Crystal structure of sodium trigallium pentaselenide, NaGa₃Se₅

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Received February 13, 1997, transferred to 1st update of database ICSD in 1998, CSD-No. 402880

Source of material: Single crystals of the new nonmetallic filled-up β -Mn phase NaGa₃Se₅ could be prepared by direct reaction of stoichiometric mixtures of the elements at 1030 K.

Compared to all known chalcogenides with this structure type (for example Ag₂Ga₆Te₁₀, SnGa₆Te₁₀, Ga₇Te₁₀ see refs. 1–3), the Ga³⁺ are ordered in a hitherto unknown way. The ordering is characterized by a framework of corner-, edge- and face-sharing GaSe₄-tetrahedra, which compared to NaGa₃Te₅ (see ref. 4) is much more complex. This is indicated by the lower symmetry of this space group and by the increased unit cell volume.

Ga₆Na₂Se₁₀, orthorhombic, $P2_12_12_1$ (No. 19), $a=9.730(2)$ Å, $b=26.939(5)$ Å, $c=13.597(3)$ Å, $V=3564.0$ Å³, $Z=8$, $R(F)=0.036$, $R_w(F^2)=0.084$.

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

Crystal:	red, fragment of a needle, size 0.05 x 0.06 x 0.09 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	293.90 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	4923
Criterion for I_0 :	$I_0 > 2 \sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	361
Programs:	SHELXL-93, NRCVAX

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}
Se(1)	4a	0.8167(2)	0.43840(6)	0.5610(1)	0.020(1)	0.012(1)	0.0192(9)	0.0016(8)	-0.0001(7)	-0.0002(6)
Se(2)	4a	0.4225(2)	0.41967(6)	0.4565(1)	0.018(1)	0.015(1)	0.029(1)	0.0010(8)	0.0003(7)	-0.0023(7)
Se(3)	4a	0.3205(2)	0.51971(7)	0.1492(1)	0.020(1)	0.020(1)	0.0217(9)	0.0022(9)	-0.0001(7)	-0.0005(7)
Se(4)	4a	0.4857(2)	0.40138(7)	0.7507(1)	0.026(1)	0.016(1)	0.0196(9)	0.0019(9)	0.0028(7)	0.0019(7)
Se(5)	4a	0.5541(2)	0.42089(6)	0.0262(1)	0.025(1)	0.018(1)	0.0213(9)	-0.0035(9)	-0.0010(7)	0.0008(7)
Se(6)	4a	0.6883(2)	0.51556(7)	0.3500(1)	0.025(1)	0.023(1)	0.0233(9)	-0.0012(9)	-0.0020(7)	0.0025(7)
Se(7)	4a	0.1665(2)	0.43795(6)	-0.0825(1)	0.019(1)	0.013(1)	0.0182(9)	-0.0006(8)	0.0008(7)	0.0001(7)
Se(8)	4a	-0.0657(2)	0.33284(6)	0.0345(1)	0.022(1)	0.016(1)	0.0201(9)	-0.0032(8)	0.0017(7)	-0.0021(7)
Se(9)	4a	-0.0112(2)	0.34722(7)	0.7521(1)	0.022(1)	0.016(1)	0.0179(9)	-0.0022(8)	-0.0012(7)	0.0011(7)
Se(10)	4a	0.1842(2)	0.23372(6)	0.1655(1)	0.020(1)	0.012(1)	0.0206(9)	-0.0019(8)	-0.0029(7)	0.0025(7)
Se(11)	4a	0.2473(2)	0.37588(7)	0.1877(1)	0.023(1)	0.016(1)	0.023(1)	0.0047(9)	-0.0015(7)	-0.0029(7)
Se(12)	4a	0.0802(2)	0.46107(6)	0.3633(1)	0.019(1)	0.016(1)	0.0173(9)	-0.0018(9)	-0.0017(7)	0.0000(6)
Se(13)	4a	-0.0695(2)	0.46764(6)	0.1302(1)	0.020(1)	0.015(1)	0.0207(9)	-0.0008(9)	-0.0003(7)	-0.0006(6)
Se(14)	4a	0.7487(2)	0.37379(6)	0.3004(1)	0.025(1)	0.014(1)	0.0212(9)	-0.0019(9)	-0.0029(7)	0.0018(7)
Se(15)	4a	-0.2111(2)	0.23525(7)	0.3468(1)	0.019(1)	0.014(1)	0.024(1)	0.0028(8)	0.0012(7)	0.0022(7)
Se(16)	4a	0.0674(2)	0.33568(6)	0.4575(1)	0.020(1)	0.015(1)	0.0255(9)	0.0002(8)	-0.0014(7)	0.0026(7)
Se(17)	4a	0.6722(2)	0.31506(6)	0.5751(1)	0.018(1)	0.016(1)	0.0191(9)	-0.0009(8)	-0.0004(7)	-0.0003(7)
Se(18)	4a	0.4322(2)	0.28739(6)	0.3810(1)	0.018(1)	0.013(1)	0.0179(9)	0.0001(8)	-0.0002(7)	-0.0016(6)
Se(19)	4a	0.3142(2)	0.30803(6)	-0.0747(1)	0.017(1)	0.014(1)	0.0177(9)	-0.0006(8)	-0.0005(7)	-0.0002(6)
Se(20)	4a	0.5645(2)	0.28636(6)	0.1089(1)	0.017(1)	0.011(1)	0.0160(9)	-0.0005(8)	-0.0009(6)	-0.0006(6)
Ga(1)	4a	0.6040(2)	0.47402(7)	0.4932(1)	0.018(1)	0.018(1)	0.022(1)	-0.0003(9)	0.0008(7)	-0.0009(8)
Ga(2)	4a	0.2558(2)	0.48281(7)	0.4827(1)	0.020(1)	0.016(1)	0.019(1)	0.0006(9)	-0.0009(7)	0.0003(7)
Ga(3)	4a	0.0972(2)	0.51707(7)	0.2210(1)	0.021(1)	0.017(1)	0.017(1)	-0.001(1)	0.0012(7)	-0.0015(7)
Ga(4)	4a	0.3857(2)	0.39471(7)	-0.0899(1)	0.020(1)	0.016(1)	0.021(1)	-0.0015(9)	0.0006(8)	0.0003(8)
Ga(5)	4a	0.6073(2)	0.49699(7)	-0.0571(1)	0.019(1)	0.019(1)	0.022(1)	-0.0016(9)	-0.0005(8)	-0.0001(8)
Ga(6)	4a	0.0796(2)	0.40155(7)	0.0699(1)	0.022(1)	0.015(1)	0.021(1)	0.0000(9)	0.0009(8)	-0.0005(7)
Ga(7)	4a	0.5643(2)	0.19522(7)	0.1032(1)	0.020(1)	0.013(1)	0.017(1)	0.0012(9)	0.0016(8)	-0.0005(7)
Ga(8)	4a	0.3325(2)	0.21550(7)	0.3005(1)	0.018(1)	0.014(1)	0.015(1)	-0.0013(9)	0.0000(7)	0.0005(7)
Ga(9)	4a	0.3146(2)	0.30195(7)	0.1049(1)	0.021(1)	0.013(1)	0.018(1)	0.0019(9)	-0.0004(8)	0.0005(8)
Ga(10)	4a	0.6386(2)	0.29614(7)	0.2775(1)	0.020(1)	0.016(1)	0.016(1)	-0.0002(9)	-0.0020(7)	0.0001(8)
Ga(11)	4a	0.1139(2)	0.25704(7)	0.5282(1)	0.021(1)	0.016(1)	0.018(1)	0.0020(9)	0.0012(8)	-0.0003(8)
Ga(12)	4a	-0.1715(2)	0.36026(7)	0.4659(1)	0.019(1)	0.017(1)	0.019(1)	-0.002(1)	-0.0001(8)	0.0009(7)
Na(1)	4a	0.0023(7)	0.3091(3)	0.2516(5)	0.024(5)	0.040(6)	0.023(4)	0.006(4)	0.006(3)	0.002(3)
Na(2)	4a	0.2579(8)	0.6286(3)	0.1301(5)	0.046(6)	0.016(5)	0.029(4)	-0.005(4)	0.005(3)	0.004(3)
Na(3)	4a	0.5016(8)	0.4400(3)	0.2404(5)	0.045(5)	0.025(5)	0.032(4)	0.008(4)	-0.002(4)	-0.004(3)
Na(4)	4a	0.2535(7)	0.1220(3)	0.1175(5)	0.029(5)	0.022(5)	0.038(5)	-0.006(4)	-0.001(3)	-0.005(3)

Acknowledgment. This work was supported by the Deutsche Forschungsgemeinschaft.

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