CdI_2	*hP*6	(186) $P6_3mc$ – b^2a

CdI_2 4H [1], Strukturbericht notation C27
Structural features: Close-packed I layers in hc stacking; Cd in octahedral voids (stacking sequence AbC AcB). Layer structure with sandwiches consisting of three sublayers in c stacking (I-Cd-I). CdI_6 octahedra share edges to form infinite slabs. See Fig. IV.17.

Hassel O. (1933) [1]
CdI_2
a = 0.425, c = 1.367 nm, c/a = 3.216, V = 0.2138 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.25		non-coplanar triangle Cd_3
Cd2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.625		octahedron I_6
I3	2*a*	3*m*.	0	0	0.0		non-coplanar triangle Cd_3

Transformation from published data ($P6_3mc$ *): origin shift $^2/_3$ $^1/_3$ 0.375
Experimental: single crystal, rotation photographs, X-rays

Remarks: Idealized coordinates, we deduced the space group from the coordinates of all the atoms in the unit cell. The *a*-parameter is given as 0.424-0.425 nm; cell parameters a = 0.42445(1), c = 0.68642(3) nm were refined in [4]. In [1] the origin of the cell is shifted by $^2/_3$ $^1/_3$ 0 from the description in the International Tables for Crystallography. A report on SnS_2 4H with this structure type [3] is superseded (see [2]).

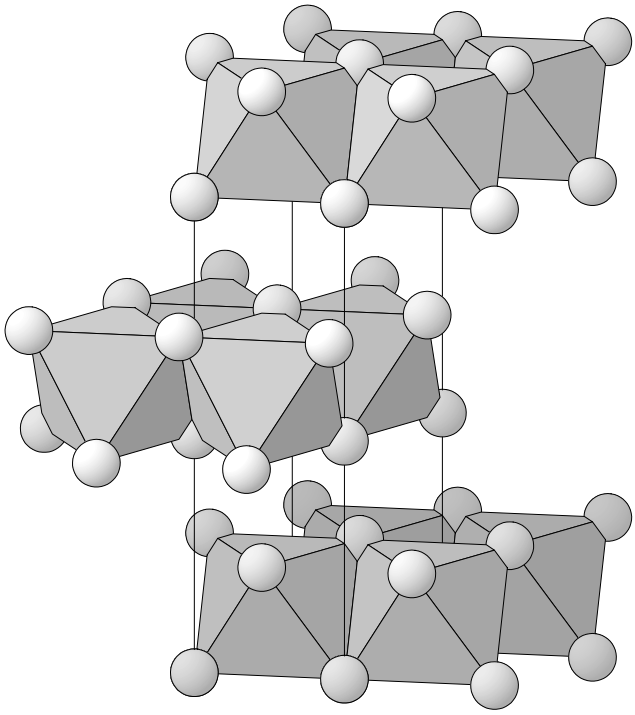

Fig. IV.17. **CdI_2 4H**

Arrangement of CdI_6 octahedra.

References: [1] Hassel O. (1933), Z. Phys. Chem., Abt. B 22, 333-334. [2] Palosz B., Steurer W., Schulz H. (1990), Acta Crystallogr. B 46, 449-455. [3] Guenter J.R., Oswald H.R. (1968), Naturwissenschaften 55, 177. [4] Palosz B., Salje E. (1989), J. Appl. Crystallogr. 22, 622-623.