

13 Estrutura do CdI₂

1. Os dados cristalográficos do Iodeto de cádmio - CdI₂ - são os seguintes.

Sistema Cristalino	Trigonal
Grupo de espaço	$P\bar{3}m1$
Z (moléculas por malha)	1
<i>a</i>	4.24 Å
<i>c</i>	6.84 Å
Coordenada do Cd	Wyckoff Symbol <i>a</i>
Coordenada do I	Wyckoff Symbol <i>d</i>

(a) Com a ajuda das informações contidas na Tabela Internacional, esquematize a projeção da estrutura do CdI₂ segundo as direções [001] (2×2 malhas) e [100] (2×2 malhas) deixando explícito nos desenhos os átomos ligados e indicando por + e - as cotas com relação ao eixo z. (b) Calcule as distâncias CdI mais curtas. (c) Calcule os ângulos entre as duas ligações CdI(1) e CdI(2). (d) Determine o número de coordenação do cádmio pelos iodetos e dos iodetos pelo cádmio.

$P\bar{3}m1$

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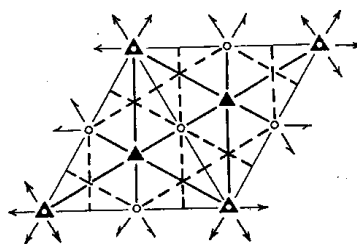
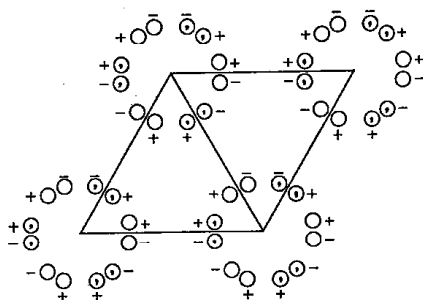
D_{3d}^3

$P\bar{3}2/m1$

$\bar{3}m1$

Trigonal

Patterson symmetry $P\bar{3}m1$



Origin at centre ($\bar{3}m1$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1; x \leq (1+y)/2; y \leq x/2$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0$
 $0,0,1 \quad \frac{1}{2},0,1 \quad \frac{1}{2},\frac{1}{2},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) 2 $x,x,0$ (5) 2 $x,0,0$ (6) 2 $0,y,0$
(7) $\bar{1}$ $0,0,0$ (8) $\bar{3}^+$ $0,0,z; 0,0,0$ (9) $\bar{3}^-$ $0,0,z; 0,0,0$
(10) m x,\bar{x},z (11) m $x,2x,z$ (12) m $2x,x,z$

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 $P\bar{3}m1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

12	<i>j</i>	1	(1) x, y, z	(2) $\bar{y}, x-y, z$	(3) $\bar{x}+y, \bar{x}, z$
			(4) y, x, \bar{z}	(5) $x-y, \bar{y}, \bar{z}$	(6) $\bar{x}, \bar{x}+y, \bar{z}$
			(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x}+y, \bar{z}$	(9) $x-y, x, \bar{z}$
			(10) \bar{y}, \bar{x}, z	(11) $\bar{x}+y, y, z$	(12) $x, x-y, z$

General:

no conditions

Special: no extra conditions

6	<i>i</i>	.m.	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	\bar{x}, x, \bar{z}	$2x, x, \bar{z}$	$\bar{x}, 2\bar{x}, \bar{z}$
6	<i>h</i>	.2.	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$
6	<i>g</i>	.2.	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$
3	<i>f</i>	.2/m.	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3	<i>e</i>	.2/m.	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	<i>d</i>	3m.	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$				
2	<i>c</i>	3m.	$0, 0, z$	$0, 0, \bar{z}$				
1	<i>b</i>	$\bar{3}m$.	$0, 0, \frac{1}{2}$					
1	<i>a</i>	$\bar{3}m$.	$0, 0, 0$					

Symmetry of special projections

Along [001] $p6mm$ $a' = a$ $b' = b$ Origin at $0, 0, z$ Along [100] $p2$ $a' = \frac{1}{2}(a+2b)$ $b' = c$ Origin at $x, 0, 0$ Along [210] $p2mm$ $a' = \frac{1}{2}b$ $b' = c$ Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P321$	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11(P\bar{3})$	1; 2; 3; 7; 8; 9
	[2] $P3m1$	1; 2; 3; 10; 11; 12
	[3] $P12/m1(C2/m)$	1; 4; 7; 10
	[3] $P12/m1(C2/m)$	1; 5; 7; 11
	[3] $P12/m1(C2/m)$	1; 6; 7; 12

IIa none

IIb [3] $H\bar{3}m1(a' = 3a, b' = 3b)(P\bar{3}1m)$; [2] $P\bar{3}c1(c' = 2c)$

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}m1(c' = 2c)$; [4] $P\bar{3}m1(a' = 2a, b' = 2b)$

Minimal non-isomorphic supergroups

I	[2] $P6/mmm$; [2] $P6_3/mmc$
II	[3] $H\bar{3}m1(P\bar{3}1m)$; [3] $R\bar{3}m$ (obverse); [3] $R\bar{3}m$ (reverse)