Supporting Information

A₅InPb₈ (A = K, Rb): An Apparent Zintl Phase With Lead Tetrahedra**Interbridged by μ_6 -In Atoms.****Michael T. Klem and John D. Corbett**Table S1. Some data collection and refinement parameters for K₅InPb₈

Formula Weight	961.21
Crystal system, space group, Z	trigonal, $R\bar{3}m$, 3
Unit cell dimensions ($\text{\AA}$) ^a	
<i>a</i>	6.8835(6)
<i>c</i>	37.591(5)
<i>V</i> ($\text{\AA}^3$)	1543.9(2)
Calculated density, g cm ⁻³	8.508
Diffractometer	Rigaku
Octants, 2 θ_{max} (deg)	$\pm h, \pm k, l$; 55°
Observ. refl. (> 2 σ_I)	2563
unique	502
Absorp. coeff. (Mo K α , cm ⁻¹)	902.59
Rel. trans. coeff. range	0.568 – 1.000
variables	20
<i>R</i> , <i>R_w</i> ^b	0.057, 0.070
Largest ΔF , e ⁻ / $\text{\AA}^3$	3.02, 0.70 $\text{\AA}$ from In1
GOF	1.69

^a Guinier powder pattern data, $\lambda = 1.540562 \text{ \AA}$, 23 C.^b $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; $R_w = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w(F_o)^2]^{1/2}$; $w = \sigma_F^{-2}$.

Table S2. Anisotropic displacement parameters for $K_5\text{InPb}_8$ phases

$K_5\text{InPb}_8$	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pb1	0.038(1)	0.038	0.012(2)	0.019	0.0000	0.0000
Pb2	0.0199(5)	0.020	0.0197(7)	0.0139(6)	0.0002	-0.0002(3)
In1	0.019(2)	0.02	0.007(4)	0.0095	0.0000	0.0000
K1	0.026(5)	0.026	0.007(8)	0.013	0.0000	0.00000
K2	0.031(5)	0.031	0.017(9)	0.0155	0.0000	0.0000
K3	0.04(1)	0.04	0.08(3)	0.02	0.00000	0.00000

$$^aT = \exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk - 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Fig. S1 : Densities of States and COOP curves for InPb_8 in which the intercluster separation has been increased. The solid DOS line represents the total density of states. The solid, dotted, and dashed lines in the COOP represent intracuster overlap, Pb-Pb overlap, and In-Pb overlap respectively.