Crystal structure of sodium strontium monogermanide, $Na_xSr_{1-x}Ge$ (x = 0.14)

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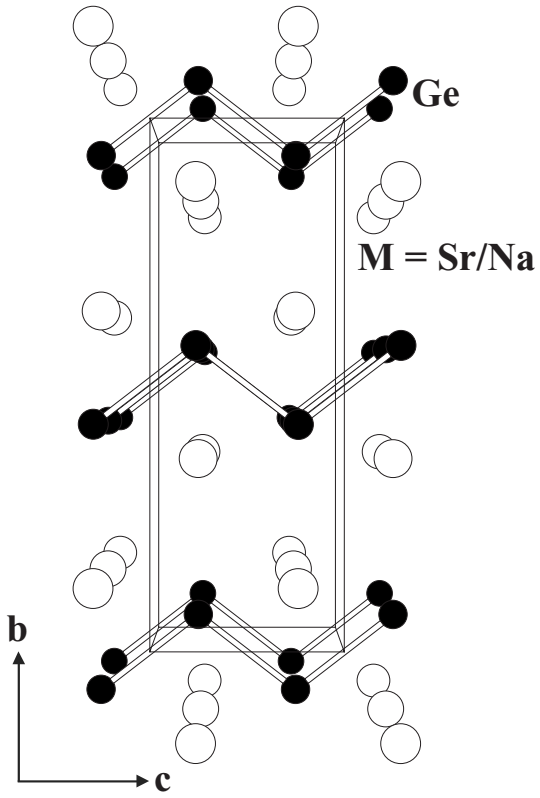
Received June 10, 2003, accepted and available on-line July 28, 2003; CSD-No. 409712



Abstract

$GeNa_{0.14}Sr_{0.86}$, orthorhombic, *Cmcm* (No. 63), a = 4.828(1) Å, b = 11.309(3) Å, c = 4.124(1) Å, V = 225.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.049, $wR_{ref}(F^2)$ = 0.115, T = 293 K.

Source of material

$Na_{0.14}Sr_{0.86}Ge$ was synthesized from a mixture of pure elements at stoichiometric amounts via direct heating in argon atmosphere up to 1173 K for 50 h. After cooling down with a rate of 25 K/h, the product was obtained as black layered crystals with metallic lustre.

Discussion

$Na_{0.14}Sr_{0.86}Ge$ crystallizes with the α-TlI structure type (also known as CrB type) similar to other MGe (M = Ca, Sr, Ba) compounds [1-3]. The Zintl anion is a one-dimensional planar chain in *all-trans* conformation (d(Ge—Ge) = 2.602(3) Å; ∠Ge–Ge–Ge = 104.8(1)°). $Na_{0.14}Sr_{0.86}Ge$ can be formulated as $(Na^+)_{0.14}(Sr^{2+})_{0.86}(Ge^{1.86-})$ according to the Zintl-Klemm concept [4-6]. Unlike MGe compounds, every germanium atom has a formal charge of q = –1.86 which is reasonable in the case of a polyethylene-like chain [7]. SrGe is also a suitable case in investigating charge acquisition tendency of planar chain anions by doping mono-valent alkaline cations. The exchange of Sr for Na withdraws electrons from the bond system leading to significant changes in bond distances, angles and lattice parameters of the unit cell.

Table 1. Data collection and handling.

Crystal:	black plate, size 0.14 × 0.16 × 0.28 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	333.05 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω
$2\theta_{max}$:	52.5°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1112, 147
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 116
$N(param)_{refined}$:	10
Programs:	SHELXS-97 [8], SHELXL-97 [9], ATOMS [10]

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}
Sr/Na(1) [a]	4c	0	0.1378(2)	1/4	0.020(1)	0.023(1)	0.015(1)	0	0	0
Ge(1)	4c	0	0.4298(2)	1/4	0.021(1)	0.023(1)	0.013(1)	0	0	0

a: Sr/Na(1) = 0.86(1)Sr + 0.14Na

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Acknowledgment. This work was supported by the Swiss National Foundation.

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