Crystal structure of tetrapotassium diarsenidomercurate(II), $K_4[HgAs_2]$

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As_2HgK_4 , trigonal, $R\bar{3}m$ (No. 166), $a = 5.763(1)$ Å, $c = 27.696(2)$ Å, $V = 796.6$ Å³, $Z = 3$, $R(F) = 0.040$, $R_w(F^2) = 0.099$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K(1)	6c	0	0	0.2083(1)	0.027(1)	U_{11}	0.033(2)	$U_{11}/2$	0	0
K(2)	6c	0	0	0.3879(2)	0.022(1)	U_{11}	0.062(2)	$U_{11}/2$	0	0
Hg	3a	0	0	0	0.0169(3)	U_{11}	0.0243(4)	$U_{11}/2$	0	0
As	6c	0	0	0.08893(5)	0.0192(5)	U_{11}	0.0244(7)	$U_{11}/2$	0	0

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Source of material: $K_4[HgAs_2]$ was synthesized from stoichiometric amounts of the elements in sealed niobium ampoules. The samples were heated to 950 K within 4 h and cooled to room temperature for 40 h. An excess of potassium (10-20 at%) was used to improve the crystallization and removed by vacuum distillation.

$K_4[HgAs_2]$ crystallizes in the $Na_4[HgP_2]$ structure type (see ref. 1) containing isolated linear $[As-Hg-As]^{4-}$ anions which are isosteric to the $HgCl_2$ molecule. The bond length $d(Hg-As) = 2.463$ Å is in good agreement with the sum of covalent radii for single bonds (see refs. 2, 3). The anion belongs to the isoelectronic series $HgCl_2$, $[CuBr_2]^-$, $[HgO_2]^{2-}$, $[AgO_2]^{3-}$, $[HgP_2]^{4-}$, $[CuSb_2]^{5-}$ (see refs. 4, 5, 6).

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

Crystal:	black prism, size 0.1 x 0.1 x 0.3 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	221.59 cm ⁻¹
Diffractometer:	Philips PW1100
Scan mode:	$\theta/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{unique}}$:	329
Criterion for I_0 :	$I_0 > 2 \sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	12
Program:	SHELXL-93