Crystal structure of sodium ytterbium(III) selenide, NaYbSe₂

A. K. Gray, B. R. Martin and P. K. Dorhout*

Colorado State University, Department of Chemistry, Fort Collins, CO 80523, USA

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Abstract

NaSe₂Yb, trigonal, $R\bar{3}m$ (No. 166), $a = 4.0568(8)$ Å, $c = 20.772(6)$ Å, $V = 296.1$ Å³, $Z = 3$, $R_{\text{gt}}(F) = 0.051$, $wR_{\text{ref}}(F^2) = 0.110$, $T = 298$ K.

Source of material

Crystals of NaYbSe₂ were formed from a molten chalcogenide flux reaction of 51.5 mg Yb, 21.8 mg Ge, 94.0 mg Se, and 40.6 mg Na₂Se₂. The reactants were combined in a fused silica ampoule in an inert atmosphere glovebox, sealed under vacuum, and heated to 998 K at a rate of 35 K / hour. After 72 hours of heating, the ampoule was cooled at 4 K / hour to room temperature. Dimethylformamide was added to dissolve remaining sodium selenide flux, resulting in well-formed hexagonal red-orange plates of NaYbSe₂.

Experimental details

Quantitative energy dispersive spectroscopy yielded atomic ratios 26(3) at% Na, 0(0) at% Ge, 47(5) at% Se and 27(4) at% Yb. The errors are associated with surface contamination, resulting

from washing the residual flux from the crystals, and represent measurements taken from many positions on several crystals. Germanium (not contained in the title compound) was involved in the formation of various sodium germanium selenides. X-ray intensity data was collected from a relatively thin plate, resulting in a small systematic absorption error after empirical absorption correction.

Discussion

NaYbSe₂ crystallizes in the NaFeO₂ structure type, and is isostructural to the family $AlnX_2$, A = alkali metal, Ln = rare earth element, X = S, Se [1]. The structure consists of layers of octahedrally coordinated Yb surrounded by Se, with Na occupying the interlayer sites.

Table 1. Data collection and handling.

Crystal:	red-orange plate, size $0.01 \times 0.1 \times 0.15$ mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	139.96 cm^{-1}
Diffraction, scan mode:	Bruker SMART CCD; 1800 frames, $\varphi = 0^\circ$, 120° , 240° ; $\Delta\omega = 0.3^\circ$
$2\theta_{\text{max}}$:	45.88°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	609, 70
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 69
$N(\text{param})_{\text{refined}}$:	9
Programs:	SHELXTL [2], SADABS [3]

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References

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	3a	0	0	0	0.025(8)	U_{11}	0.01(1)	$U_{11}/2$	0	0
Yb(1)	3b	0	0	1/2	0.010(2)	U_{11}	0.005(2)	$U_{11}/2$	0	0
Se(1)	6c	0	0	0.2424(2)	0.012(2)	U_{11}	0.003(2)	$U_{11}/2$	0	0

* Correspondence author (e-mail: pkd@lamar.colostate.edu)