Crystal structure of tetrarubidiumhexaselenodigermanate(IV), $\text{Rb}_4\text{Ge}_2\text{Se}_6$

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Source of material: $\text{Rb}_4\text{Ge}_2\text{Se}_6$ was obtained by reacting a stoichiometric mixture of Rb_2Se , Ge and Se in a sealed silica tube at 1173 K, followed by controlled slow cooling.

$\text{Rb}_4\text{Ge}_2\text{Se}_6$ is isostructural with $\text{Cs}_4\text{Sn}_2\text{Se}_6$ (see ref. 1). The crystal structure is characterized by discrete $[\text{Ge}_2\text{Se}_6]^{4-}$ anions formed by edge sharing GeSe_4 tetrahedra. Ge–Se bond distances are 2.281 Å, 2.285 Å (terminal) and 2.420 Å (bridging). Bond angles range from 94.3° to 118.5°. Both rubidium cations are coordinated by seven Se in irregular configurations ($d(\text{Rb}–\text{Se})$: 3.394 Å to 4.024 Å).

$\text{Ge}_2\text{Rb}_4\text{Se}_6$, monoclinic, $C12/m1$ (No. 12), $a = 13.885(6)$ Å, $b = 7.133(1)$ Å, $c = 9.984(5)$ Å, $\beta = 124.41(2)^\circ$, $V = 815.8$ Å³, $Z = 2$, $R(F) = 0.044$, $R_w(F) = 0.033$.

Table 1. Parameters used for the X-ray data collection

Crystal:	pale yellow, prismatic, size 0.1 x 0.05 x 0.025 mm
Wavelength:	Mo $K\alpha$ radiation (0.71070 Å)
μ :	284.00 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	2 θ
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	54°
$N(hkl)_{\text{unique}}$:	952
Criterion for I_o :	$I_o > 3 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	37
Programs:	DIFABS, MolEN

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb(1)	4i	0.5860(2)	0	0.3691(2)	0.0262(9)	0.029(1)	0.0290(9)	0	0.0133(6)	0
Rb(2)	4i	0.8099(2)	0	0.1821(2)	0.038(1)	0.043(1)	0.0342(9)	0	0.0190(8)	0
Ge	4i	0.1197(2)	0	0.1854(2)	0.0194(9)	0.016(1)	0.0211(8)	0	0.0124(5)	0
Se(1)	4i	0.1117(2)	0	0.4078(2)	0.0295(9)	0.034(1)	0.0261(8)	0	0.0199(5)	0
Se(2)	4i	0.2984(2)	0	0.2248(2)	0.0243(9)	0.043(1)	0.0343(8)	0	0.0200(6)	0
Se(3)	4g	0	0.2486(4)	0	0.039(1)	0.013(1)	0.0267(8)	0	0.0127(6)	0

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References

- Sheldrick, W. S.; Braunbeck, H. G.: Darstellung und Kristallstruktur von $\text{Cs}_4\text{Sn}_2\text{Se}_6$. *Z. Naturforsch.* **44b** (1989) 851–852.
- Walker, N.; Stuart, D.: DIFABS: An empirical method for correcting diffractometer data for absorption effects. *Acta Crystallogr.* **A39** (1983) 158–160.
- Fair, C. K.: MolEN, An Interactive Intelligent System for Crystal Structure Analysis. Enraf-Nonius Delft, The Netherlands 1990.