Supporting Information

$K_6Tl_2Sb_3$, A Zintl Phase with a Novel Heteroatomic $^1_\infty[Tl_4Sb_6^{12-}]$ Chain.

Lisheng Chi and John D. Corbett*

Table S1. Crystal data and structure refinement for $K_6Tl_2Sb_3$.

Empirical formula	$K_6Tl_2Sb_3$	
Formula weight	1008.59	
Temperature, K	293(2)	
Wavelength, Å	0.71073	
Crystal system	Monoclinic	
Space group, *Z*	*C*2/*c* (No. 15), 8	
Unit cell dimensions,[a] Å, deg.	a = 9.951(1)	α= 90°.
	b = 17.137(3)	β= 104.26(3)°.
	c = 19.640(6)	γ= 90°.
Volume, Å^3	3245.8(9)	
Density (calculated) μg/m^3	4.140	
Absorption coefficient, mm^{-1}	26.294	
F(000)	3432	
Crystal size, mm	0.1 ×0.15 ×0.45	
Theta range for data collection	2.13 to 27.59°.	
Index ranges	$0 \le h \le 12$, $0 \le k \le 22$, $-25 \le l \le 24$	
Reflections collected	3952	
Independent reflections	3741 [R(int) = 0.1515, I > 0]	
Completeness	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1758 / 0 / 102	
Goodness-of-fit on F^2	1.029	
Final R[b] indices [I>2σ(I)]	R1 = 0.0415, wR2 = 0.1002	
R indices (all data)	R1 = 0.1504, wR2 = 0.1291	
Extinction coefficient(10^{-5})	2(1)	
Largest diff. peak and hole	3.59 and -2.04 e.Å^{-3}	

[a] Guinier data 23 °C, λ = 1.54056 Å.

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

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $K_6Tl_2Sb_3$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Tl(1)	29(1)	22(1)	23(1)	0(1)	1(1)	0(1)
Tl(2)	22(1)	27(1)	30(1)	0(1)	5(1)	1(1)
Sb(1)	19(1)	23(1)	23(1)	3(1)	4(1)	0(1)
Sb(2)	19(1)	24(1)	22(1)	1(1)	4(1)	1(1)
Sb(3)	20(1)	22(1)	26(1)	-2(1)	5(1)	0(1)
K(1)	27(4)	40(4)	20(3)	0	2(3)	0
K(2)	21(4)	35(4)	39(4)	0	10(3)	0
K(3)	41(3)	39(3)	31(2)	-1(2)	3(2)	0(3)
K(4)	29(2)	29(2)	48(3)	-3(3)	11(2)	6(3)
K(5)	25(2)	29(2)	38(2)	5(2)	9(2)	1(2)
K(6)	36(3)	34(3)	26(2)	1(2)	6(2)	-1(2)
K(7)	19(2)	40(3)	38(2)	2(2)	6(2)	4(2)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \cdots + 2\,hka^*b^*U_{12}\cdots]$.

Table S3. Bond lengths [Å] in $K_6Tl_2Sb_3$.

Tl(1) - Sb(1)	3.049(2)	K(2) - Sb(1)H2	3.622(2)
Tl(1) - Sb(3)	3.078(2)	K(2) - K(1)	3.821(9)
Tl(1) - Sb(2)	3.147(2)	K(2) - Tl(1)H2	3.964(3)
Tl(1) - Tl(1)	3.217(2)	K(2) - K(6)H2	3.974(5)
Tl(1) - K(5)	3.424(5)	K(2) - K(5)H2	4.019(5)
Tl(1) - K(4)	3.427(5)	K(2) - Tl(2)	4.139(3)
Tl(1) - K(7)	3.652(5)	K(3) - Sb(2)	3.544(4)
Tl(1) - Tl(2)	3.714(1)	K(3) - Tl(2)	3.577(6)
Tl(1) - K(1)	3.918(3)	K(3) - Sb(2)	3.634(6)
Tl(1) - K(2)	3.964(4)	K(3) - Sb(1)	3.733(5)
Tl(2) - Sb(1)	3.179(2)	K(3) - K(4)	3.803(7)
Tl(2) - Sb(3)	3.195(2)	K(3) - Sb(3)	3.815(6)
Tl(2) - Sb(2)	3.236(2)	K(3) - Tl(2)	3.831(5)
Tl(2) - K(3)	3.577(6)	K(3) - K(7)	3.857(7)
Tl(2) - K(6)	3.602(5)	K(3) - K(6)	3.932(7)
Tl(2) - K(7)	3.719(5)	K(3) - K(3)	3.96(1)
Tl(2) - K(6)	3.802(5)	K(3) - K(5)	3.996(7)
Tl(2) - K(3)	3.831(5)	K(4) - Tl(1)	3.427(5)
Tl(2) - K(7)	3.872(5)	K(4) - Sb(2)	3.580(6)
Sb(1) - K(5)	3.559(5)	K(4) - Sb(1)	3.613(6)
Sb(1) - K(4)	3.613(6)	K(4) - Sb(3)	3.644(5)
Sb(1) - K(6)	3.615(5)	K(4) - K(3)	3.803(7)
Sb(1) - K(2)	3.622(2)	K(4) - K(6)	3.809(7)
Sb(1) - K(6)	3.680(5)	K(4) - K(7)	3.845(7)
Sb(1) - K(5)	3.683(4)	K(4) - K(4)	3.901(9)
Sb(1) - K(7)	3.687(5)	K(4) - K(1)	4.009(5)
Sb(1) - K(3)	3.733(6)	K(4) - K(2)	4.150(8)
Sb(2) - Tl(2)	3.236(2)	K(5) - Tl(1)	3.424(5)
Sb(2) - K(2)	3.451(4)	K(5) - Sb(2)	3.512(5)
Sb(2) - K(1)	3.464(4)	K(5) - Sb(3)	3.538(5)
Sb(2) - K(5)	3.512(5)	K(5) - Sb(1)	3.683(4)
Sb(2) - K(3)	3.544(4)	K(5) - K(5)	3.819(9)
Sb(2) - K(7)	3.557(5)	K(5) - K(3)	3.996(7)
Sb(2) - K(4)	3.580(6)	K(5) - K(2)	4.019(5)
Sb(2) - K(3)	3.634(6)	K(5) - K(6)	4.054(7)
Sb(2) - K(6)	3.744(5)	K(5) - K(7)	4.114(7)
Sb(3) - K(5)	3.538(5)	K(5) - K(1)	4.212(8)
Sb(3) - K(7)	3.540(5)	K(6) - Sb(1)	3.615(5)
Sb(3) - K(1)	3.555(2)	K(6) - Sb(3)	3.742(5)
Sb(3) - K(4)	3.644(5)	K(6) - Sb(2)	3.744(5)
Sb(3) - K(4)	3.648(5)	K(6) - Tl(2)	3.802(5)
Sb(3) - K(7)	3.697(5)	K(6) - K(4)	3.809(7)
Sb(3) - K(6)	3.742(5)	K(6) - K(7)	3.852(7)
Sb(3) - K(3)	3.815(6)	K(6) - K(3)	3.932(7)

K(1) - Sb(2)		3.464(4)	K(6) - K(2)	3.974(5)
K(1) - Sb(3)		3.555(2)	K(6) - K(6)	3.995(10)
K(1) - K(2)		3.821(9)	K(6) - K(5)	4.054(7)
K(1) - Tl(1)	×2	3.918(3)	K(7) - Sb(2)	3.557(5)
K(1) - K(3)	×2	3.980(5)	K(7) - Sb(3)	3.697(5)
K(1) - K(4)	×2	4.009(5)	K(7) - K(6)	3.852(7)
K(1) - Tl(2)		4.086(3)	K(7) - Tl(2)	3.872(5)
K(2) - Sb(2)	×2	3.451(4)	K(7) - K(7)	4.013(10)