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Crystal structure of decasodium di-μ-arsenido-bis(diarsenidosilicate), $Na_{10}Si_2As_6$

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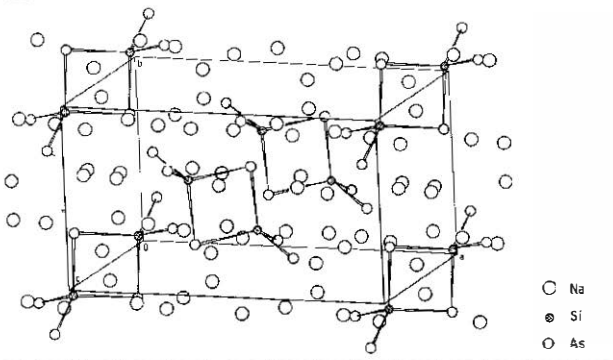

Source of material: $Na_{10}[Si_2As_6]$ was prepared from stoichiometric mixtures of the elements in evacuated iron ampoules at 973 K.
$Na_{10}[Si_2As_6]$ belongs to the $Na_{10}[Si_2P_6]$-type compounds (see refs. 1, 2, 3). In the anionic part of the structure two $SiAs_4$ – tetrahedra are connected by a common edge forming isolated dimers $[Si_2As_6]^{10-}$ (mean bond lengths: $d(Si\text{-}As)_{endo} = 2.435$ Å, $d(Si\text{-}As)_{exo} = 2.364$ Å; bond angle Si-As-Si = 85.8°).

Monoclinic, $P12_1/n1$ (no 14), $a = 13.466(5)$, $b = 7.529(4)$, $c = 8.177(5)$ Å, $\beta = 90.5(1)°$, $V = 829.0$ Å^3, $Z = 2$, $R = 0.086$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	2426
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_o < 2.5\sigma(I_o)$
Crystal characteristics:	red plate	Number of refined parameters:	83
Temperature of measurement:	293 K	Scan mode:	$\omega/2\theta$-scan
$2\theta_{max}$:	60°	μ:	129.84 cm^{-1}
		Structure solution program used:	SHELX

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

Atom	x	y	z	U_{eq}/U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si(1)	0.0840(2)	0.1399(5)	0.4280(4)	0.004(1)	0.006(1)	0.003(1)	−0.001(1)	−0.000(1)	−0.000(1)
As(1)	0.2236(1)	0.2335(2)	0.5797(2)	0.0074(6)	0.0091(6)	0.0080(6)	−0.0008(5)	−0.0027(4)	−0.0009(5)
As(2)	0.0796(1)	0.2500(2)	0.1596(2)	0.0090(6)	0.0092(6)	0.0048(5)	−0.0002(5)	−0.0005(4)	0.0029(4)
As(3)	0.9338(1)	0.1824(2)	0.5855(2)	0.0072(6)	0.0044(5)	0.0077(6)	0.0008(4)	0.0019(4)	−0.0005(4)
Na(1)	0.7406(5)	0.1514(9)	0.4242(7)	0.018(3)	0.020(3)	0.013(3)	0.001(2)	−0.001(2)	−0.001(2)
Na(2)	0.4189(5)	0.1646(9)	0.4214(8)	0.016(3)	0.023(3)	0.016(3)	−0.002(3)	0.002(2)	0.002(3)
Na(3)	0.0881(5)	0.015(1)	0.8253(8)	0.026(3)	0.021(3)	0.021(3)	0.004(3)	−0.000(3)	0.002(3)
Na(4)	0.0811(6)	0.531(1)	0.6652(9)	0.013(5)	0.026(4)	0.026(4)	0.014(3)	0.016(3)	0.009(3)
Na(5)	0.2584(6)	0.994(1)	0.1860(8)	0.032(4)	0.023(3)	0.017(3)	0.009(3)	−0.003(3)	−0.005(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. 300188 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.