

CdI ₂	<i>hP</i> 24	(186) <i>P</i> 6 ₃ <i>mc</i> – b ⁸ a ⁴
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CdI₂ 16H₈ [1]

Structural features: Close-packed I layers in h₂chc₂ stacking; Cd occupies all octahedral voids in every second interlayer. Layer structure with infinite slabs of edge-linked CdI₆ octahedra.

Jain P.C., Trigunayat G.C. (1978) [1]

CdI₂

a = 0.424, *c* = 5.468 nm, *c/a* = 12.896, *V* = 0.8513 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.03125		non-coplanar triangle Cd ₃
I2	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.15625		non-coplanar triangle Cd ₃
I3	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.28125		non-coplanar triangle Cd ₃
Cd4	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.375		octahedron I ₆
I5	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.46875		non-coplanar triangle Cd ₃
Cd6	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.625		octahedron I ₆
I7	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.71875		non-coplanar triangle Cd ₃
I8	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.90625		non-coplanar triangle Cd ₃
Cd9	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		octahedron I ₆
I10	2 <i>a</i>	3 <i>m.</i>	0	0	0.09375		non-coplanar triangle Cd ₃
Cd11	2 <i>a</i>	3 <i>m.</i>	0	0	0.25		octahedron I ₆
I12	2 <i>a</i>	3 <i>m.</i>	0	0	0.34375		non-coplanar triangle Cd ₃

Transformation from published data: origin shift 0 0 0.15625

Experimental: single crystal, oscillation photographs, X-rays

Remarks: Zhdanov notation (22211)₂. We derived idealized atom coordinates from the stacking sequence.

References: [1] Jain P.C., Trigunayat G.C. (1978), Acta Crystallogr. B 34, 2677-2684.