Zeitschrift für Kristallographie 197, 275–276 (1991)
 – 0044-2968/91 $3.00+0.00

Crystal structure of trisodium dipotassium triphosphidosilicate, $Na_3K_2SiP_3$

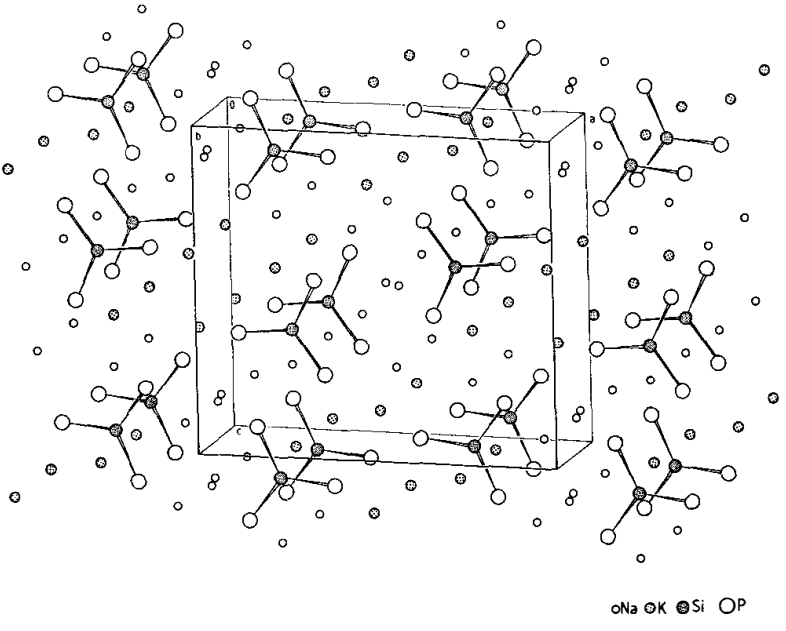
B. Eisenmann and J. Klein

Eduard-Zintl-Institut der Technischen Hochschule, Hochschulstr. 10, D-6100 Darmstadt

and M. Somer

Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-7000 Stuttgart 80

(Received March 26, 1991, transferred to database ICSD July 1, 1991)



Source of material: $Na_3K_2[SiP_3]$ was prepared from stoichiometric mixtures of Na_3P and $K_2[SiP_2]$ in evacuated tantalum ampoules at 973 K.
The crystal structure of $Na_3K_2[SiP_3]$ is not strictly isotypic but strongly related to the $Cs_5[SiP_3]$-type (see ref. 1). The anionic sublattice is characterized by isolated $[SiP_3]^{5-}$ anions isosteric to $[CO_3]^{2-}$ with bond lengths d(Si-P) = 2.171–2.182 Å and bond angles P-Si-P = 118.2– 121.1°.

Orthorhombic, Pnma (no 62), $a = 14.580(4)$, $b = 4.750(2)$, $c = 13.020(4)$ Å, $V = 901.7$ Å^3, $Z = 4$, $R = 0.084$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	1473
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_\bullet < 3.5\sigma(I_\bullet)$
Crystal characteristics:	black metallic prism	Number of refined parameters:	55
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	16.98 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)	0.5595(3)	0.25	0.4286(4)	0.020(2)	0.021(2)	0.031(3)	0.0	0.002(2)	0.0
Na(2)	0.0842(4)	0.25	0.8160(4)	0.033(3)	0.020(2)	0.021(2)	0.0	−0.002(2)	0.0
Na(3)	0.2570(3)	0.25	0.2352(4)	0.026(2)	0.025(2)	0.022(2)	0.0	−0.008(2)	0.0
K(1)	0.2984(2)	0.25	0.9401(2)	0.043(2)	0.028(1)	0.027(1)	0.0	0.002(1)	0.0
K(2)	0.5132(2)	0.25	0.1341(2)	0.024(1)	0.025(1)	0.034(1)	0.0	−0.004(1)	0.0
Si(1)	0.2958(2)	0.25	0.5843(2)	0.011(1)	0.010(1)	0.014(1)	0.0	−0.001(1)	0.0
P(1)	0.1475(2)	0.25	0.6008(2)	0.012(1)	0.027(2)	0.022(1)	0.0	0.004(1)	0.0
P(2)	0.3594(2)	0.25	0.4326(2)	0.018(1)	0.020(1)	0.014(1)	0.0	0.004(1)	0.0
P(3)	0.3848(2)	0.25	0.7180(2)	0.018(1)	0.023(2)	0.019(1)	0.0	−0.007(1)	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. 300203 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.