

$Fddd$

D_{2h}^{24}

mmm

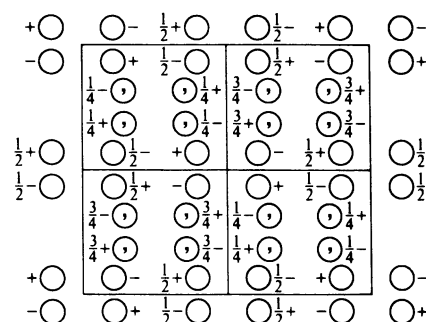
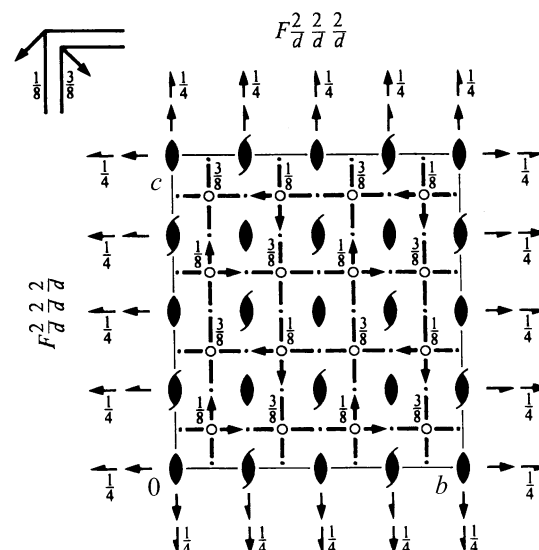
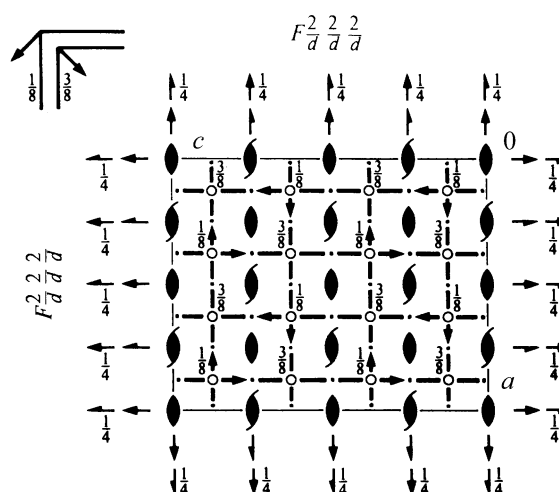
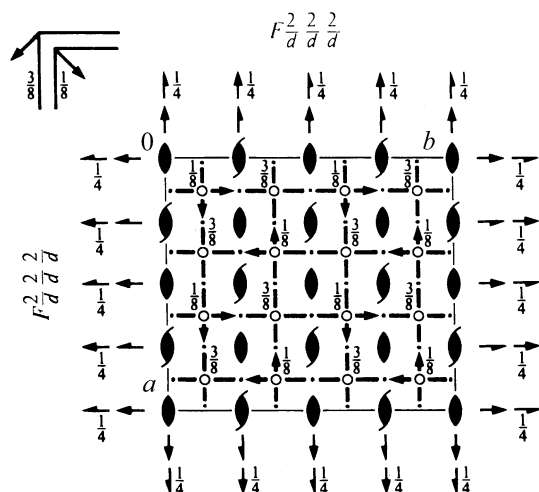
Orthorhombic

No. 70

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

Patterson symmetry $Fmmm$

ORIGIN CHOICE 1



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

Asymmetric unit $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

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

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

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

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

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

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

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

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

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

hkl: $h + k = 2n$ and
 $h + l, k + l = 2n$
*Ok*l: $k + l = 4n$ and
 $k, l = 2n$
hOl: $h + l = 4n$ and
 $h, l = 2n$
hk0: $h + k = 4n$ and
 $h, k = 2n$
h00: $h = 4n$
Ok0: $k = 4n$
00l: $l = 4n$

Special: as above, plus

16 *g* ..2 $0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}$ }
16 *f* .2. $0, y, 0$ $0, \bar{y}, 0$ $\frac{1}{4}, \bar{y} + \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, y + \frac{1}{4}, \frac{1}{4}$ }
16 *e* 2.. $x, 0, 0$ $\bar{x}, 0, 0$ $\bar{x} + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $x + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ }

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

16 *d* $\bar{1}$ $\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$ $\frac{3}{8}, \frac{3}{8}, \frac{5}{8}$ $\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$ $\frac{5}{8}, \frac{3}{8}, \frac{3}{8}$ }
16 *c* $\bar{1}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{7}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$ $\frac{1}{8}, \frac{7}{8}, \frac{7}{8}$ }

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

8 *b* 222 $0, 0, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ }
8 *a* 222 $0, 0, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ }

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 $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0, y, 0$

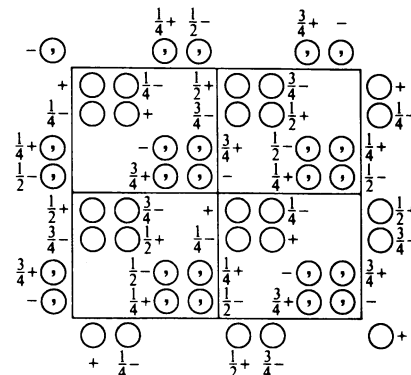
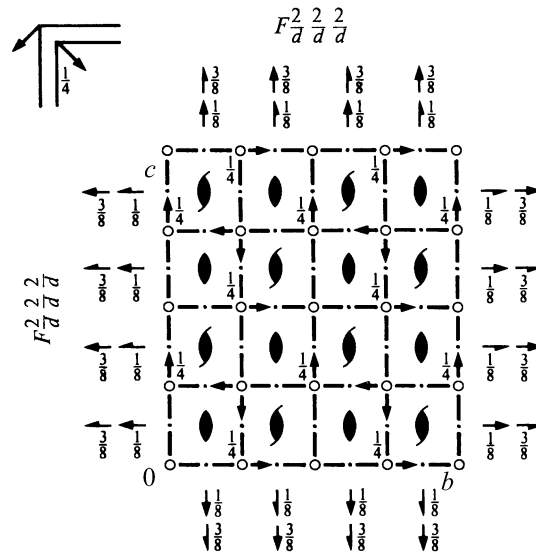
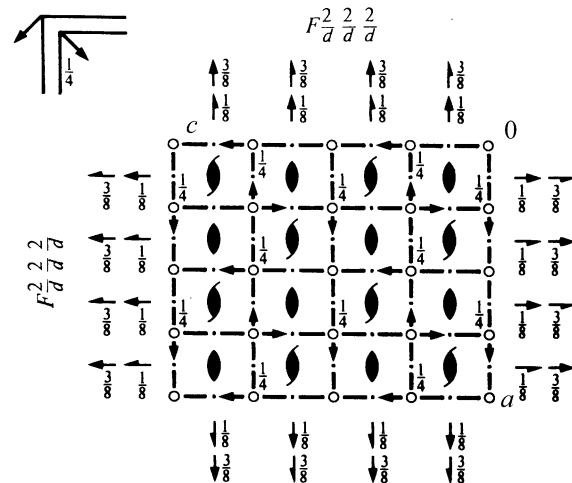
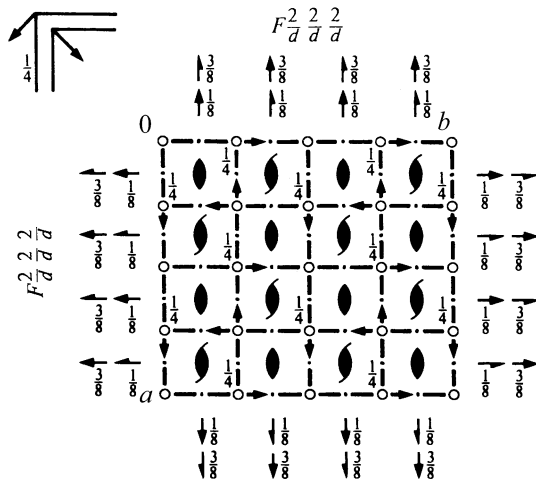
$Fddd$ D_{2h}^{24} mmm

Orthorhombic

No. 70

 $F 2/d 2/d 2/d$ Patterson symmetry $Fmmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at ddd , 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) $2 \begin{smallmatrix} \frac{1}{8} \\ \frac{3}{8} \\ \frac{1}{8} \end{smallmatrix}, z$ | (3) $2 \begin{smallmatrix} \frac{3}{8} \\ \frac{1}{8} \\ \frac{3}{8} \end{smallmatrix}, y, z$ | (4) $2 \begin{smallmatrix} x \\ \frac{3}{8} \\ \frac{3}{8} \end{smallmatrix}$ |
| (5) $\bar{1} \quad 0,0,0$ | (6) $d(\frac{1}{4}, \frac{1}{4}, 0) \quad x,y,0$ | (7) $d(\frac{1}{4}, 0, \frac{1}{4}) \quad x,0,z$ | (8) $d(0, \frac{1}{4}, \frac{1}{4}) \quad 0,y,z$ |

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

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

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

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

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

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

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) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$

$hkl: h+k, h+l, k+l = 2n$
 $OkI: k+l = 4n, k, l = 2n$
 $hOl: h+l = 4n, h, l = 2n$
 $hk0: h+k = 4n, h, k = 2n$
 $h00: h = 4n$
 $Ok0: k = 4n$
 $00l: l = 4n$

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.. $x, \frac{1}{8}, \frac{1}{8}$ $\bar{x} + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}$ $\bar{x}, \frac{7}{8}, \frac{7}{8}$ $x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}$ }

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

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* $\bar{1}$ $0, 0, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, 0, \frac{3}{4}$ $0, \frac{3}{4}, \frac{3}{4}$ }

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

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 $h+k+l = 4n$

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 $\frac{1}{8}, y, \frac{1}{8}$