

$F d d d$

D_{2h}^{24}

$m m m$

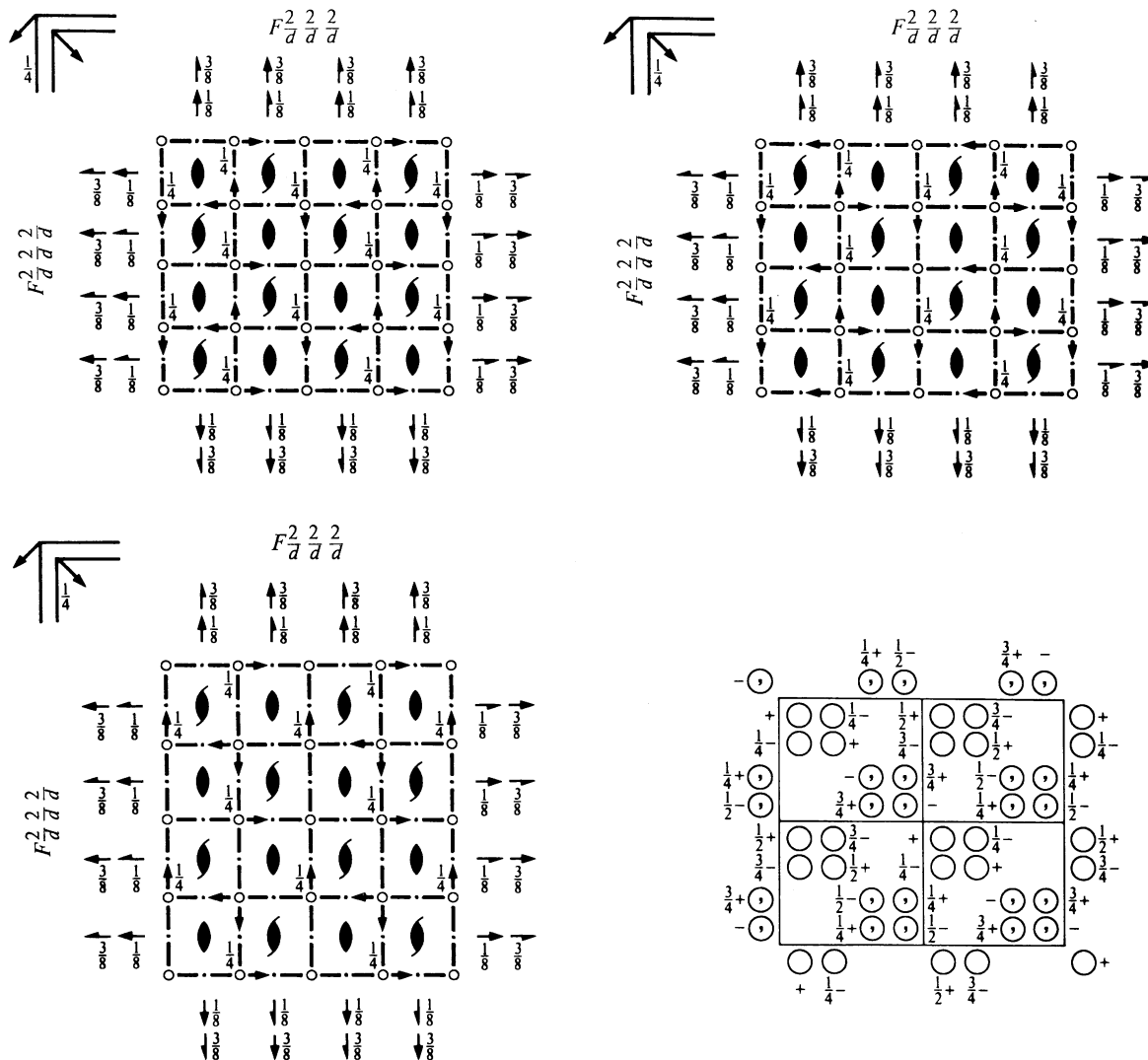
Orthorhombic

No. 70

$F 2/d 2/d 2/d$

Patterson symmetry $F m m m$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $d d d$, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 222

Asymmetric unit $0 \leq x \leq \frac{1}{8}; -\frac{1}{8} \leq y \leq \frac{1}{8}; 0 \leq z \leq 1$

Symmetry operations

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

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

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

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

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

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

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

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

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); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

32 *h* 1 (1) x, y, z (2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, z$ (3) $\bar{x} + \frac{3}{4}, y, \bar{z} + \frac{3}{4}$ (4) $x, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$
 (5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z}$ (7) $x + \frac{1}{4}, \bar{y}, z + \frac{1}{4}$ (8) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$

$hkl : h+k, h+l, k+l = 2n$
 $Ok_l : k+l = 4n, k, l = 2n$
 $h0l : h+l = 4n, h, l = 2n$
 $hk0 : h+k = 4n, h, k = 2n$
 $h00 : h = 4n$
 $0k0 : k = 4n$
 $00l : l = 4n$

Special: as above, plus

16 *g* ..2 $\frac{1}{8}, \frac{1}{8}, z$ $\frac{5}{8}, \frac{1}{8}, \bar{z} + \frac{3}{4}$ $\frac{7}{8}, \frac{7}{8}, \bar{z}$ $\frac{3}{8}, \frac{7}{8}, z + \frac{1}{4}$
 16 *f* .2. $\frac{1}{8}, y, \frac{1}{8}$ $\frac{5}{8}, \bar{y} + \frac{3}{4}, \frac{1}{8}$ $\frac{7}{8}, \bar{y}, \frac{7}{8}$ $\frac{3}{8}, y + \frac{1}{4}, \frac{7}{8}$
 16 *e* 2.. $x, \frac{1}{8}, \frac{1}{8}$ $\bar{x} + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}$ $\bar{x}, \frac{7}{8}, \frac{7}{8}$ $x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}$
 16 *d* $\bar{1}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$
 16 *c* $\bar{1}$ 0,0,0 $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, 0, \frac{3}{4}$ $0, \frac{3}{4}, \frac{3}{4}$
 8 *b* 222 $\frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ $\frac{7}{8}, \frac{7}{8}, \frac{3}{8}$
 8 *a* 222 $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$

$hkl : h = 2n + 1$
 or $h+k+l = 4n$

$hkl : h = 2n + 1$
 or $h, k, l = 4n + 2$
 or $h, k, l = 4n$

$hkl : h = 2n + 1$
 or $h+k+l = 4n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, \frac{1}{8}, \frac{1}{8}$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $\frac{1}{8}, y, \frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $Fdd2$ (43) (1; 2; 7; 8)+
 [2] $Fd2d$ ($Fdd2$, 43) (1; 3; 6; 8)+
 [2] $F2dd$ ($Fdd2$, 43) (1; 4; 6; 7)+
 [2] $F222$ (22) (1; 2; 3; 4)+
 [2] $F112/d$ ($C2/c$, 15) (1; 2; 5; 6)+
 [2] $F12/d1$ ($C2/c$, 15) (1; 3; 5; 7)+
 [2] $F2/d11$ ($C2/c$, 15) (1; 4; 5; 8)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $Fddd$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (70)**Minimal non-isomorphic supergroups****I** [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)**II** [2] $Pnnn$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (48)