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Crystal structure of decasodium di-μ-arsenido-bis(diarsenidogermanate), $Na_{10}Ge_2As_6$

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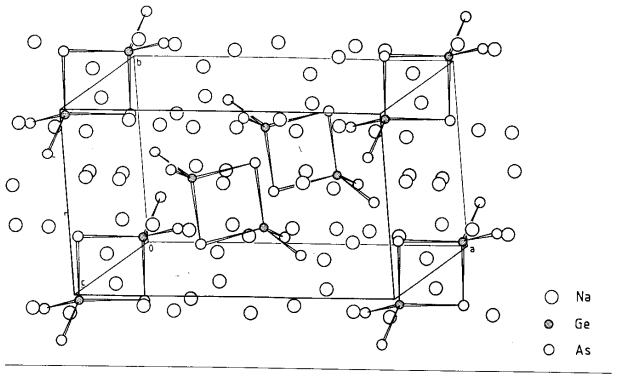

Source of material: $Na_{10}[Ge_2As_6]$ was prepared from stoichiometric mixtures of the elements in evacuated iron ampoules at 973 K.
$Na_{10}[Ge_2As_6]$ belongs to the $Na_{10}[Si_2P_6]$-type compounds (see refs. 1, 2, 3). In the anionic part of the structure two $GeAs_4$ – tetrahedra are connected by a common edge forming isolated dimers $[Ge_2As_6]^{10-}$ (mean bond lengths: $d(Ge\text{-}As)_{endo} = 2.510$ Å, $d(Ge\text{-}As)_{exo} = 2.442$ Å; bond angle Ge-As-Ge = 85.1°).

Monoclinic, $P12_1/n1$ (no 14), $a = 13.531(5)$, $b = 7.544(4)$, $c = 8.298(5)$ Å, $\beta = 90.2(1)°$, $V = 847.0$ Å^3, $Z = 2$, $R = 0.070$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	2468
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_O < 2\sigma(I_O)$
Crystal characteristics:	dark red plate	Number of refined parameters:	83
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	162.62 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}
Ge(1)	0.0863(1)	0.1427(2)	0.4281(1)	0.0076(5)	0.0073(5)	0.0071(5)	0.0003(4)	−0.0011(4)	−0.0003(4)
As(1)	0.2283(1)	0.2385(2)	0.5863(1)	0.0097(5)	0.0131(6)	0.0114(5)	−0.0014(4)	−0.0029(4)	−0.0010(4)
As(2)	0.0808(1)	0.2631(2)	0.1540(1)	0.0116(5)	0.0135(6)	0.0082(5)	−0.0003(4)	−0.0007(4)	0.0025(4)
As(3)	0.9322(1)	0.1892(2)	0.5882(1)	0.0102(5)	0.0091(5)	0.0112(5)	0.0001(4)	0.0009(4)	−0.0003(4)
Na(1)	0.7410(4)	0.1480(8)	0.4254(7)	0.017(2)	0.025(3)	0.018(3)	0.002(2)	−0.001(2)	−0.000(2)
Na(2)	0.4186(4)	0.1645(8)	0.4222(7)	0.017(2)	0.027(3)	0.018(3)	−0.002(2)	−0.000(2)	−0.001(2)
Na(3)	0.0880(5)	0.0155(9)	0.8264(8)	0.026(3)	0.024(3)	0.030(3)	−0.003(2)	0.001(2)	0.001(3)
Na(4)	0.0847(5)	0.531(1)	0.6702(8)	0.036(4)	0.031(4)	0.033(3)	0.016(3)	0.012(3)	0.012(3)
Na(5)	0.2586(5)	0.9954(9)	0.1807(7)	0.030(3)	0.026(3)	0.024(3)	0.009(3)	−0.005(2)	−0.002(3)

Further details of the structure determination (e.g. structure factors) have been deposited within the relevant database and can be accessed as Collection No. 300187 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

References:

1. Eisenmann, B., Somer, M.: Zur Kenntnis von Oligophosphidosilikaten(IV) und -germanaten(IV): $Na_{10}Si_2P_6$ und $Na_{10}Ge_2P_6$. Z. Naturforsch. **40b** (1985) 886–890.
2. Eisenmann, B., Klein, J., Hofmann, A.: Arsenido- und Antimonidostannate der Alkali- und Erdalkalimetalle. Z. Kristallogr. **182** (1988) 78–79.
3. Eisenmann, B., Klein, J.: Dimere Zintl-Anionen $[Sn_2As_6]^{10-}$ und $[Sn_2Sb_6]^{10-}$ in Alkaliverbindungen. Z. Kristallogr. **196** (1991) 213–229.