SUPPORTING INFORMATION

Synthesis and Structure of the Metallic K_6Tl_{17} — A Unique Layered Structure Related to That of Cr_3Si

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Table S1. Selected Details of Data Collection and Structural Refinement for K_6Tl_{17}

Formula weight	3708.89
Crystal system, space group, *Z*	orthorhombic, *Cccm* (no. 66), 8
Unit cell dimens. (Å, Å^3)[a]	
a	16.625(1)
b	23.594(2)
c	15.369(2)
V	6029(1)
Calculated density, g/cm^3	8.173
F(000)	11928
Crystal size, mm	0.08 × 0.12 × 0.25
Diffractometer	Siemens CCD
θ range for data collec., deg.	1.50 – 23.29
Limiting indices	$-18 \le h \le 18$, $-26 \le k \le 25$, $-17 \le l \le 17$
Reflects. collec./unique (all)	17375/2277 [*R*(int) = 0.0828]
Completeness to theta = 23.29	100.0%
Absorp. coeffic. μ (Mo Kα, mm^{-1})	91.297
Absorp. correction	SADABS
Refinement method	Full-matrix least-squares on F^2
Obs. data/restraints/parameters	1322 / 0 / 118
Sec. ext. coeff. (10^{-6})	3(2)
Goodness-of-fit on F^2	0.929
*R*1, *wR*2 [I>2σ$_I$][b]	0.059, 0.136
Largest diff. peak and hole	2.401 and –2.219 e/Å^3

[a] Guinier powder data, λ = 1.540562 Å, 23 °C.

[b] $R1=\sum||F_o|-|F_c||/\sum|F_o|$, $wR2=\{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$.

Table S2. Anisotropic Displacement Parameters for K_6Tl_{17}

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Tl1	0.029(1)	0.025(1)	0.030 (1)	0.0012(8)	-0.0009(9)	-0.0009(8)
Tl2	0.034(2)	0.035(2)	0.029(2)	0.000	0.000	0.003(2)
Tl3	0.034(2)	0.0218	0.044(2)	0.000	0.002	0.000
Tl4	0.033(2)	0.026(2)	0.076(3)	0.000	0.000	0.000
Tl5	0.032(1)	0.030(1)	0.036(1)	-0.0014(9)	0.0055(9)	-0.0053(8)
Tl6	0.032(1)	0.027(1)	0.035(1)	-0.0058(9)	0.0030(9)	-0.0019(8)
Tl7	0.034(1)	0.035(1)	0.034(1)	-0.0041(9)	-0.003(1)	0.0030(9)
Tl8	0.033(2)	0.026(1)	0.030(2)	0.000	0.000	-0.001(1)
Tl9	0.038(1)	0.032(1)	0.040(1)	0.006(1)	0.003(1)	0.006(2)
Tl10	0.034(1)	0.030(1)	0.031(1)	-0.0002(9)	-0.0008(9)	-0.0072(8)
Tl11	0.036(2)	0.023(1)	0.064(2)	0.000	0.000	0.001(1)
Tl12	0.035(2)	0.046(2)	0.041(2)	0.000	0.000	0.005(1)
K1	0.027(8)	0.04(1)	0.032(9)	0.000	0.000	-0.005(7)
K2	0.04(1)	0.040(9)	0.04(1)	0.000	0.000	0.003(8)
K3	0.06(1)	0.024(8)	0.04(1)	0.000	0.000	0.001(8)
K4	0.033(7)	0.036(6)	0.047(7)	0.000(6)	-0.003(6)	0.010(5)
K5	0.03(1)	0.05(1)	0.07(1)	-0.03(1)	0.000	0.000

[a] $-2\pi^2[h^2 a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12} + \ldots]$

Table S3. Bond distances (Å) and Tl–Tl Overlap Populations in K_6Tl_{17}

Tl1–Tl1		3.208(4)	0.325	Tl9–Tl6		3.396(3)	0.299
Tl1–Tl2		3.209(2)	0.341	Tl9–Tl6		3.473(3)	0.204
Tl1–Tl3		3.211(3)	0.333	Tl9–Tl7		3.473(3)	0.256
Tl1–Tl5		3.341(3)	0.327	Tl9–K4		3.54(1)	
Tl1–Tl5		3.352(2)	0.322	Tl9–Tl5		3.589(3)	0.309
Tl1–Tl1		3.403(4)	0.173	Tl9–K1		3.63(1)	
Tl1–Tl5		3.420(3)	0.187	Tl9–K1		3.67(1)	
Tl1–Tl1		3.421(4)	0.175	Tl9–Tl9		3.711(4)	—
Tl1–K2		3.68(1)		Tl9–K3		3.87(2)	
Tl1–K5		3.69(2)		Tl10–Tl10		3.313(4)	0.193
Tl1–K4		3.75(1)		Tl10–Tl7		3.357(3)	0.237
Tl1–K3		3.88(1)		Tl10–Tl7		3.365(3)	0.288
Tl2–Tl1	×4	3.209(2)	0.341	Tl10–Tl4		3.367(2)	0.335
Tl2–Tl5	×4	3.316(2)	0.291	Tl10–Tl6		3.427(2)	0.137
Tl2–K2	×2	3.77(2)		Tl10–Tl12		3.429(3)	0.255
Tl2–K3	×2	4.00(2)		Tl10–Tl11		3.444(3)	0.275
Tl3–Tl6	×2	3.205(3)	0.387	Tl10–Tl11		3.478(3)	0.288
Tl3–Tl1	×2	3.211(3)	0.333	Tl10–K5		3.61(1)	
Tl3–Tl9	×2	3.313(2)	0.302	Tl10–K2		3.65(2)	
Tl3–Tl5	×2	3.336(2)	0.256	Tl10–K4		3.86(1)	
Tl3–K4	×2	3.80(1)		Tl11–Tl11		3.269(6)	0.394
Tl3–K3	×2	3.954(4)		Tl11–Tl8		3.367(4)	0.134
Tl4–Tl10	×4	3.367(2)	0.335	Tl11–Tl7	×2	3.373(2)	0.355
Tl4–Tl7	×4	3.377(2)	0.211	Tl11–Tl10	×2	3.444(3)	0.275

Tl4–K5	×2	3.712(16)	
Tl5–Tl2		3.316(2)	0.291
Tl5–Tl3		3.336(2)	0.256
Tl5–Tl1		3.341(3)	0.322
Tl5–Tl1		3.352(2)	0.327
Tl5–Tl1		3.420(3)	0.187
Tl5–K1		3.55(1)	
Tl5–Tl9		3.589(3)	0.309
Tl5–Tl5		3.619(4)	(~0.25)
Tl5–K4		3.69(1)	
Tl5–K2		3.70(1)	
Tl5–K3		3.84(2)	
Tl5–K5		3.94(1)	
Tl6–Tl8		3.190(2)	0.282
Tl6–Tl7		3.231(3)	0.354
Tl6–Tl12		3.335(3)	0.498
Tl6–Tl9		3.396(3)	0.299
Tl6–Tl10		3.427(2)	0.137
Tl6–Tl6		3.451(4)	0.035
Tl6–Tl9		3.473(3)	0.204
Tl6–Tl7		3.527(3)	0.136
Tl6–K4		3.62(1)	
Tl6–K4		3.71(1)	
Tl11–Tl10	×2	3.478(3)	0.288
Tl11–K1		3.67(2)	
Tl11–K2		3.73(2)	
Tl12–Tl6	×2	3.335(3)	0.498
Tl12–Tl8		3.368(14)	0.176
Tl12–Tl12		3.340(6)	0.544
Tl12–Tl10	x2	3.429(3)	0.255
Tl2–K4		3.63(1)	
Tl12–K3		4.02(1)	
K1–Tl5		3.55(1)	
K1–Tl9	×2	3.63(1)	
K1–Tl9		3.67(1)	
K1–Tl11		3.67(2)	
K1–Tl8		3.68(2)	
K1–Tl7	×2	3.79(1)	
K2–Tl7	×2	3.651(1)	
K2–Tl1		3.68(1)	
K2–Tl5	×2	3.70(1)	
K2–Tl11		3.73(2)	
K2–Tl2		3.77(2)	
K2–K5		3.998(6)	
K3–Tl6		3.78(1)	
K3–Tl5	×2	3.84(2)	

Tl6–K3		3.78(1)		K3–Tl8		3.87(2)
Tl7–Tl8		3.316(2)	0.188	K3–Tl9	×2	3.87(2)
Tl7–Tl10		3.357(3)	0.237	K3–Tl1		3.88(1)
Tl7–Tl10		3.365(3)	0.288	K3–Tl3	×2	3.954(4)
Tl7–Tl4		3.372(2)	0.211	K3–Tl12		4.02(1)
Tl7–Tl11		3.373(2)	0.355	K4–Tl9		3.54(1)
Tl7–Tl7		3.470(4)	0.119	K4–Tl6		3.62(1)
Tl7–Tl9		3.473(3)	0.256	K4–Tl12		3.63(1)
Tl7–Tl6		3.527(3)	0.136	K4–Tl7		3.68(1)
Tl7–K4		3.68(1)		K4–Tl3		3.80(1)
Tl7–K1		3.79(1)		K4–Tl10		3.86(1)
Tl7–K5		3.86(1)		K4–K5		4.02(1)
Tl8–Tl6	×2	3.190(2)	0.282	K4–K4		4.09(2)
Tl8–Tl9		3.252(3)	0.400	K5–Tl10	×2	3.69(1)
Tl8–Tl7	×2	3.316(2)	0.188	K5–Tl1		3.69(2)
Tl8–Tl10	×2	3.326(3)	0.166	K5–Tl4		3.71(2)
Tl8–Tl11		3.367(4)	0.134	K5–Tl7	×2	3.89(1)
Tl8–Tl12		3.368(4)	0.176	K5–Tl5		3.94(1)
Tl8–K1		3.68(2)		K5–K2		3.998(6)
Tl8–K3		3.87(2)		K5–K4		4.02(1)
Tl9–Tl8		3.252(3)	0.400			
Tl9–Tl3		3.313(2)	0.302			

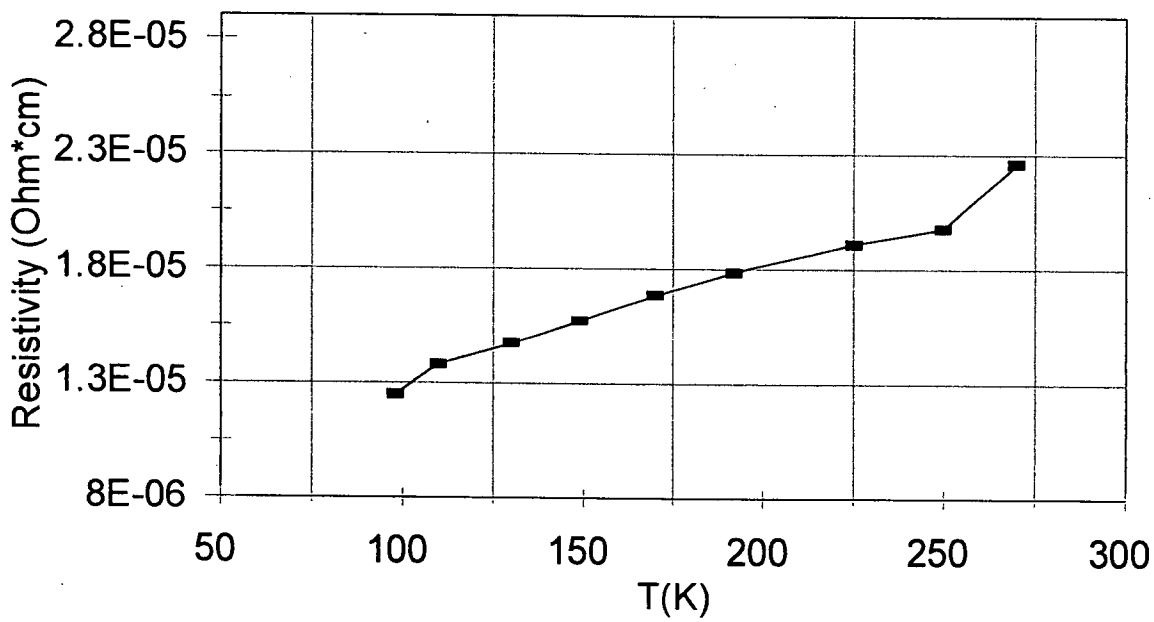

Table S1. Resistivity of K_6Tl_{17} by the "Q" method, Ω·cm vs T.

Fig. S1

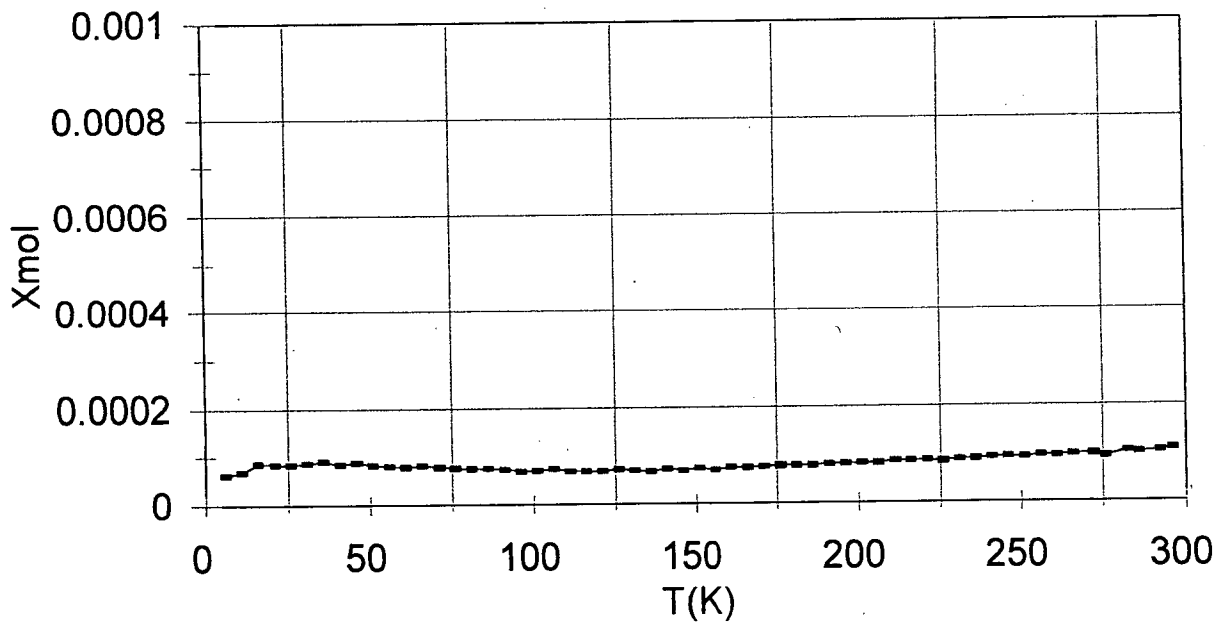

Table S2. Molar paramagnetic susceptibility of K_6Tl_{17} (emu) vs T at 3 Tesla.

Fig. S2