

$Pmmm$

D_{2h}^1

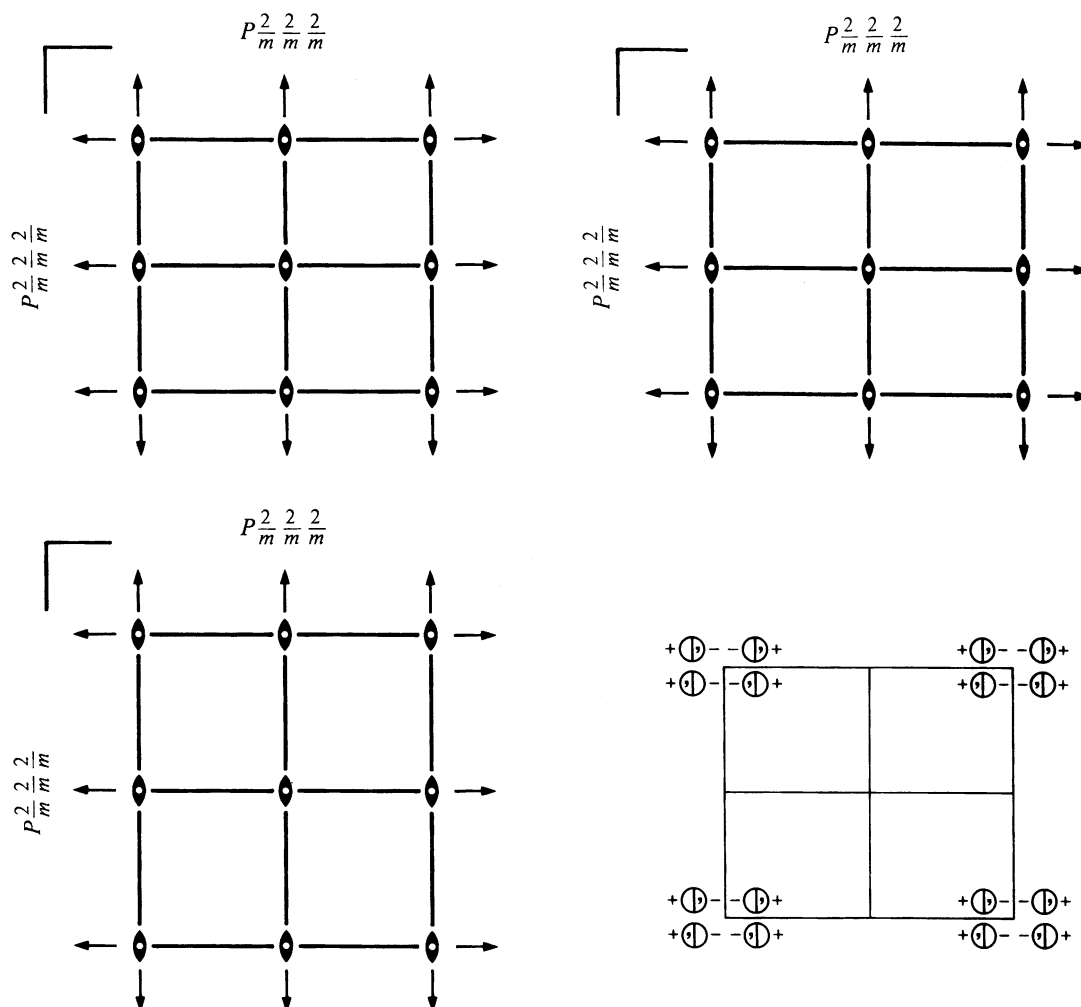
mmm

Orthorhombic

No. 47

$P 2/m 2/m 2/m$

Patterson symmetry $Pmmm$



Origin at centre (mmm)

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

- | | | | |
|---------------------|-------------|-------------|-------------|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) $\bar{1}$ 0,0,0 | (6) m x,y,0 | (7) m x,0,z | (8) m 0,y,z |

Maximal non-isomorphic subgroups (*continued*)

IIa none

IIb [2] $Pmma$ ($\mathbf{a}' = 2\mathbf{a}$) (51); [2] $Pmam$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pmma$, 51); [2] $Pmaa$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pccm$, 49); [2] $Pbmm$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pmmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pbmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pccm$, 49); [2] $Pcmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pmcm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pccm$ ($\mathbf{c}' = 2\mathbf{c}$) (49); [2] $Aemm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Ammm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Bmem$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Bmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Cmme$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (67); [2] $Cmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (65); [2] $Fmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (69)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmmm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$) (47)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4_2/mmc$ (131); [3] $Pm\bar{3}$ (200)

II [2] $Ammm$ ($Cmmm$, 65); [2] $Bmmm$ ($Cmmm$, 65); [2] $Cmmm$ (65); [2] $Immm$ (71)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
						General:	
8	α 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) \bar{x}, y, \bar{z} (7) x, \bar{y}, z	(4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	no conditions	
Special: no extra conditions							
4	z . . m	$x, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$	$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$		
4	y . . m	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, 0$	$x, \bar{y}, 0$		
4	x . m .	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, \bar{z}$	$x, \frac{1}{2}, \bar{z}$		
4	w . m .	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x}, 0, \bar{z}$	$x, 0, \bar{z}$		
4	v m . .	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$	$\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, \bar{z}$		
4	u m . .	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$		
2	t $m m 2$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$				
2	s $m m 2$	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$				
2	r $m m 2$	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$				
2	q $m m 2$	$0, 0, z$	$0, 0, \bar{z}$				
2	p $m 2 m$	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	1	h $m m m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
2	o $m 2 m$	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	1	g $m m m$	$0, \frac{1}{2}, \frac{1}{2}$	
2	n $m 2 m$	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$	1	f $m m m$	$\frac{1}{2}, \frac{1}{2}, 0$	
2	m $m 2 m$	$0, y, 0$	$0, \bar{y}, 0$	1	e $m m m$	$0, \frac{1}{2}, 0$	
2	l $2 m m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	1	d $m m m$	$\frac{1}{2}, 0, \frac{1}{2}$	
2	k $2 m m$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	1	c $m m m$	$0, 0, \frac{1}{2}$	
2	j $2 m m$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	1	b $m m m$	$\frac{1}{2}, 0, 0$	
2	i $2 m m$	$x, 0, 0$	$\bar{x}, 0, 0$	1	a $m m m$	$0, 0, 0$	

Symmetry of special projections

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

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

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

Maximal non-isomorphic subgroups

I	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $Pm2m$ ($Pmm2$, 25)	1; 3; 6; 8
	[2] $P2mm$ ($Pmm2$, 25)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6
	[2] $P12/m1$ ($P2/m$, 10)	1; 3; 5; 7
	[2] $P2/m11$ ($P2/m$, 10)	1; 4; 5; 8

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