

*Iba*2

$C_{2v}^{21}$

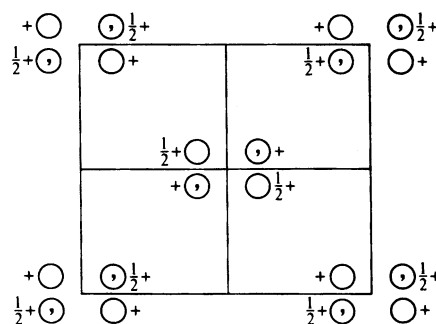
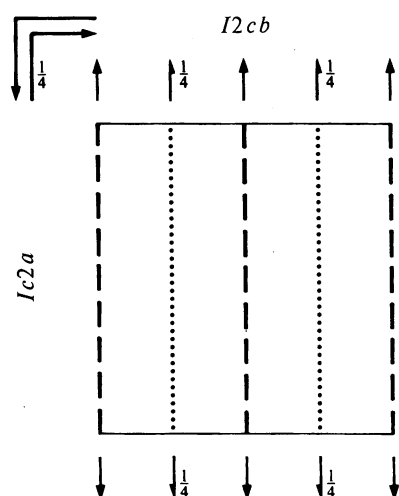
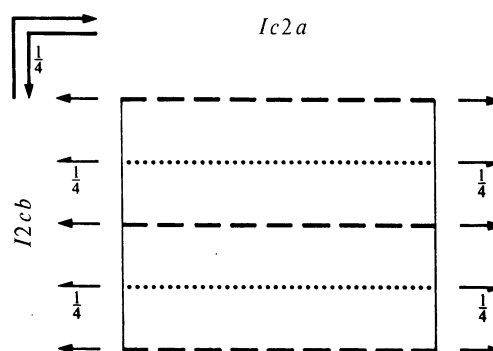
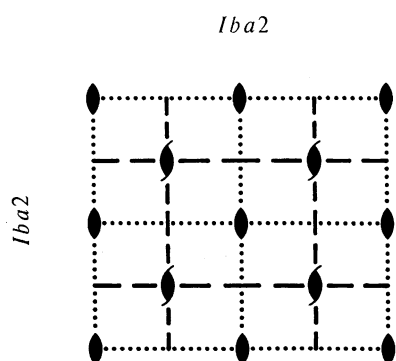
*mm*2

Orthorhombic

No. 45

*Iba*2

Patterson symmetry *Immm*



Origin on *cc*2

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

For (0,0,0)+ set

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

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

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

**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)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8 c 1	(1) $x,y,z$	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$hkl : h+k+l=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
4 b ..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			Special: as above, plus $hkl : l=2n$
4 a ..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			$hkl : l=2n$

**Symmetry of special projections**

Along [001]  $c2mm$

$\mathbf{a}' = \mathbf{a}$   $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [100]  $p1m1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$   $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,0,0

Along [010]  $p11m$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$   $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at 0,y,0

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I1a1 (Cc, 9)$	(1; 3)+
	[2] $Ib11 (Cc, 9)$	(1; 4)+
	[2] $I112 (C2, 5)$	(1; 2)+
<b>IIa</b>	[2] $Pba2 (32)$	1; 2; 3; 4
	[2] $Pca2_1 (29)$	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbc2_1 (Pca2_1, 29)$	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcc2 (27)$	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
<b>IIb</b>	none	

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $Iba2 (\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}) (45)$ ; [3]  $Iba2 (\mathbf{c}' = 3\mathbf{c}) (45)$

**Minimal non-isomorphic supergroups**

**I** [2]  $Ibam (72)$ ; [2]  $Ibca (73)$ ; [2]  $I4cm (108)$ ; [2]  $I4_1cd (110)$ ; [2]  $I\bar{4}c2 (120)$   
**II** [2]  $Cmm2 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (35)$ ; [2]  $Aem2 (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (39)$ ; [2]  $Bme2 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (Aem2, 39)$