Crystal structure of tribromoselenium(IV) tetrabromogallate(III), $[SeBr_3][GaBr_4]$

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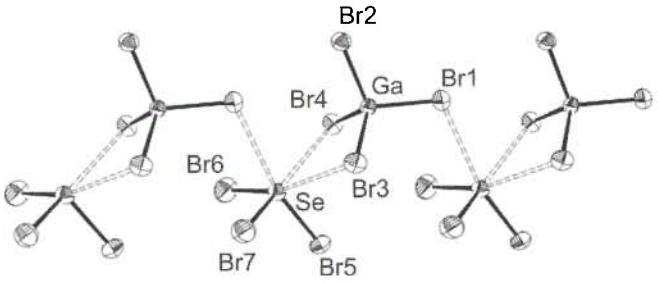

Abstract

Br_7GaSe, monoclinic, $P1c1$ (No. 7), $a = 6.594(1)$ Å, $b = 6.547(2)$ Å, $c = 14.316(3)$ Å, $\beta = 101.10(2)°$, $V = 606.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.081$, $wR_{ref}(F^2) = 0.264$, $T = 208$ K.

Source of material

The compound is formed when selenium, gallium and bromine in the molar ratio 1:1:4 are heated in sealed glass ampoule. To obtain high quality crystals it is essential that the temperature is slowly increased between 570 K and 620 K. After cooling, $[SeBr_3][GaBr_4]$ deposits as yellow single crystals.

Discussion

The structure of this compound is isotypic with those of $[SCl_3][AlCl_4]$ [1], $[TeI_3][AlI_4]$ [2] and $[TeI_3][GaI_4]$ [3], consisting of trigonal-pyramidal units of $SeBr_3^+$ and tetrahedral units of $GaBr_4^-$. The selenium atom also has three weak interactions: two with bromine atoms of the $GaBr_4^-$ tetrahedron of the same asymmetric unit and a third with a neighbouring $GaBr_4^-$ unit. The coordination geometry around the Se atom could be considered distorted octahedral. The structure may then be regarded as built up of octahedrons and tetrahedrons, where each octahedron shares an edge or a vertex of two neighboring tetrahedrons to form chains parallel to the crystallographic b axis.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.25 × 0.35 × 0.40 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	282.65 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω scan
$2\theta_{max}$:	54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2562, 2562
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1366
$N(param)_{refined}$:	82
Programs:	HELENA[4], PLATON [4], SHELXS-97 [5], SHELXL-97 [6], DIFABS [7]

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ga	2a	0.2836(6)	0.5035(7)	0.8104(3)	0.030(2)	0.028(2)	0.028(2)	0.001(2)	0.008(1)	−0.002(2)
Se	2a	−0.0067(5)	0.9216(6)	0.6460(3)	0.033(2)	0.033(2)	0.030(2)	−0.005(2)	0.007(1)	0.002(2)
Br(1)	2a	0.3150(6)	0.1518(6)	0.8205(3)	0.049(2)	0.032(2)	0.045(3)	0.003(2)	0.003(2)	0.001(2)
Br(2)	2a	0.5014(5)	0.6520(6)	0.9388(3)	0.033(2)	0.043(2)	0.035(2)	0.006(2)	0.001(2)	−0.002(2)
Br(3)	2a	0.3708(5)	0.6147(7)	0.6689(3)	0.037(2)	0.050(3)	0.035(2)	−0.001(2)	0.018(2)	0.005(2)
Br(4)	2a	−0.0523(5)	0.6085(6)	0.8120(3)	0.030(2)	0.042(2)	0.042(2)	0.003(2)	0.014(2)	0.005(2)
Br(5)	2a	0.1995(5)	0.6984(7)	0.5392(3)	0.040(2)	0.044(2)	0.037(3)	0.007(2)	0.001(2)	0.008(2)
Br(6)	2a	0.2689(6)	1.1212(8)	0.6804(4)	0.041(2)	0.063(3)	0.071(4)	0.016(2)	0.000(2)	0.015(3)
Br(7)	2a	0.1269(8)	1.1242(8)	0.5417(4)	0.086(3)	0.052(3)	0.045(3)	0.019(2)	0.018(2)	0.008(2)

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