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Crystal structure of tetrasodium monopotassium triarsenidogermanate, Na_4KGeAs_3

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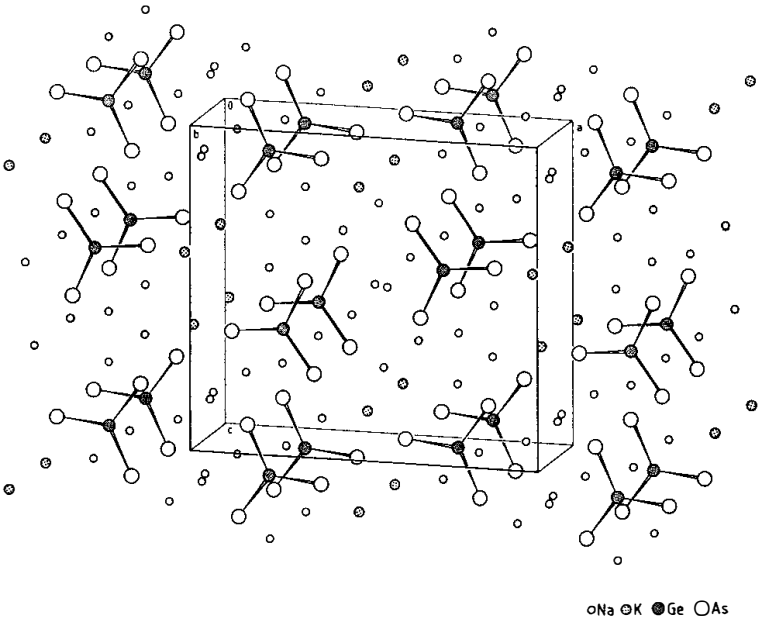

Source of material: $Na_4K[GeAs_3]$ was prepared from stoichiometric amounts of the elements in graphitized evacuated quartz glass ampoules at 973 K.

The crystal structure of $Na_4K[SiAs_3]$ is not strictly isotypic but strongly related to the $Cs_5[SiP_3]$-type (see ref. 1). The anionic sublattice is characterized by isolated $[GeAs_3]^{5-}$ anions isosteric to $[CO_3]^{2-}$ with bond lengths d(Ge-As) = 2.330–2.350 Å and bond angles As-Ge-As = 117.8–122.5°.

Orthorhombic, Pnma (no 62), $a = 15.161(4)$, $b = 4.813(2)$, $c = 13.168(4)$ Å, $V = 960.9$ Å^3, $Z = 4$, $R = 0.055$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	1554
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_O < 2.5\sigma(I_O)$
Crystal characteristics:	black metallic prism	Number of refined parameters:	55
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	147.11 cm^{-1}
$2\theta_{max}$:	60°	Structure solution program used:	SHELX

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	x	y	z	U_{iso}/U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	0.5626(4)	0.25	0.4276(5)	0.020(3)	0.026(3)	0.034(3)	0.0	0.001(3)	0.0
Na(2)	0.0815(4)	0.25	0.8111(5)	0.026(3)	0.018(3)	0.021(3)	0.0	−0.006(2)	0.0
Na(3)	0.2555(5)	0.25	0.2370(5)	0.035(4)	0.028(3)	0.033(3)	0.0	−0.016(3)	0.0
Na(4)	0.2888(4)	0.25	0.9393(5)	0.034(3)	0.023(3)	0.024(3)	0.0	0.007(3)	0.0
K(1)	0.5160(2)	0.25	0.1288(3)	0.026(2)	0.019(2)	0.028(2)	0.0	−0.001(1)	0.0
Ge(1)	0.2941(1)	0.25	0.5845(1)	0.0142(6)	0.0074(6)	0.0144(6)	0.0	0.0001(5)	0.0
As(1)	0.1405(1)	0.25	0.5923(1)	0.0138(6)	0.0288(8)	0.0203(7)	0.0	0.0014(5)	0.0
As(2)	0.3649(1)	0.25	0.4258(1)	0.0182(6)	0.0171(6)	0.0139(6)	0.0	0.0018(5)	0.0
As(3)	0.3828(1)	0.25	0.7305(1)	0.0171(6)	0.0169(6)	0.0164(6)	0.0	−0.0026(5)	0.0

Further details of the structure determination (e.g. structure factors) have been deposited within the relevant database and can be accessed as Collection No. 300204 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

References:

1. Eisenmann, B., Klein, J., Somer, M.: CO_3^{2-}-isostere Anionen in Cs_5SiP_3, Cs_5SiAs_3, Cs_5GeP_3 und Cs_5GeAs_3. Angew. Chem. **102** (1990) 92–93.