

CdI <sub>2</sub>	<i>hP</i> 12	(186) $P6_3mc - b^4a^2$
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**CdI<sub>2</sub> 8H<sub>2</sub> [1]**

Structural features: Close-packed I layers in h<sub>3</sub>c stacking; Cd in octahedral voids in every second interlayer. Layer structure with sandwiches consisting of three sublayers (I-Cd-I).

Chadha G.K., Trigunayat G.C. (1967) [1]

CdI<sub>2</sub>

$a = 0.424$ ,  $c = 2.734$  nm,  $c/a = 6.448$ ,  $V = 0.4257$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.125		non-coplanar triangle Cd <sub>3</sub>
I2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.375		non-coplanar triangle Cd <sub>3</sub>
Cd3	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5625		octahedron I <sub>6</sub>
Cd4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.8125		octahedron I <sub>6</sub>
I5	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		non-coplanar triangle Cd <sub>3</sub>
I6	2 <i>a</i>	3 <i>m</i> .	0	0	0.25		non-coplanar triangle Cd <sub>3</sub>

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Zhdanov notation (211)<sub>2</sub>. We derived idealized atom coordinates from the stacking sequence.

References: [1] Chadha G.K., Trigunayat G.C. (1967), Acta Crystallogr. 23, 726-729.