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K₄Au(TlSn₃): A Novel Zintl Phase with an Anionic Chain
 Daping Huang and John D. Corbett*

Table S1. Data Collection and Refinement Parameters for K₄Au(Sn₃Tl)

Form. wt.	913.81
Crystal system	Monoclinic
Space group, Z	C2/c (No. 15), 4
Lattice constants (Å, °, Å ³) ^a	
<i>a</i>	15.101(3)
<i>b</i>	6.6925(9)
<i>c</i>	14.389(3)
β	118.56 (1)
<i>V</i>	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.	± <i>h</i> , <i>k</i> , ± <i>l</i>
Total refl.: meas	3764
unique	1885
<i>R</i> _{ave} (<i>I</i> > 0), %	5.82
observed (<i>I</i> > 2σ _{<i>I</i>})	1385
Absorption corr. type	Psi-scan
μ, cm ⁻¹ , Mo Kα	310.45
Ref. trans. coeff. range	0.53–1.00
Variables	47
<i>R</i> 1(<i>F</i>)/w <i>R</i> 2(<i>F</i> ²) (<i>I</i> > 2σ _{<i>I</i>}), %	3.83/8.44
<i>R</i> 1(<i>F</i>)/w <i>R</i> 2(<i>F</i> ²) (<i>I</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)

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|; wR2 = \{w[\sum(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}, w = 1/\sigma^2(F_o^2) + (aP)^2 + bP],$$

$$P = [2F_c^2 + \text{Max}(F_o^2, 0)]^{1/3}.$$

Table S2. Anisotropic thermal parameters for $K_4(AuSn_3Ti)$

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)
Ti1	0.0261(3)	0.0172(3)	0.0188(3)	-0.0007(2)	0.0047(2)	0.0003(2)
Ti2	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)