

Inorganic Chemistry

including bioinorganic chemistry

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Table S1. Some Data Collection and Refinement Parameters for $\text{Rb}_5\text{TaAs}_4\text{Te}_2$

Formula wt	1316.71
Crystal system	Orthorhombic
Space group, Z	<i>Pnma</i> (No.62), 4
Lattice constants ($\text{\AA}$) ^a	$a = 19.200(5)$ $b = 11.123(5)$ $c = 7.824(4)$
Volume ($\text{\AA}^3$)	1683(2)
Crystal habit, dimensions	plate-like, $0.3 \times 0.2 \times 0.03 \text{ mm}$
Temperature ($^\circ\text{C}$)	23
d_c (g/cm^3)	5.195
μ , cm^{-1} (Mo $K\alpha$)	474.36
Octants meas.	$\pm h, k, \ell$
Total refl. meas	3237
unique	1778
observed ($I > 3\sigma_I$)	635
R_{ave} ($I > 0$), %	18
Rel. trans. coeff. range	0.19–1.00
Variables	65
R/R_w ^b (%)	4.4/4.9
Largest residual peaks ^c	2.33, -2.13 $\text{e/\AA}^3$
GOF	1.74
Second extinction (10^{-7})	0.43(9)

^a Guinier powder pattern data, $\lambda = 1.540\,562\, \text{\AA}$, 23°C .

^b $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; $R_w = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w(F_o)^2]^{1/2}$; $w = \sigma_F^{-2}$.

^c At 0.2344, 1/4, 0.5122 and 0.1660, 1/4, 0.7430, respectively.

Table S2 Anisotropic Thermal Factors for $\text{Rb}_5\text{TaAs}_4\text{Tl}_2$

Atoms	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tl1	0.026(1)	0.028(2)	0.030(2)	0	0.008(1)	0
Tl2	0.029(2)	0.031(2)	0.024(1)	0	0.005(1)	0
Ta1	0.019(2)	0.015(2)	0.017(1)	0	0.002	0
As1	0.030(3)	0.019(3)	0.029(3)	-0.006(2)	0.006(3)	0.001(3)
As2	0.033(5)	0.029(5)	0.015(4)	0	0.004(3)	0
As3	0.024(3)	0.016(4)	0.021(3)	0	-0.005(3)	0
Rb1	0.040(3)	0.030(3)	0.018(2)	0.001(2)	0.000(2)	0.001(3)
Rb2	0.039(4)	0.064(6)	0.049(5)	0	-0.006(4)	0
Rb3	0.027(3)	0.039(4)	0.080(4)	0.005(3)	-0.001(3)	-0.007(4)

$$U_{ij} = \exp(-2\pi^2 \{u_{11}k^2a^2 + \dots + u_{23}klb^*c^*\})$$