Zeitschrift für Kristallographie 197, 273–274 (1991)
 – 0044-2968/91 $3.00+0.00

Crystal structure of pentarubidium triarsenidosilicate, Rb_5SiAs_3

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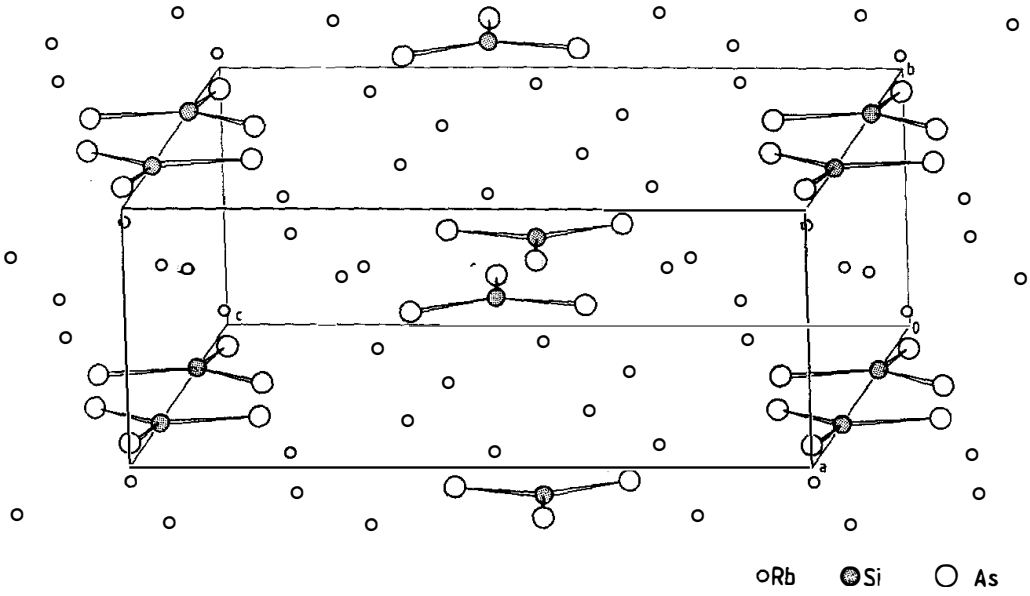
(Received April 12, 1991, transferred to database ICSD July 1, 1991)



Source of material: $Rb_5[SiAs_3]$ was prepared from mixtures of the elements in the ratio Rb:Si:As = 7:1:3 in evacuated tantalum ampoules at 973 K. The excess Rb was removed by distillation in a high vaccum.
$Rb_5[SiAs_3]$ crystallizes in the $Cs_5[SiP_3]$-type (see ref. 1). The anionic sublattice is characterized by isolated $[SiAs_3]^{5-}$ anions isostructural to $[CO_3]^{2-}$, with bond lengths d(Si-As) = 2.265 – 2.316 Å and bond angles As-Si-As = 117.4 – 122.0°.

Orthorhombic, Pnma (no 62), $a = 14.169(4)$, $b = 5.671(2)$, $c = 15.479(4)$ Å, $V = 1243.8$ 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:	1227
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_O < 3\sigma(I_O)$
Crystal characteristics:	black metallic prism	Number of refined parameters:	55
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	289.95 cm^{-1}
$2\theta_{max}$:	50°	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}
Rb(1)	0.5673(2)	0.25	0.4448(2)	0.023(2)	0.022(2)	0.030(2)	0.0	−0.004(1)	0.0
Rb(2)	0.6156(3)	0.25	0.6822(2)	0.034(2)	0.021(2)	0.024(2)	0.0	0.004(2)	0.0
Rb(3)	0.8538(2)	0.25	0.5449(2)	0.026(2)	0.026(2)	0.031(2)	0.0	−0.005(2)	0.0
Rb(4)	0.2811(2)	0.25	0.2126(2)	0.030(2)	0.018(2)	0.019(2)	0.0	−0.005(1)	0.0
Rb(5)	0.0558(3)	0.25	0.3493(3)	0.032(2)	0.034(2)	0.042(2)	0.0	−0.002(2)	0.0
Si(1)	0.2599(6)	0.25	0.5749(5)	0.016(4)	0.003(4)	0.013(4)	0.0	−0.002(3)	0.0
As(1)	0.1016(2)	0.25	0.5951(2)	0.010(2)	0.021(2)	0.020(2)	0.0	0.001(1)	0.0
As(2)	0.3137(2)	0.25	0.4354(2)	0.018(2)	0.021(2)	0.013(2)	0.0	0.001(1)	0.0
As(3)	0.3649(2)	0.25	0.6895(2)	0.020(2)	0.018(2)	0.020(2)	0.0	−0.010(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. 300191 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.