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Supporting Information

$K_4Au(TlSn_3)$: A Novel Zintl Phase with an Anionic Chain

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Table S1. Data Collection and Refinement Parameters **for $K_4Au(Sn_3Tl)$**

Form. wt.	913.81
Crystal system	Monoclinic
Space group, Z	*C2/c* (No. 15), 4
Lattice constants (Å, °, Å^3)[a]	
a	15.101(3)
b	6.6925(9)
c	14.389(3)
β	118.56 (1)
V	1277.2(4)
Color, habit	Black, bar-like
Dimension (mm)	0.06×0.05×0.05
Temperature (°C)	23
D_c (g/cm^3)	4.752
Octants meas.	$\pm h$, k, $\pm \ell$
Total refl.: meas	3764
unique	1885
R_{ave} ($I>0$), %	5.82
observed ($I>2\sigma_I$)	1385
Absorption corr. type	Psi-scan
μ, cm^{-1}, Mo Kα	310.45
Ref. trans. coeff. range	0.53–1.00
Variables	47
$R1(F)/wR2(F^2)$ ($I>2\sigma_I$), %	3.83/8.44
$R1(F)/wR2(F^2)$ ($I > 0$), %	6.79/9.40
Largest residual peaks (e/Å^3)	2.51, -2.77
Goof	1.019
Sec. extinc. coeff., 10^{-4}	5.3(6)

$R1=\Sigma||Fo|-|Fc||/\Sigma|Fo|$; $wR2=\{w[\Sigma(Fo^2-Fc^2)^2]/\Sigma[w(Fo^2)^2]\}^{1/2}$, $w=1/\sigma^2(F_o^2)+(aP)^2+bP]$, $P=[2F_c^2+\mathrm{Max}(F_o2,0)]^{1/3}$.

Table S2. Anisotropic thermal parameters for $K_4(AuSn_3Tl)$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au1	0.0432(3)	0.0141(3)	0.0234(3)	0	0.0166(2)	0
Sn1	0.0261(3)	0.0172(3)	0.0188(3)	-0.0007(2)	0.0047(2)	0.0003(2)
Sn2	0.0279(3)	0.0183(3)	0.0326(3)	-0.0012(2)	0.0177(2)	-0.0022(2)
Tl1	0.0261(3)	0.0172(3)	0.0188(3)	-0.0007(2)	0.0047(2)	0.0003(2)
Tl2	0.0279(3)	0.0183(3)	0.0326(3)	-0.0012(2)	0.0177(2)	-0.0022(2)
K1	0.035(1)	0.031(1)	0.032(1)	0.0007(9)	0.0194(9)	-0.0014(9)
K2	0.032(1)	0.037(1)	0.027(1)	0.0028(9)	0.0100(9)	-0.0023(9)