

*I*222

D_2^8

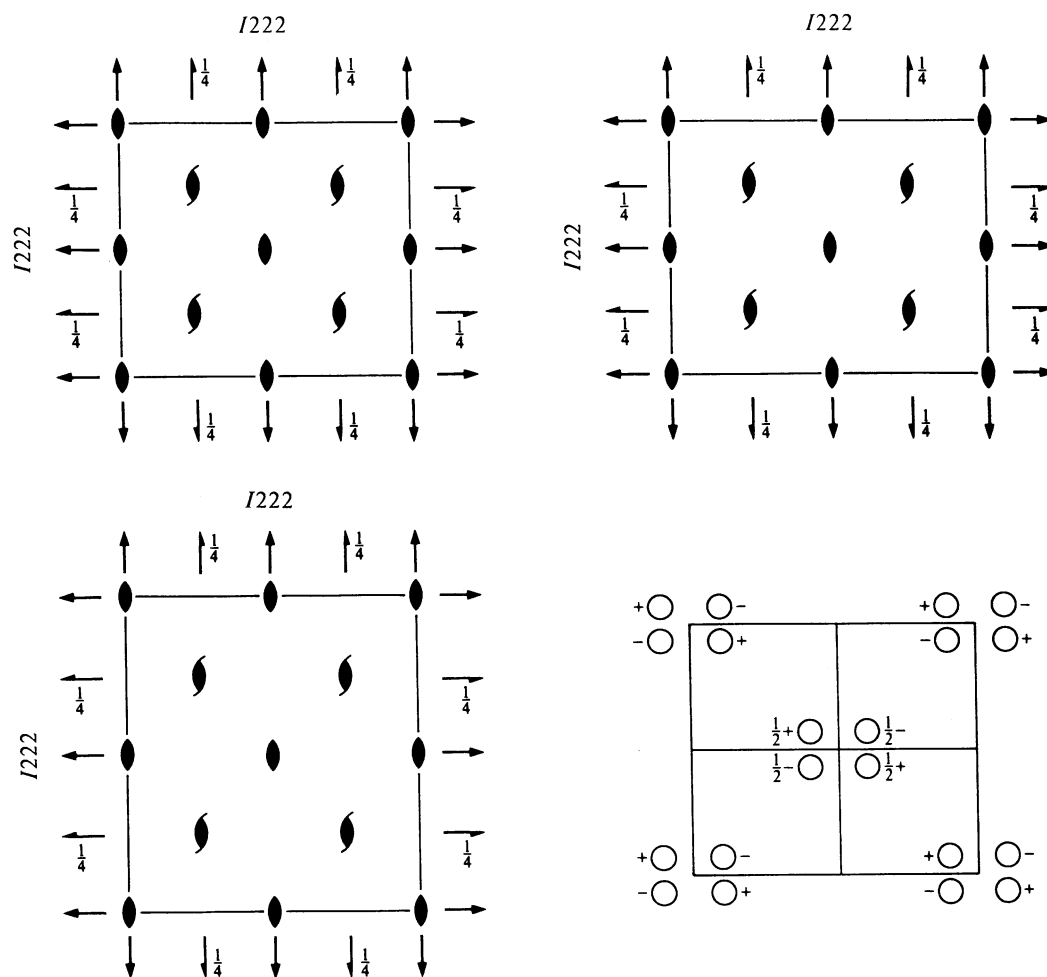
222

Orthorhombic

No. 23

*I*222

Patterson symmetry *Immm*



Origin at 222

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- (1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0,0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ (3) 2 $(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{1}{4}$ (4) 2 $(\frac{1}{2}, 0, 0) x, \frac{1}{4}, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		(0,0,0)+	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$			General:
8	<i>k</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	$hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
4	<i>j</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$			Special: no extra conditions
4	<i>i</i> ..2	$0, 0, z$	$0, 0, \bar{z}$			
4	<i>h</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$			
4	<i>g</i> .2.	$0, y, 0$	$0, \bar{y}, 0$			
4	<i>f</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$			
4	<i>e</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$			
2	<i>d</i> 222	$0, \frac{1}{2}, 0$				
2	<i>c</i> 222	$0, 0, \frac{1}{2}$				
2	<i>b</i> 222	$\frac{1}{2}, 0, 0$				
2	<i>a</i> 222	$0, 0, 0$				

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x,0,0

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $I112$ (C2, 5)	(1; 2)+
	[2] $I121$ (C2, 5)	(1; 3)+
	[2] $I211$ (C2, 5)	(1; 4)+
IIa	[2] $P2_12_12_1$ (18)	1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P2_12_12_1$ ($P2_12_12_1$, 18)	1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P22_12_1$ ($P2_12_12_1$, 18)	1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P222$ (16)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I222$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (23)

Minimal non-isomorphic supergroups

I [2] $Immm$ (71); [2] $Ibam$ (72); [2] $I422$ (97); [2] $I\bar{4}2m$ (121); [3] $I23$ (197)
II [2] $A222$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (C222, 21); [2] $B222$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (C222, 21); [2] $C222$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (21)