Crystal structure of sodium gallium germanium oxide, $NaGaGeO_4$

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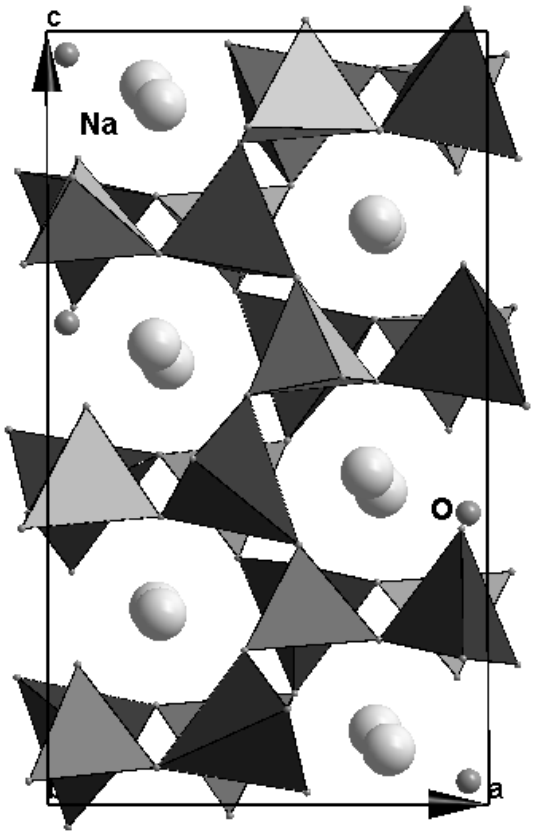
Received March 24, 2010, accepted and available on-line May 12, 2010; CSD no. 710045



Abstract

$GaGeNaO_4$, monoclinic, $P2_1/n$ (no. 14), a = 8.8794(5) Å, b = 8.2679(5) Å, c = 15.5969(9) Å, β = 90.129(5)°, V = 1144.20 Å^3, Z = 12, $R(I)$ = 0.013, $R(P)$ = 0.056, T = 293 K.

Source of material

The $NaGaGeO_4$ sample material was prepared by mixing 10 mmol GeO_2, 5 mmol Ga_2O_3 and 5 mmol Na_2CO_3 in a ball mill for 15 minutes. This mixture was molten in a platinum crucible at 1200 °C for 24 h and subsequently quenched at room temperature. Crystallisation of the resulting glass was achieved by further heat treatment at 800 °C for 48 hours.

Experimental details

In the refinement the displacement parameters of the atoms and the framework atoms were constrained.

Discussion

$NaGaGeO_4$ crystallizes in space group $P12_1/n1$ as reported for the room temperature polytype by Barbier and Fleet [1]. The unit cell parameters obtained here are in good agreement with the values given in [1]. The structure is analogous to beryllonite ($NaBePO_4$) as given in ICSD file (no. 9271) [2], which provided the starting values for the refinement of the atomic coordinates. In the $NaGaGeO_4$ structure, GaO_2 (figure, light grey) and GeO_2 (dark grey) corner-sharing tetrahedra form a three-dimensional network with channel-like openings parallel to [010]. In these channels the sodium cations are regularly distributed.

Table 1. Data collection and handling.

Powder:	colorless, particle size < 63 μm
Wavelength:	Cu $K_{\alpha1}$,$K_{\alpha2}$ radiation (1.540596, 1.544493 Å)
μ:	186.45 cm^{-1}
Diffractometer, scan mode:	Bruker AXS D8 Advance, Debye-Scherrer
$2\theta_{max}$, stepwidth:	117°, 0.02
$N(points)_{measured}$:	5351
$N(hkl)_{measured}$:	1628
$N(parameter)_{refined}$:	80
Programs:	DIAMOND [3] , TOPAS [4]

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

Atom	Site	x	y	z	U_{iso}
Na(1)	4*e*	0.254(3)	–0.009(3)	0.247(3)	0.038(5)
Na(2)	4*e*	0.742(4)	0.434(4)	0.095(3)	0.038
Na(3)	4*e*	0.771(3)	0.022(4)	0.071(2)	0.038
Ge(1)	4*e*	0.920(2)	0.172(1)	0.2353(7)	0.014(2)
Ge(2)	4*e*	0.405(1)	0.172(2)	0.4227(7)	0.014
Ge(3)	4*e*	0.443(2)	0.164(2)	0.0897(7)	0.014
Ga(1)	4*e*	0.585(2)	0.280(1)	0.2661(7)	0.014
Ga(2)	4*e*	0.111(1)	0.273(2)	0.0836(8)	0.014
Ga(3)	4*e*	0.060(1)	0.270(1)	0.4075(8)	0.014
O(1)	4*e*	0.446(5)	0.264(4)	0.199(3)	0.014
O(2)	4*e*	0.066(5)	0.270(5)	0.181(3)	0.014
O(3)	4*e*	0.253(5)	0.255(6)	0.374(3)	0.014
O(4)	4*e*	0.749(5)	0.260(5)	0.215(3)	0.014
O(5)	4*e*	0.954(5)	0.233(5)	0.029(3)	0.014
O(6)	4*e*	0.589(4)	0.265(5)	0.015(3)	0.014
O(7)	4*e*	0.574(5)	0.176(4)	0.337(3)	0.014
O(8)	4*e*	0.250(5)	0.137(5)	0.047(3)	0.014
O(9)	4*e*	0.937(5)	0.151(4)	0.354(3)	0.014
O(10)	4*e*	0.559(4)	0.454(5)	0.312(2)	0.014
O(11)	4*e*	0.177(4)	0.456(6)	0.053(2)	0.014
O(12)	4*e*	–0.046(3)	0.464(5)	0.379(2)	0.014

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References

1. Barbier, J.; Fleet, M. E.: Investigation of structural states in the series $MGaSiO_4$, $MAlGeO_4$, $MGaGeO_4$ (M = Na, K). J. Sol. State. Chem. **71** (1987) 361-370.
2. ICSD: Inorganic Crystal Structure Database; Fachinformationszentrum Karlsruhe and National Institute of Standards and Technology, 2009.
3. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 3.2. Crystal Impact, Bonn, Germany 1998.
4. TOPAS: Version 4.2, Bruker AXS GmbH, Karlsruhe, Germany 1999.