

$K_{14}Tl_{21}Cd_9$	$hP44$	(189) $P-62m - ki^4hgfec$
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$K_{14}Cd_9Tl_{21}$ [1]

Structural features: Layers containing single Tl_{11} units (pentacapped trigonal prism) alternate with layers containing (Cd_5Tl_2) pentagonal bipyramids and (Cd_3Tl_2) trigonal bipyramids sharing edges and vertices.

Tillard Charbonnel M. et al. (1995) [1]

$Cd_9K_{14}Tl_{21}$

$a = 0.9884$, $c = 1.7173$ nm, $c/a = 1.737$, $V = 1.4529$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	$6k$	$m..$	0.2991	0.4719	$\frac{1}{2}$		pseudo Frank-Kasper $Cd_5Tl_6K_2$
K2	$6i$	$..m$	0.389	0	0.1842		pseudo Frank-Kasper Tl_8K_5
Tl3	$6i$	$..m$	0.3993	0	0.3927		icosahedron $Cd_5Tl_3K_4$
Tl4	$6i$	$..m$	0.706	0	0.0938		bicapped square antiprism Tl_4K_6
K5	$6i$	$..m$	0.747	0	0.3175		16-vertex Frank-Kasper $Tl_7Cd_4K_5$
Tl6	$4h$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.3344		icosahedron $Tl_3Cd_3K_6$
Cd7	$3g$	$m2m$	0.165	0	$\frac{1}{2}$		6-vertex polyhedron Cd_4Tl_2
Tl8	$3f$	$m2m$	0.2211	0	0		icosahedron Tl_8K_4
Tl9	$2e$	$3.m$	0	0	0.1526		icosahedron Tl_6K_6
K10	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		15-vertex polyhedron Tl_9K_6

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.059$, $T = 293$ K

Remarks: In table 2 of [1] the x -coordinate of former Tl(5) and the y -coordinate of former K(3) are misprinted as $\frac{1}{6}$ instead of $\frac{2}{3}$ (agreement with Wyckoff positions $4h$ and $2d$, respectively; checked on interatomic distances) and the Wyckoff position of former Cd(1) as $6i$ instead of $6j$.

References: [1] Tillard Charbonnel M., Chahine A., Belin C. (1995), Z. Kristallogr. 210, 162.