

TlCdS ₂	<i>hP4</i>	(187) <i>P-6m2</i> – ida
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CdTiS₂ [1]

Structural features: Directly superposed close-packed S layers; Cd and Tl in trigonal prismatic voids (stacking sequence AbAγ). CdS₆ trigonal prisms share edges to form infinite slabs; Tl in trigonal prismatic voids between the slabs.

Guseinov G.D. et al. (1967) [1]

CdS₂Tl

$a = 0.3645$, $c = 0.681$ nm, $c/a = 1.868$, $V = 0.0784$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	<i>2i</i>	<i>3m.</i>	$\frac{2}{3}$	$\frac{1}{3}$	0.25		octahedron Cd ₃ Tl ₃
Tl2	<i>1d</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism S ₆
Cd3	<i>1a</i>	<i>-6m2</i>	0	0	0		trigonal prism S ₆

Experimental: single crystal, Weissenberg and rotation photographs, X-rays

Remarks: The description in space group (156) *P3m1* in [1] does not take into consideration all symmetry elements of the proposed structure. In the abstract of [1] the compound is misprinted as GdTiS₂ instead of CdTiS₂.

References: [1] Guseinov G.D., Ismailov M.Z., Guseinov G.G. (1967), Mater. Res. Bull. 2, 765-772.