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Crystal structure of dipotassium catena-phosphidoaurate(I), K_2AuP

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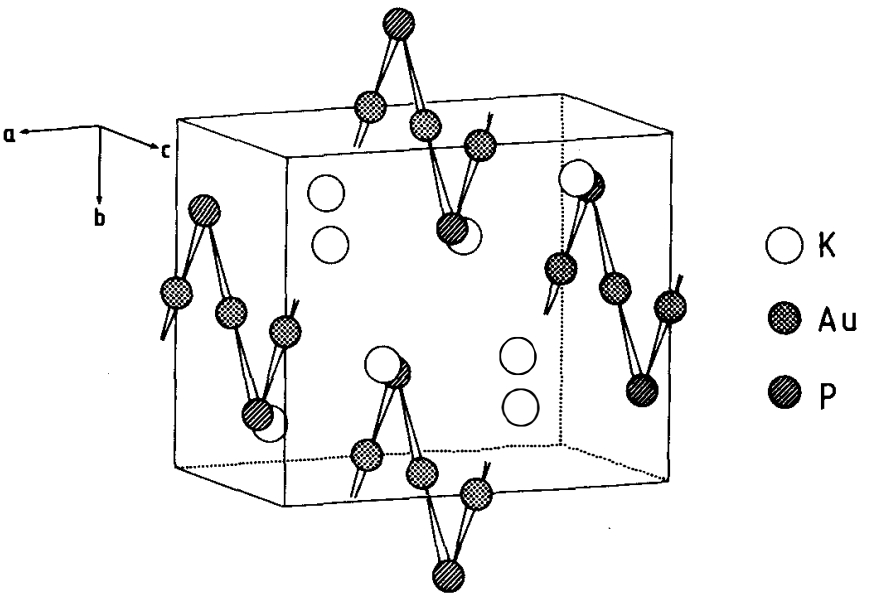

Source of material: $K_2[AuP]$ was prepared from stoichiometric mixtures of the elements in a sealed steel ampoule at 925 K.
$K_2[AuP]$ crystallizes in the $Na_2[CuAs]$ – type (see refs. 1–4). In the infinite planar Au-P zigzag chains, two collinear bonds are formed by Au (d(Au-P) = 2.395 Å, angle Au-P-Au = 80.1°).

Orthorhombic, Cmcm (no 63), $a = 9.787(4)$, $b = 7.395(3)$, $c = 6.168(2)$ Å, $V = 446.4$ Å^3, $Z = 4$, $R = 0.030$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	378
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_O < 2.5\sigma(I_\bullet)$
Crystal characteristics:	black prism	Number of refined parameters:	15
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	358.75 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}
Au(1)	0.0	0.5	0.0	0.0120(3)	0.0118(3)	0.0115(3)	0.0	0.0	−0.0005(2
P(1)	0.0	0.2521(6)	0.25	0.008(2)	0.011(2)	0.010(2)	0.0	0.0	0.0
K(1)	0.3279(3)	0.3549(4)	0.25	0.016(1)	0.018(1)	0.028(1)	−0.001(1)	0.0	0.0

Further details of the structure determination (e.g. structure factors) have been deposited with the relevant database and can be accessed as Collection No. 300201 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

References:

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