ (0.5 mmol), Yb (Alfa Aesar, 99.9%, 1.0 mmol) and Se (Aldrich, 99.9%, 0.5 mmol). The Cs₂Se₃ reactive flux was prepared by the stoichiometric reaction of Cs (Aldrich, 99.5%) and Se in liquid

NH₃. The reactants were loaded in a fused-silica tube that was then evacuated to 10^{−4} Torr (1 Torr = 133.322 Pa). The tube was heated to 1173 K, kept at 1173 K for 72 h and cooled at 4 K h^{−1} to 373 K, and then the furnace was turned off. The reaction mixture was washed with water and then dried with acetone. The yield was about 30%, based on Yb. Qualitative energy dispersive spectroscopy (EDS) analysis verified the presence of Cs, Yb and Se.

Crystal data

CsYbSe ₂	Mo $K\alpha$ radiation
$M_r = 463.87$	Cell parameters from 2727 reflections
Hexagonal, $P6_3/mmc$	$\theta = 2.5\text{--}29.0^\circ$
$a = 4.1539$ (3) Å	$\mu = 40.78 \text{ mm}^{-1}$
$c = 16.508$ (2) Å	$T = 153$ (2) K
$V = 246.68$ (4) Å ³	Plate, red
$Z = 2$	$0.080 \times 0.074 \times 0.040 \text{ mm}$
$D_x = 6.245 \text{ Mg m}^{-3}$	

Data collection

Bruker SMART 1000 CCD diffractometer	158 independent reflections
ω scans	153 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (face-indexed; <i>SHELXTL</i> ; Sheldrick, 2003)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.051$, $T_{\text{max}} = 0.201$	$\theta_{\text{max}} = 29.0^\circ$
2727 measured reflections	$h = -5 \rightarrow 5$
	$k = -5 \rightarrow 5$
	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.019$	$\Delta\rho_{\text{max}} = 1.11 \text{ e \AA}^{-3}$
$wR(F^2) = 0.041$	$\Delta\rho_{\text{min}} = -1.58 \text{ e \AA}^{-3}$
$S = 1.70$	$\Delta\rho_{\text{rms}} = -0.26 \text{ e \AA}^{-3}$
158 reflections	Extinction correction: <i>SHELXL97</i>
9 parameters	Extinction coefficient: 0.0231 (15)
$w = 1/[\sigma^2(F_o^2) + (0.017P)^2]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Table 1

Selected geometric parameters (Å, °).

Cs–Se ⁱ	3.5370 (6)	Yb–Se ⁱⁱ	2.8432 (5)
Se ⁱ –Cs–Se ⁱⁱⁱ	140.365 (8)	Se ⁱⁱ –Yb–Se ^v	93.855 (19)
Se ⁱ –Cs–Se ^{iv}	71.918 (15)	Se ⁱ –Yb–Se ^v	86.145 (19)
Se ⁱⁱⁱ –Cs–Se ^{iv}	94.617 (19)		

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

The highest residual electron density is located 2.40 Å from Cs; the deepest hole is located 0.67 Å from Yb.

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

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