

$Fm\bar{3}$

T_h^3

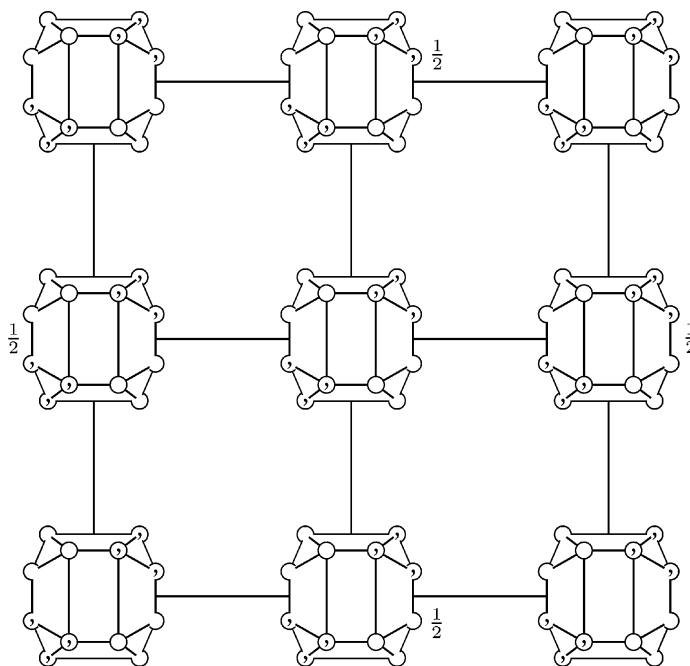
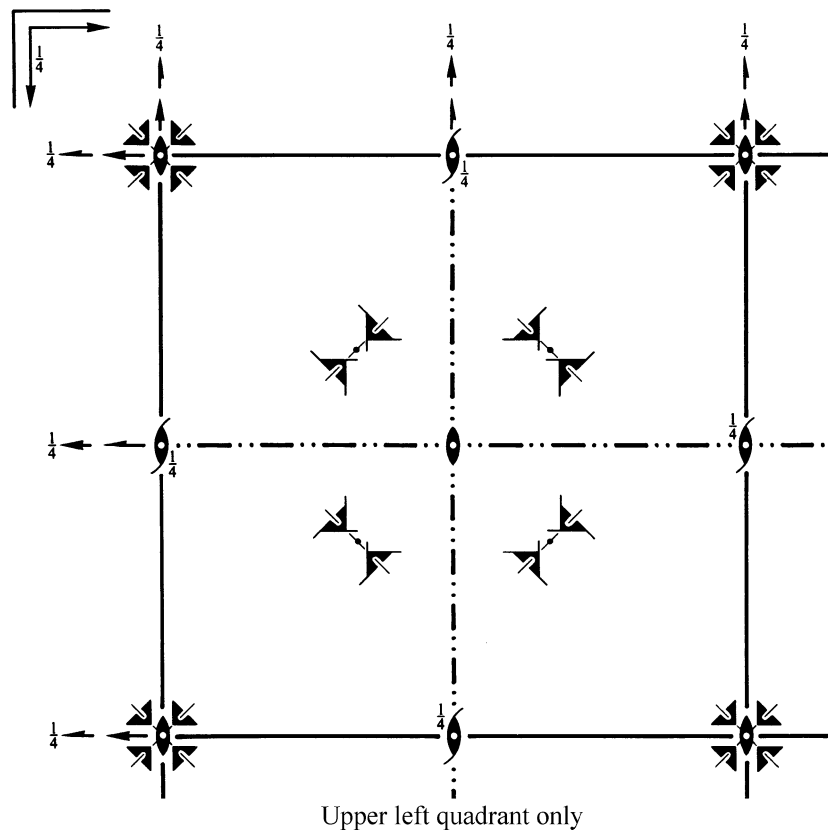
$m\bar{3}$

Cubic

No. 202

$F2/m\bar{3}$

Patterson symmetry $Fm\bar{3}$



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; y \leq x; z \leq \min(\frac{1}{2} - x, y)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

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) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) $\bar{1}$ 0,0,0 | (14) m x,y,0 | (15) m x,0,z | (16) m 0,y,z |
| (17) $\bar{3}^+$ x,x,x; 0,0,0 | (18) $\bar{3}^+$ \bar{x},x,\bar{x} ; 0,0,0 | (19) $\bar{3}^+$ x, \bar{x},\bar{x} ; 0,0,0 | (20) $\bar{3}^+$ \bar{x},\bar{x},x ; 0,0,0 |
| (21) $\bar{3}^-$ x,x,x; 0,0,0 | (22) $\bar{3}^-$ x, \bar{x},\bar{x} ; 0,0,0 | (23) $\bar{3}^-$ \bar{x},\bar{x},x ; 0,0,0 | (24) $\bar{3}^-$ \bar{x},x,\bar{x} ; 0,0,0 |

Symmetry operations (continued)

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

- | | | | |
|--|---|--|---|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \quad 0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2 \quad x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+ \quad \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{3}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \quad \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- \quad \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \quad \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $\bar{1} \quad 0, \frac{1}{4}, \frac{1}{4}$ | (14) $b \quad x, y, \frac{1}{4}$ | (15) $c \quad x, \frac{1}{4}, z$ | (16) $n(0, \frac{1}{2}, \frac{1}{2}) \quad 0, y, z$ |
| (17) $\bar{3}^+ \quad x, x + \frac{1}{2}, x; \quad 0, \frac{1}{2}, 0$ | (18) $\bar{3}^+ \quad \bar{x} - 1, x + \frac{1}{2}, \bar{x}; \quad -\frac{1}{2}, 0, \frac{1}{2}$ | (19) $\bar{3}^+ \quad x, \bar{x} + \frac{1}{2}, \bar{x}; \quad 0, \frac{1}{2}, 0$ | (20) $\bar{3}^+ \quad \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \quad \frac{1}{2}, 0, \frac{1}{2}$ |
| (21) $\bar{3}^- \quad x - \frac{1}{2}, x - \frac{1}{2}, x; \quad 0, 0, \frac{1}{2}$ | (22) $\bar{3}^- \quad x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; \quad 0, 0, \frac{1}{2}$ | (23) $\bar{3}^- \quad \bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; \quad -\frac{1}{2}, \frac{1}{2}, 0$ | (24) $\bar{3}^- \quad \bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}; \quad \frac{1}{2}, \frac{1}{2}, 0$ |

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

- | | | | |
|--|---|---|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2 \quad \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^+ \quad x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \quad \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x - \frac{1}{6}, x - \frac{1}{6}, x$ | (10) $3^- \quad x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^- \quad \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ |
| (13) $\bar{1} \quad \frac{1}{4}, 0, \frac{1}{4}$ | (14) $a \quad x, y, \frac{1}{4}$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, 0, z$ | (16) $c \quad \frac{1}{4}, y, z$ |
| (17) $\bar{3}^+ \quad x - \frac{1}{2}, x - \frac{1}{2}, x; \quad 0, 0, \frac{1}{2}$ | (18) $\bar{3}^+ \quad \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; \quad 0, 0, \frac{1}{2}$ | (19) $\bar{3}^+ \quad x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \quad \frac{1}{2}, \frac{1}{2}, 0$ | (20) $\bar{3}^+ \quad \bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \quad \frac{1}{2}, -\frac{1}{2}, 0$ |
| (21) $\bar{3}^- \quad x + \frac{1}{2}, x, x; \quad \frac{1}{2}, 0, 0$ | (22) $\bar{3}^- \quad x + \frac{1}{2}, \bar{x} - 1, \bar{x}; \quad 0, -\frac{1}{2}, \frac{1}{2}$ | (23) $\bar{3}^- \quad \bar{x} + \frac{1}{2}, \bar{x} + 1, x; \quad 0, \frac{1}{2}, \frac{1}{2}$ | (24) $\bar{3}^- \quad \bar{x} + \frac{1}{2}, x, \bar{x}; \quad \frac{1}{2}, 0, 0$ |

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

- | | | | |
|--|---|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \quad \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, x + \frac{1}{6}, x$ | (6) $3^+ \quad \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ \quad x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{6}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^- \quad x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- \quad \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, 0$ | (14) $n(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, 0$ | (15) $a \quad x, \frac{1}{4}, z$ | (16) $b \quad \frac{1}{4}, y, z$ |
| (17) $\bar{3}^+ \quad x + \frac{1}{2}, x, x; \quad \frac{1}{2}, 0, 0$ | (18) $\bar{3}^+ \quad \bar{x} - \frac{1}{2}, x + 1, \bar{x}; \quad 0, \frac{1}{2}, \frac{1}{2}$ | (19) $\bar{3}^+ \quad x - \frac{1}{2}, \bar{x} + 1, \bar{x}; \quad 0, \frac{1}{2}, -\frac{1}{2}$ | (20) $\bar{3}^+ \quad \bar{x} + \frac{1}{2}, \bar{x}, x; \quad \frac{1}{2}, 0, 0$ |
| (21) $\bar{3}^- \quad x, x + \frac{1}{2}, x; \quad 0, \frac{1}{2}, 0$ | (22) $\bar{3}^- \quad x + 1, \bar{x} - \frac{1}{2}, \bar{x}; \quad \frac{1}{2}, 0, \frac{1}{2}$ | (23) $\bar{3}^- \quad \bar{x}, \bar{x} + \frac{1}{2}, x; \quad 0, \frac{1}{2}, 0$ | (24) $\bar{3}^- \quad \bar{x} + 1, x - \frac{1}{2}, \bar{x}; \quad \frac{1}{2}, 0, -\frac{1}{2}$ |

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); (13)

Positions

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates | | | | Reflection conditions | | |
|---|---|--|--|--|--|--|---------------------|
| | $(0, 0, 0)+$ | $(0, \frac{1}{2}, \frac{1}{2})+$ | $(\frac{1}{2}, 0, \frac{1}{2})+$ | $(\frac{1}{2}, \frac{1}{2}, 0)+$ | | | |
| 96 $i \quad 1$ | (1) x, y, z (5) z, x, y (9) y, z, x (13) $\bar{x}, \bar{y}, \bar{z}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (21) $\bar{y}, \bar{z}, \bar{x}$ | (2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) x, y, \bar{z} (18) \bar{z}, x, y (22) y, \bar{z}, x | (3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) x, \bar{y}, z (19) z, x, \bar{y} (23) \bar{y}, z, x | (4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{x}, y, z (20) z, \bar{x}, y (24) y, z, \bar{x} | $hkl: h + k, h + l, k + l = 2n$ $Ok: k, l = 2n$ $hhl: h + l = 2n$ $h00: h = 2n$ | | |
| 48 $h \quad m..$ | $0, y, z$ $\bar{z}, 0, y$ | $0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ | $0, y, \bar{z}$ $y, z, 0$ | $0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ | $z, 0, y$ $y, \bar{z}, 0$ | $z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ | no extra conditions |
| 48 $g \quad 2..$ | $x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ | $\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$ | $\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ | $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ | $\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$ | $\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$ | $hkl: h = 2n$ |
| 32 $f \quad .3.$ | x, x, x $\bar{x}, \bar{x}, \bar{x}$ | \bar{x}, \bar{x}, x x, x, \bar{x} | \bar{x}, x, \bar{x} x, \bar{x}, x | x, \bar{x}, \bar{x} \bar{x}, x, x | no extra conditions | | |
| 24 $e \quad mm2..$ | $x, 0, 0$ | $\bar{x}, 0, 0$ | $0, x, 0$ | $0, \bar{x}, 0$ | $0, 0, x$ | $0, 0, \bar{x}$ | no extra conditions |
| 24 $d \quad 2/m..$ | $0, \frac{1}{4}, \frac{1}{4}$ | $0, \frac{3}{4}, \frac{1}{4}$ | $\frac{1}{4}, 0, \frac{1}{4}$ | $\frac{1}{4}, 0, \frac{3}{4}$ | $\frac{1}{4}, \frac{1}{4}, 0$ | $\frac{3}{4}, \frac{1}{4}, 0$ | $hkl: h = 2n$ |
| 8 $c \quad 23.$ | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ | | | | $hkl: h = 2n$ | |
| 4 $b \quad m\bar{3}.$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | | | | | no extra conditions |
| 4 $a \quad m\bar{3}.$ | $0, 0, 0$ | | | | | | no extra conditions |

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a} \quad \mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along [111] $p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$