

$F 222$

D_2^7

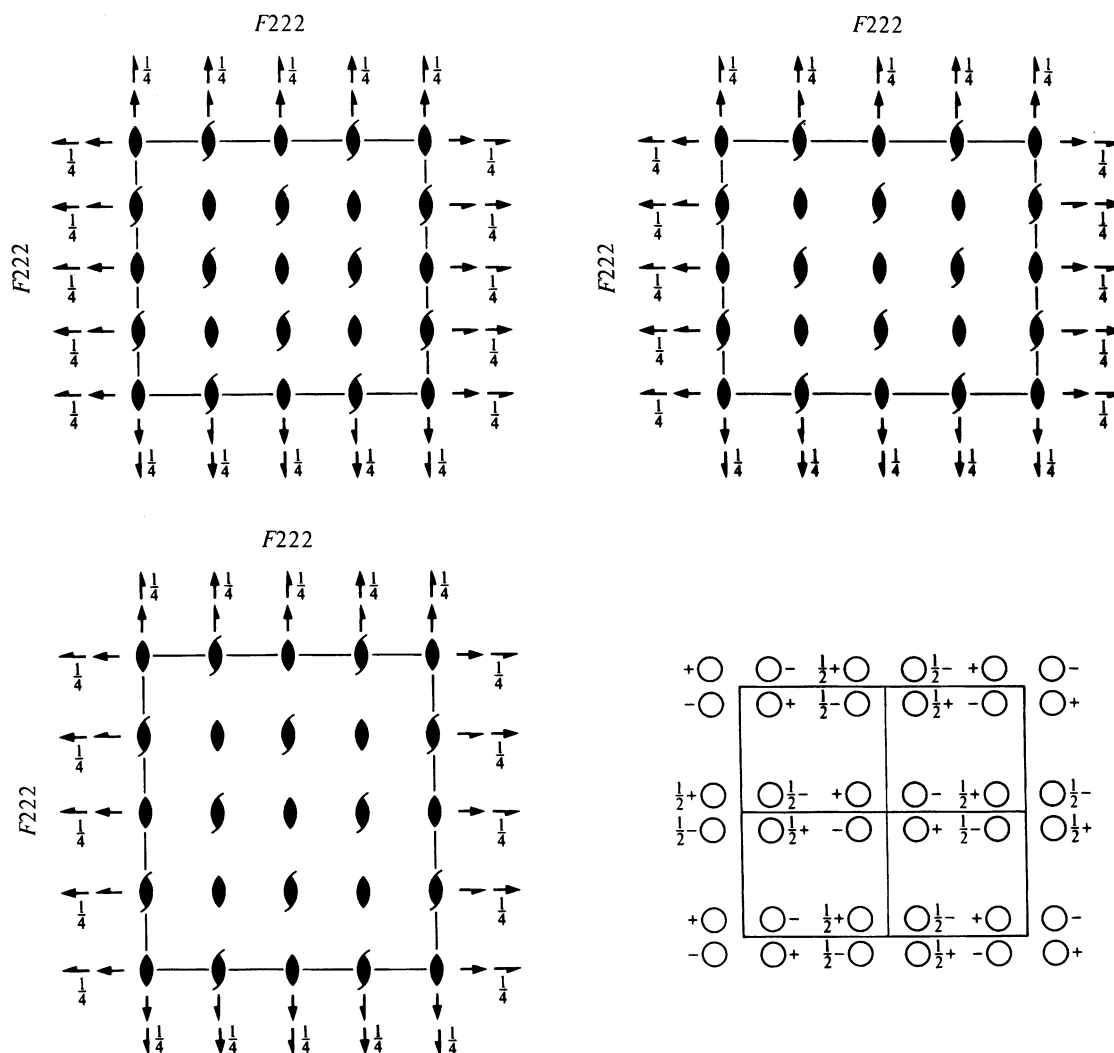
222

Orthorhombic

No. 22

$F 222$

Patterson symmetry $F m m m$



Origin at 222

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

Symmetry operations

For $(0,0,0)+$ set

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

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

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

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

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

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

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

Maximal isomorphic subgroups of lowest index

Ic [3] $F 222$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (22)

Minimal non-isomorphic supergroups

I [2] $F m m m$ (69); [2] $F d d d$ (70); [2] $I 4 2 2$ (97); [2] $I 4_1 2 2$ (98); [2] $I \bar{4} m 2$ (119); [2] $I \bar{4} c 2$ (120); [3] $F 2 3$ (196)

II [2] $P 222$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (16)

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

Positions

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

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0, 0, z$

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

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

Maximal non-isomorphic subgroups

I	[2] $F112 (C2, 5)$	(1; 2)+
	[2] $F121 (C2, 5)$	(1; 3)+
	[2] $F211 (C2, 5)$	(1; 4)+
IIa	[2] $A222 (C222, 21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $A222 (C222, 21)$	1; 4; (1; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $B222 (C222, 21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $B222 (C222, 21)$	1; 3; (1; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $C222 (21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C222 (21)$	1; 2; (1; 2) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $A2_122 (C222_1, 20)$	1; 2; (1; 2) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $A2_122 (C222_1, 20)$	1; 3; (1; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $B22_12 (C222_1, 20)$	1; 2; (1; 2) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $B22_12 (C222_1, 20)$	1; 4; (1; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $C222_1 (20)$	1; 3; (1; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $C222_1 (20)$	1; 4; (1; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$
IIb	none	

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