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Crystal structure of tetrapotassium diarsenidocadmate, K_4CdAs_2

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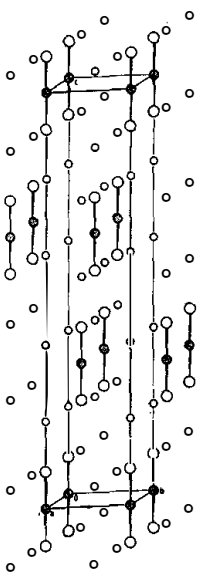

Source of material: $K_4[CdAs_2]$ was prepared from stoichiometric mixtures of the elements with a slight excess of potassium in evacuated iron ampoules at 973 K, the excess K was removed by distillation.
$K_4[CdAs_2]$ crystallizes in the $Na_4[HgP_2]$-type (see ref. 1). Linear units $[As\text{-}Cd\text{-}As]^{4-}$ with bond lengths d(Cd-As) = 2.473 Å, which are isosteric to the molecule $HgCl_2$, represent the characteristic structural elements.

Trigonal, $R\bar{3}m$ (no 166), $a = 5.797(2)$, $c = 27.724(6)$ Å, $V = 806.9$ Å^3, $Z = 3$, $R = 0.028$.

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

Diffractometer type:	Philips PW1100	Number of unique reflections:	338
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_O < 2.5\sigma(I_O)$
Crystal characteristics:	black plate	Number of refined parameters:	12
Temperature of measurement:	293 K	Scan mode:	$\Theta/2\Theta$-scan
		μ:	98.84 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}
K(1)	0.0	0.0	0.2086(1)	0.0321(7)	0.0321(7)	0.030(1)	0.0160(4)	0.0	0.0
K(2)	0.0	0.0	0.3917(1)	0.0254(7)	0.0254(7)	0.072(2)	0.0127(4)	0.0	0.0
Cd(1)	0.0	0.0	0.0	0.0245(3)	0.0245(3)	0.0201(4)	0.0123(2)	0.0	0.0
As(1)	0.0	0.0	0.0892(1)	0.0238(3)	0.0238(3)	0.0218(5)	0.0119(2)	0.0	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. 300190 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

References:

1. Eisenmann, B., Somer, M.: Intermetallische Verbindungen mit $HgCl_2$-isosteren Anionen: Strukturelle und schwingungsspektroskopische Untersuchung von Na_4HgP_2, K_4ZnP_2, K_4CdP_2 und K_4HgP_2. Z. Naturforsch. **44b** (1989) 1228–1232.