

$C222$

$D_2^6$

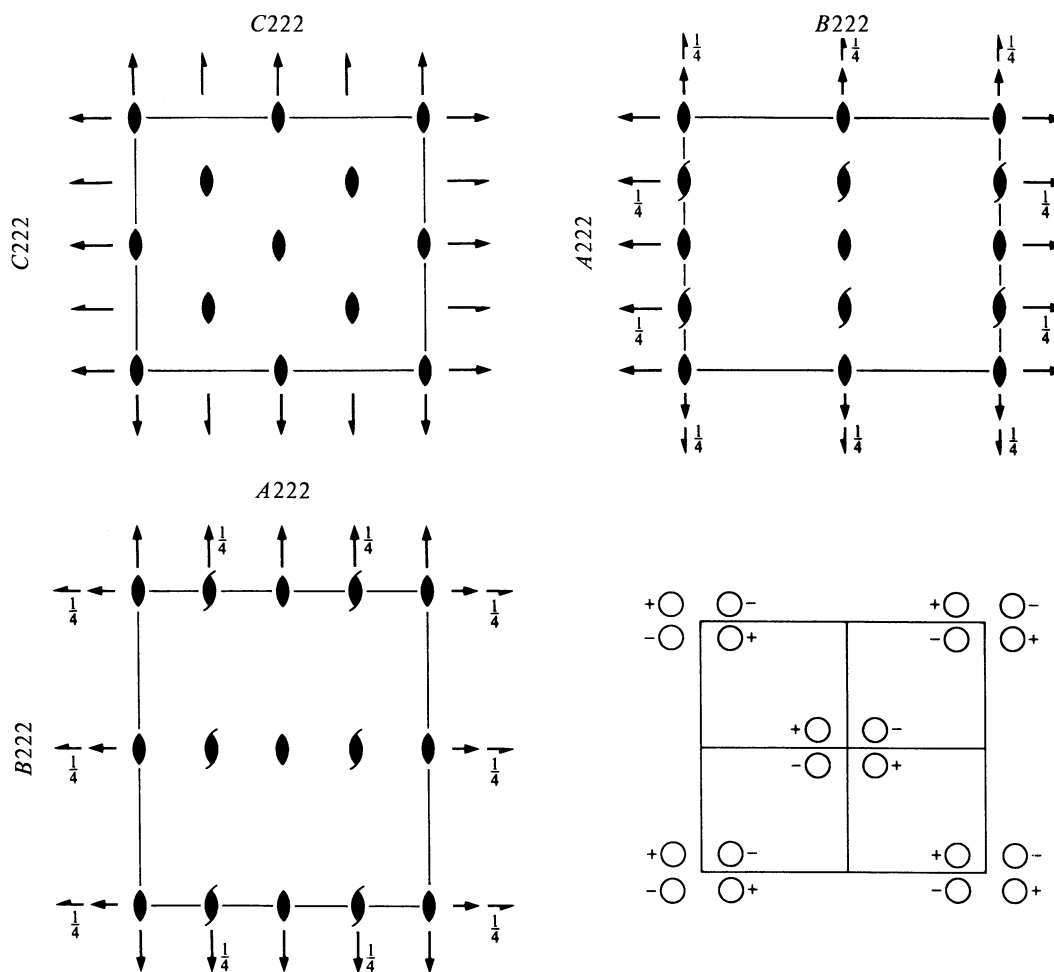
222

Orthorhombic

No. 21

$C222$

Patterson symmetry  $Cmmm$



Origin at 222

Asymmetric unit  $0 \leq x \leq \frac{1}{4}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq 1$

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  $(\frac{1}{2},\frac{1}{2},0)+$  set

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

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

**Positions**

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

**Symmetry of special projections**

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

Along [100]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$   $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x,0,0$

Along [010]  $p2mm$   
 $\mathbf{a}' = \mathbf{c}$   $\mathbf{b}' = \frac{1}{2}\mathbf{a}$   
 Origin at  $0,y,0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $C121$ ( $C2, 5$ )	(1; 3)+
	[2] $C211$ ( $C2, 5$ )	(1; 4)+
	[2] $C112$ ( $P2, 3$ )	(1; 2)+
<b>IIa</b>	[2] $P2_12_12_1$ (18)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P2_12_2$ ( $P222_1, 17$ )	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P22_12$ ( $P222_1, 17$ )	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P222$ (16)	1; 2; 3; 4
<b>IIb</b>	[2] $I2_12_12_1$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (24); [2] $I222$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (23); [2] $C222_1$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (20)	

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $C222$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (21); [3]  $C222$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (21)

**Minimal non-isomorphic supergroups**

<b>I</b>	[2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P422$ (89); [2] $P4_22$ (90); [2] $P4_22$ (93); [2] $P4_22_12$ (94); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118); [3] $P622$ (177); [3] $P6_22$ (180); [3] $P6_422$ (181)
<b>II</b>	[2] $F222$ (22); [2] $P222$ ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) (16)