

$P222_1$

$D_2^2$

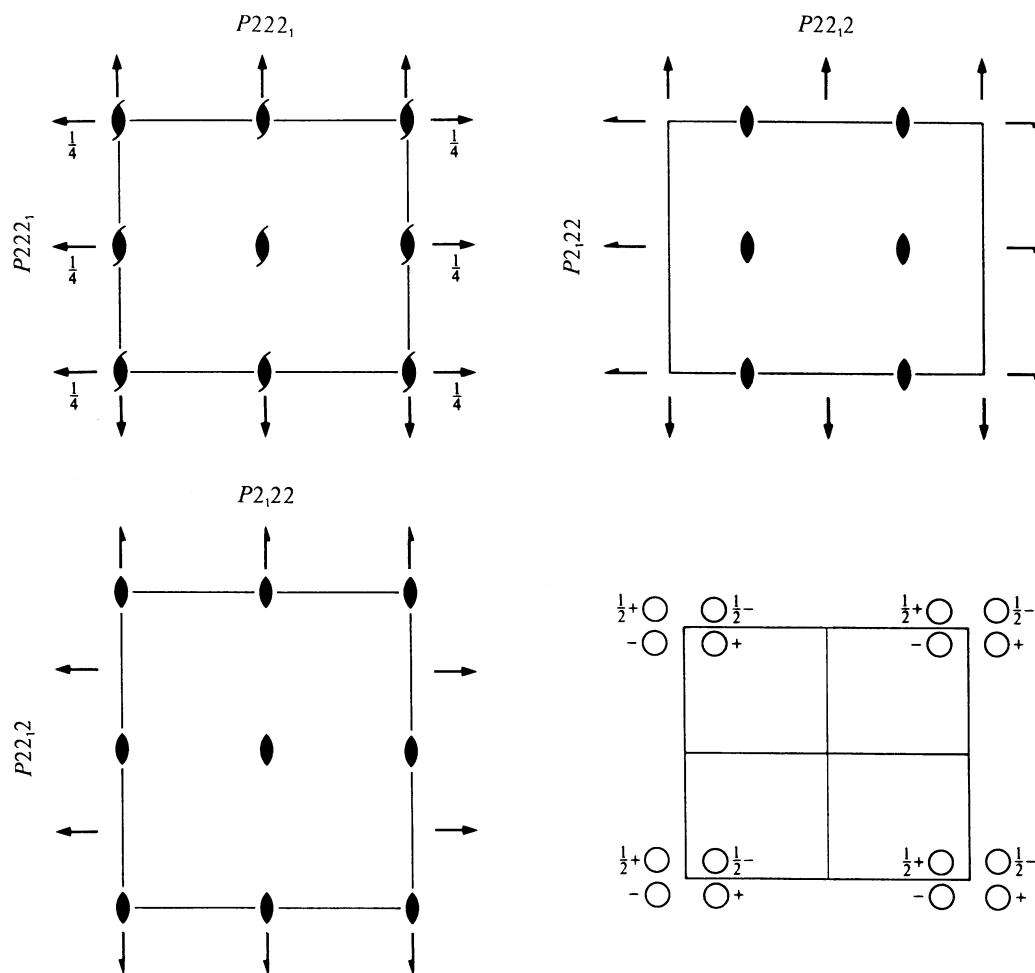
222

Orthorhombic

No. 17

$P222_1$

Patterson symmetry  $Pmmm$



Origin at  $212_1$

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

Symmetry operations

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

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(4) $x, \bar{y}, \bar{z}$	General: $00l : l = 2n$ Special: as above, plus $h0l : l = 2n$ $h0l : l = 2n$ $0kl : l = 2n$ $0kl : l = 2n$
2 <i>d</i> .2.	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$			
2 <i>c</i> .2.	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$			
2 <i>b</i> 2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$			
2 <i>a</i> 2..	$x, 0, 0$	$\bar{x}, 0, \frac{1}{2}$			

**Symmetry of special projections**

Along [001]  $p2mm$   
 $\mathbf{a}' = \mathbf{a}$   $\mathbf{b}' = \mathbf{b}$   
Origin at  $0, 0, z$

Along [100]  $p2gm$   
 $\mathbf{a}' = \mathbf{b}$   $\mathbf{b}' = \mathbf{c}$   
Origin at  $x, 0, 0$

Along [010]  $p2mg$   
 $\mathbf{a}' = \mathbf{c}$   $\mathbf{b}' = \mathbf{a}$   
Origin at  $0, y, \frac{1}{4}$

**Maximal non-isomorphic subgroups**

**I** [2]  $P112_1$  ( $P2_1, 4$ ) 1; 2  
[2]  $P121$  ( $P2, 3$ ) 1; 3  
[2]  $P211$  ( $P2, 3$ ) 1; 4

**IIa** none

**IIb** [2]  $P2_122_1$  ( $\mathbf{a}' = 2\mathbf{a}$ ) ( $P2_12_12, 18$ ); [2]  $P22_12_1$  ( $\mathbf{b}' = 2\mathbf{b}$ ) ( $P2_12_12, 18$ ); [2]  $C222_1$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (20)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $P222_1$  ( $\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{b}' = 2\mathbf{b}$ ) (17); [3]  $P222_1$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (17)

**Minimal non-isomorphic supergroups**

**I** [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $P4_122$  (91); [2]  $P4_322$  (95)

**II** [2]  $C222_1$  (20); [2]  $A222$  ( $C222, 21$ ); [2]  $B222$  ( $C222, 21$ ); [2]  $I2_12_12_1$  (24); [2]  $P222$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (16)