

Ibca

D_{2h}^{27}

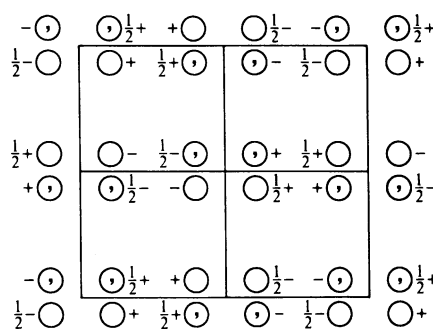
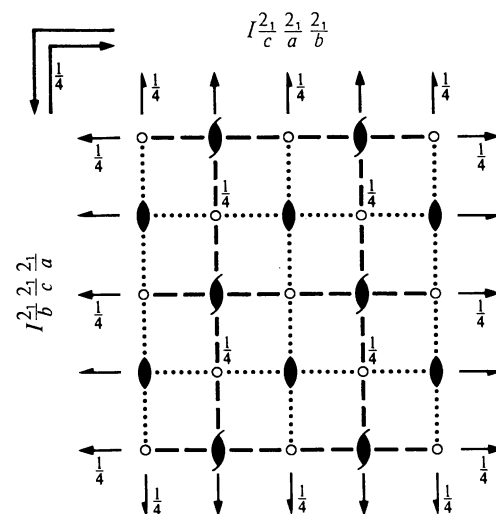
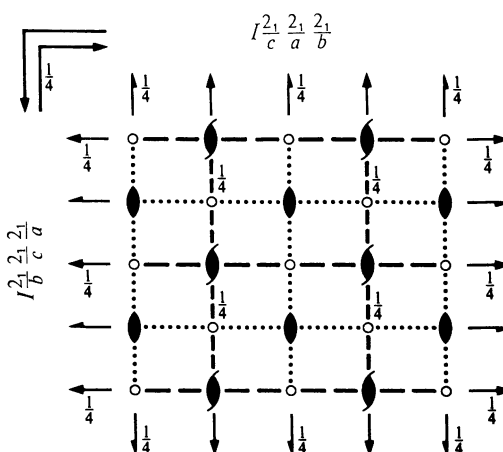
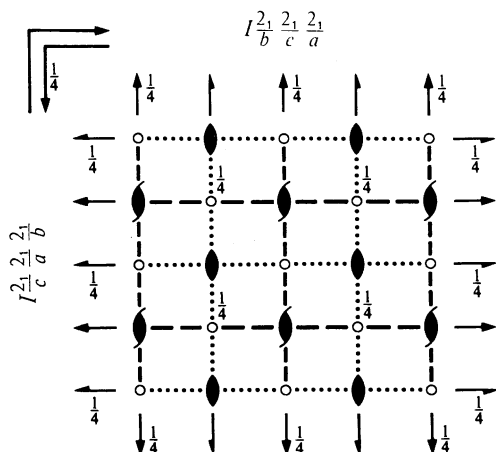
mmm

Orthorhombic

No. 73

$I 2_1/b 2_1/c 2_1/a$

Patterson symmetry *Immm*



Origin at $\bar{1}$ at *cab*

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

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-------------------------|--|--|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) <i>a</i> $x, y, \frac{1}{4}$ | (7) <i>c</i> $x, \frac{1}{4}, z$ | (8) <i>b</i> $\frac{1}{4}, y, z$ |

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

- | | | | |
|---|-----------------------------|-----------------------------|-----------------------------|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, 0$ | (4) 2 $x, 0, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) <i>b</i> $x, y, 0$ | (7) <i>a</i> $x, 0, z$ | (8) <i>c</i> $0, y, z$ |

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); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ +				General:
16 <i>f</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$hkl : h+k+l=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8 <i>e</i> ..2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},z+\frac{1}{2}$	$hkl : l=2n$
8 <i>d</i> .2.	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,\frac{1}{2}$	$hkl : k=2n$
8 <i>c</i> 2..	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$hkl : h=2n$
8 <i>b</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$hkl : k,l=2n$
8 <i>a</i> $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$hkl : k,l=2n$

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] <i>Ibc2</i> (<i>Iba2</i> , 45)	(1; 2; 7; 8)+
	[2] <i>Ib2a</i> (<i>Iba2</i> , 45)	(1; 3; 6; 8)+
	[2] <i>I2ca</i> (<i>Iba2</i> , 45)	(1; 4; 6; 7)+
	[2] <i>I2</i> , $2_1, 2_1$ (24)	(1; 2; 3; 4)+
	[2] <i>I112/a</i> (<i>C2/c</i> , 15)	(1; 2; 5; 6)+
	[2] <i>I12/c1</i> (<i>C2/c</i> , 15)	(1; 3; 5; 7)+
	[2] <i>I2/b11</i> (<i>C2/c</i> , 15)	(1; 4; 5; 8)+
	IIa	[2] <i>Pbca</i> (61)
[2] <i>Pcab</i> (<i>Pbca</i> , 61)		1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pcaa</i> (<i>Pcca</i> , 54)		1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pccb</i> (<i>Pcca</i> , 54)		1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pbab</i> (<i>Pcca</i> , 54)		1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pbcb</i> (<i>Pcca</i> , 54)		1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pbaa</i> (<i>Pcca</i> , 54)		1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] <i>Pcca</i> (54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] *Ibca* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (73)

Minimal non-isomorphic supergroups

I [2] *I4*, *acd* (142); [3] *Ia3* (206)

II [2] *Aemm* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Cmme*, 67); [2] *Bmem* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Cmme*, 67); [2] *Cmme* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)