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Crystal structure of pentarubidium triphosphidogermanate, Rb_5GeP_3

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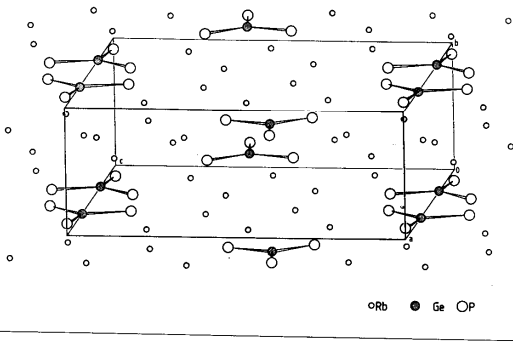

Source of material: $Rb_5[GeP_3]$ was prepared from mixtures of the elements in the ratio Rb:Ge:P = 7:1:3 in evacuated tantalum ampoules at 973 K. The excess of Rb was removed by distillation in a high vacuum. $Rb_5[GeP_3]$ crystallizes in the $Cs_5[SiP_3]$-type (see ref. 1). The anionic sublattice is characterized by isolated $[GeP_3]^{5-}$ anions isostructural to $[CO_3]^{2-}$ with bond lengths d(Ge-P) = 2.240–2.281 Å and bond angles P-Ge-P = 117.3–121.3°.

Orthorhombic, Pnma (no 62), $a = 13.966(4)$, $b = 5.582(2)$, $c = 15.256(4)$ Å, $V = 1189.3$ Å^3, $Z = 4$, $R = 0.058$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	1175
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:	244.84 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)	0.5653(2)	0.25	0.4451(2)	0.015(1)	0.023(1)	0.028(1)	0.0	−0.001(1)	0.0
Rb(2)	0.6152(2)	0.25	0.6829(2)	0.035(1)	0.021(1)	0.015(1)	0.0	0.002(1)	0.0
Rb(3)	0.8546(2)	0.25	0.5461(2)	0.027(1)	0.025(2)	0.029(1)	0.0	−0.008(1)	0.0
Rb(4)	0.2783(2)	0.25	0.2138(2)	0.031(1)	0.019(1)	0.015(1)	0.0	−0.003(1)	0.0
Rb(5)	0.0512(2)	0.25	0.3499(2)	0.026(1)	0.033(2)	0.054(2)	0.0	−0.006(1)	0.0
Ge(1)	0.2621(2)	0.25	0.5733(1)	0.006(1)	0.011(1)	0.008(1)	0.0	0.0008(9)	0.0
P(1)	0.1035(4)	0.25	0.5950(4)	0.011(3)	0.018(3)	0.018(3)	0.0	0.001(3)	0.0
P(2)	0.3141(5)	0.25	0.4334(4)	0.026(4)	0.020(4)	0.012(3)	0.0	0.002(3)	0.0
P(3)	0.3669(4)	0.25	0.6880(4)	0.012(3)	0.032(4)	0.018(3)	0.0	−0.006(3)	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. 300186 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.