

$Fd\bar{3}m$

O_h^7

$m\bar{3}m$

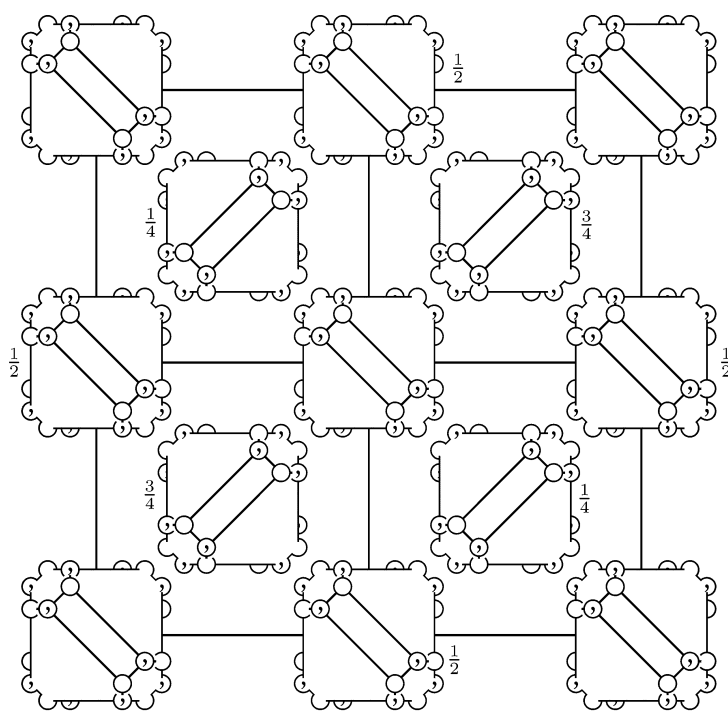
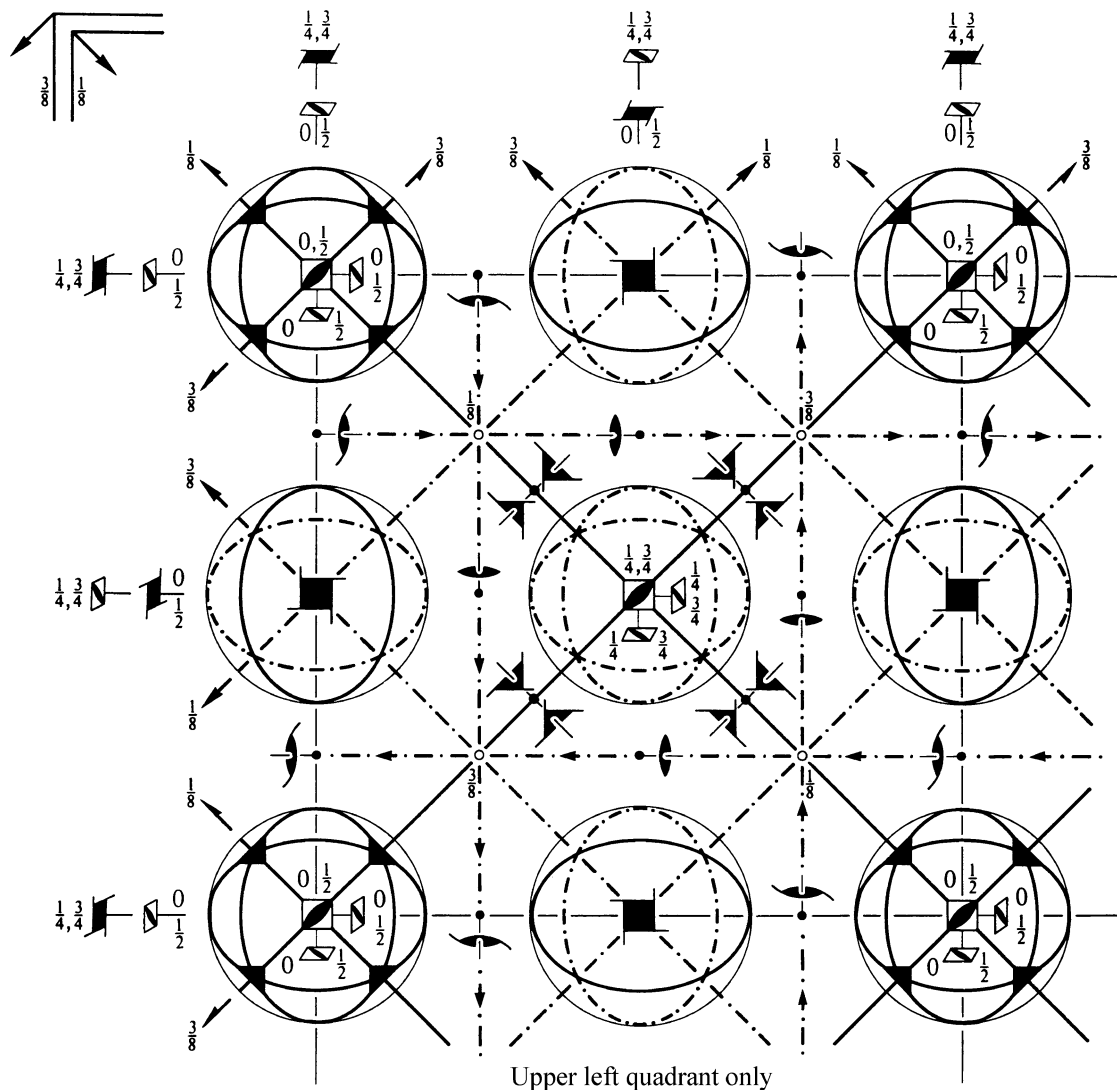
Cubic

No. 227

$F 4_1/d \bar{3} 2/m$

Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 1



Origin at $\bar{4}3m$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{8}; -\frac{1}{8} \leq z \leq \frac{1}{8}; y \leq \min(\frac{1}{2}-x, x); -y \leq z \leq y$
 Vertices $0, 0, 0 \quad \frac{3}{8}, 0, 0 \quad \frac{3}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{3}{8}, \frac{1}{8}, -\frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$

Symmetry operations

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

- | | | | |
|---|---|--|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad 0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{4}$ |
| (5) $3^+ x, x, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^+(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{3}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{3}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x - \frac{1}{4}, \frac{3}{8}$ | (14) $2 \quad x, \bar{x} + \frac{1}{4}, \frac{1}{8}$ | (15) $4^-(0, 0, \frac{3}{4}) \quad \frac{1}{2}, \frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{4}) \quad 0, \frac{3}{4}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0) \quad x, \frac{1}{2}, \frac{1}{4}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{3}{8}, y + \frac{1}{4}, y$ | (19) $2 \quad \frac{1}{8}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0) \quad x, 0, \frac{3}{4}$ |
| (21) $4^+(0, \frac{1}{4}, 0) \quad \frac{3}{4}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x - \frac{1}{4}, \frac{3}{8}, x$ | (23) $4^-(0, \frac{3}{4}, 0) \quad \frac{1}{4}, y, \frac{1}{2}$ | (24) $2 \quad \bar{x} + \frac{1}{4}, \frac{1}{8}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (26) $d(\frac{1}{4}, \frac{3}{4}, 0) \quad x, y, \frac{3}{8}$ | (27) $d(\frac{3}{4}, 0, \frac{1}{4}) \quad x, \frac{3}{8}, z$ | (28) $d(0, \frac{1}{4}, \frac{3}{4}) \quad \frac{3}{8}, y, z$ |
| (29) $\bar{3}^+ x, x, x; \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; \quad -\frac{1}{8}, \frac{1}{8}, \frac{7}{8}$ | (31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \quad \frac{1}{8}, \frac{7}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \quad \frac{7}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x, x, x; \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + \frac{3}{2}, \bar{x} - 1, \bar{x}; \quad \frac{5}{8}, -\frac{1}{8}, \frac{7}{8}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{3}{2}, x; \quad -\frac{1}{8}, \frac{7}{8}, \frac{5}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x + \frac{1}{2}, \bar{x}; \quad \frac{7}{8}, \frac{5}{8}, -\frac{1}{8}$ |
| (37) $g(\frac{1}{4}, -\frac{1}{4}, \frac{1}{2}) \quad x + \frac{1}{4}, \bar{x}, z$ | (38) $m \quad x, x, z$ | (39) $\bar{4}^- \quad -\frac{1}{4}, \frac{1}{4}, z; \quad -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (40) $\bar{4}^+ \quad \frac{1}{2}, 0, z; \quad \frac{1}{2}, 0, 0$ |
| (41) $\bar{4}^- x, -\frac{1}{4}, \frac{1}{4}; \quad \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (42) $g(\frac{1}{2}, \frac{1}{4}, -\frac{1}{4}) \quad x, y + \frac{1}{4}, \bar{y}$ | (43) $m \quad x, y, y$ | (44) $\bar{4}^+ x, \frac{1}{2}, 0; \quad 0, \frac{1}{2}, 0$ |
| (45) $\bar{4}^+ 0, y, \frac{1}{2}; \quad 0, 0, \frac{1}{2}$ | (46) $g(-\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) \quad \bar{x} + \frac{1}{4}, y, x$ | (47) $\bar{4}^- \quad \frac{1}{4}, y, -\frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ | (48) $m \quad x, y, x$ |

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

- | | | | |
|---|--|--|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, 0, z$ | (3) $2 \quad \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+ \quad \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x, \bar{x}, \bar{x}$ | (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) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- \quad \bar{x}, x, \bar{x}$ |
| (13) $2(\frac{3}{4}, \frac{3}{4}, 0) \quad x, x, \frac{1}{8}$ | (14) $2(-\frac{1}{4}, \frac{1}{4}, 0) \quad x, \bar{x} + \frac{1}{2}, \frac{3}{8}$ | (15) $4^-(0, 0, \frac{1}{4}) \quad \frac{1}{4}, 0, z$ | (16) $4^+(0, 0, \frac{3}{4}) \quad \frac{1}{4}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0) \quad x, \frac{1}{2}, -\frac{1}{4}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{3}{8}, y - \frac{1}{4}, y$ | (19) $2 \quad \frac{1}{8}, y + \frac{3}{4}, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0) \quad x, 0, \frac{1}{4}$ |
| (21) $4^+(0, \frac{3}{4}, 0) \quad \frac{1}{2}, y, -\frac{1}{4}$ | (22) $2(\frac{1}{4}, 0, \frac{1}{4}) \quad x, \frac{1}{8}, x$ | (23) $4^-(0, \frac{1}{4}, 0) \quad 0, y, \frac{3}{4}$ | (24) $2(-\frac{1}{4}, 0, \frac{1}{4}) \quad \bar{x} + \frac{1}{2}, \frac{3}{8}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (26) $d(\frac{1}{4}, \frac{1}{4}, 0) \quad x, y, \frac{1}{8}$ | (27) $d(\frac{3}{4}, 0, \frac{3}{4}) \quad x, \frac{1}{8}, z$ | (28) $d(0, \frac{3}{4}, \frac{1}{4}) \quad \frac{3}{8}, y, z$ |
| (29) $\bar{3}^+ x, x + \frac{1}{2}, x; \quad \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{3}{2}, \bar{x}; \quad -\frac{1}{8}, \frac{5}{8}, \frac{7}{8}$ | (31) $\bar{3}^+ x, \bar{x} + \frac{1}{2}, \bar{x}; \quad \frac{1}{8}, \frac{3}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x} - \frac{1}{2}, x; \quad \frac{7}{8}, -\frac{5}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; \quad \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (34) $\bar{3}^- x + 1, \bar{x} - \frac{3}{2}, \bar{x}; \quad \frac{1}{8}, -\frac{5}{8}, \frac{7}{8}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + 1, x; \quad -\frac{1}{8}, \frac{7}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x}, \bar{x}; \quad \frac{3}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $m \quad x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) \quad x - \frac{1}{4}, x, z$ | (39) $\bar{4}^- \quad 0, 0, z; \quad 0, 0, 0$ | (40) $\bar{4}^+ \quad \frac{1}{4}, -\frac{1}{4}, z; \quad \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (41) $\bar{4}^- x, \frac{1}{4}, \frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (42) $g(\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}) \quad x, y + \frac{1}{4}, \bar{y}$ | (43) $g(0, \frac{1}{2}, \frac{1}{2}) \quad x, y, y$ | (44) $\bar{4}^+ x, 0, 0; \quad 0, 0, 0$ |
| (45) $\bar{4}^+ \quad \frac{1}{4}, y, \frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (46) $m \quad \bar{x}, y, x$ | (47) $\bar{4}^- \quad \frac{1}{2}, y, 0; \quad \frac{1}{2}, 0, 0$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) \quad x - \frac{1}{4}, y, x$ |

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

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2 \quad \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2 \quad x, 0, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+ \quad \bar{x}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+ \quad \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x - \frac{1}{6}, x - \frac{1}{3}, x$ | (10) $3^-(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- \quad \bar{x}, \bar{x}, x$ | (12) $3^- \quad \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0) \quad x, x, \frac{1}{8}$ | (14) $2(\frac{1}{4}, -\frac{1}{4}, 0) \quad x, \bar{x} + \frac{1}{2}, \frac{3}{8}$ | (15) $4^-(0, 0, \frac{1}{4}) \quad \frac{3}{4}, 0, z$ | (16) $4^+(0, 0, \frac{3}{4}) \quad -\frac{1}{4}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0) \quad x, \frac{1}{4}, 0$ | (18) $2(0, \frac{3}{4}, \frac{3}{4}) \quad \frac{1}{8}, y, y$ | (19) $2(0, -\frac{1}{4}, \frac{1}{4}) \quad \frac{3}{8}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0) \quad x, \frac{1}{4}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{4}, 0) \quad \frac{1}{4}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x + \frac{1}{4}, \frac{3}{8}, x$ | (23) $4^-(0, \frac{3}{4}, 0) \quad -\frac{1}{4}, y, \frac{1}{2}$ | (24) $2 \quad \bar{x} + \frac{3}{4}, \frac{1}{8}, x$ |
| (25) $\bar{1} \quad \frac{3}{8}, \frac{1}{8}, \frac{3}{8}$ | (26) $d(\frac{3}{4}, \frac{3}{4}, 0) \quad x, y, \frac{1}{8}$ | (27) $d(\frac{1}{4}, 0, \frac{3}{4}) \quad x, \frac{3}{8}, z$ | (28) $d(0, \frac{1}{4}, \frac{1}{4}) \quad \frac{1}{8}, y, z$ |
| (29) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; \quad \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; \quad -\frac{1}{8}, \frac{1}{8}, \frac{3}{8}$ | (31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + \frac{3}{2}, \bar{x}; \quad \frac{1}{8}, \frac{7}{8}, -\frac{5}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{2}, \bar{x} + \frac{1}{2}, x; \quad \frac{7}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x, x; \quad \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + 1, \bar{x} - 1, \bar{x}; \quad \frac{1}{8}, -\frac{1}{8}, \frac{7}{8}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; \quad -\frac{1}{8}, \frac{3}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + \frac{3}{2}, x - \frac{1}{2}, \bar{x}; \quad \frac{7}{8}, \frac{1}{8}, -\frac{5}{8}$ |
| (37) $m \quad x, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) \quad x + \frac{1}{4}, x, z$ | (39) $\bar{4}^- \quad 0, \frac{1}{2}, z; \quad 0, \frac{1}{2}, 0$ | (40) $\bar{4}^+ \quad \frac{1}{4}, \frac{1}{4}, z; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (41) $\bar{4}^- x, 0, 0; \quad 0, 0, 0$ | (42) $m \quad x, y + \frac{1}{2}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) \quad x, y - \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{1}{4}, -\frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ |
| (45) $\bar{4}^+ 0, y, 0; \quad 0, 0, 0$ | (46) $g(\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}) \quad \bar{x} + \frac{1}{4}, y, x$ | (47) $\bar{4}^- \quad \frac{1}{4}, y, \frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) \quad x, y, x$ |

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

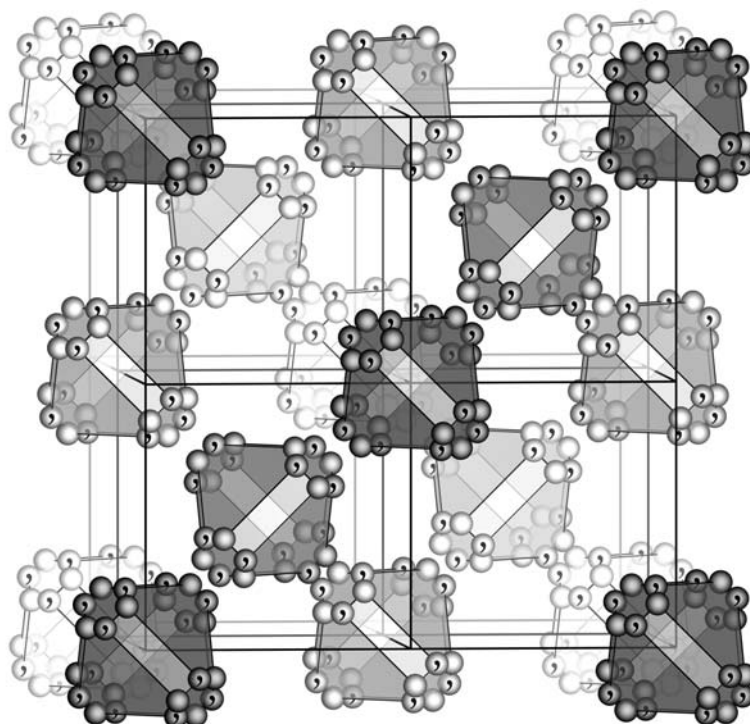
- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2 \quad 0, y, 0$ | (4) $2 \quad x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, x + \frac{1}{3}, x$ | (6) $3^+ \quad \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \quad \bar{x}, \bar{x}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^- x, \bar{x}, \bar{x}$ | (11) $3^- \quad \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x + \frac{1}{4}, \frac{3}{8}$ | (14) $2 \quad x, \bar{x} + \frac{3}{4}, \frac{1}{8}$ | (15) $4^-(0, 0, \frac{3}{4}) \quad \frac{1}{2}, -\frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{4}) \quad 0, \frac{1}{4}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0) \quad x, \frac{3}{4}, 0$ | (18) $2(0, \frac{1}{4}, \frac{1}{4}) \quad \frac{1}{8}, y, y$ | (19) $2(0, -\frac{1}{4}, -\frac{1}{4}) \quad \frac{3}{8}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0) \quad x, -\frac{1}{4}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{3}{4}, 0) \quad \frac{1}{2}, y, \frac{1}{4}$ | (22) $2(\frac{3}{4}, 0, \frac{3}{4}) \quad x, \frac{1}{8}, x$ | (23) $4^-(0, \frac{1}{4}, 0) \quad 0, y, \frac{1}{4}$ | (24) $2(\frac{1}{4}, 0, -\frac{1}{4}) \quad \bar{x} + \frac{1}{2}, \frac{3}{8}, x$ |
| (25) $\bar{1} \quad \frac{3}{8}, \frac{3}{8}, \frac{1}{8}$ | (26) $d(\frac{3}{4}, \frac{1}{4}, 0) \quad x, y, \frac{3}{8}$ | (27) $d(\frac{1}{4}, 0, \frac{1}{4}) \quad x, \frac{1}{8}, z$ | (28) $d(0, \frac{3}{4}, \frac{3}{4}) \quad \frac{1}{8}, y, z$ |
| (29) $\bar{3}^+ x + \frac{1}{2}, x, x; \quad \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - \frac{3}{2}, x + 1, \bar{x}; \quad -\frac{5}{8}, \frac{1}{8}, \frac{7}{8}$ | (31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + 1, \bar{x}; \quad \frac{5}{8}, \frac{7}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x}, \bar{x}; \quad \frac{3}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x, x + \frac{1}{2}, x; \quad \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; \quad \frac{1}{8}, -\frac{1}{8}, \frac{3}{8}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + 1, x; \quad -\frac{5}{8}, \frac{7}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x, \bar{x}; \quad \frac{7}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $g(-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) \quad x + \frac{1}{4}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, z$ | (39) $\bar{4}^- \quad \frac{1}{4}, \frac{1}{4}, z; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (40) $\bar{4}^+ 0, 0, z; \quad 0, 0, 0$ |
| (41) $\bar{4}^- x, 0, \frac{1}{2}; \quad 0, 0, \frac{1}{2}$ | (42) $m \quad x, y, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) \quad x, y + \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{1}{4}, \frac{1}{4}; \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (45) $\bar{4}^+ \quad -\frac{1}{4}, y, \frac{1}{4}; \quad -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (46) $m \quad \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- 0, y, 0; \quad 0, 0, 0$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) \quad x + \frac{1}{4}, y, x$ |

ORIGIN CHOICE 1

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); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions																																																
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+ (\frac{1}{2}, 0, \frac{1}{2})+ (\frac{1}{2}, \frac{1}{2}, 0)+$	h, k, l permutable General:																																																
192 i 1	<table border="0"> <tr> <td>(1) x, y, z</td> <td>(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$</td> <td>(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$</td> <td>(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$</td> </tr> <tr> <td>(5) z, x, y</td> <td>(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$</td> <td>(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$</td> <td>(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$</td> </tr> <tr> <td>(9) y, z, x</td> <td>(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$</td> <td>(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$</td> <td>(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$</td> </tr> <tr> <td>(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$</td> <td>(14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$</td> <td>(15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$</td> <td>(16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$</td> </tr> <tr> <td>(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$</td> <td>(18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$</td> <td>(19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$</td> <td>(20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$</td> </tr> <tr> <td>(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$</td> <td>(22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$</td> <td>(23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$</td> <td>(24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$</td> </tr> <tr> <td>(25) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$</td> <td>(26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$</td> <td>(27) $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{4}$</td> <td>(28) $\bar{x} + \frac{3}{4}, y + \frac{1}{4}, z + \frac{3}{4}$</td> </tr> <tr> <td>(29) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$</td> <td>(30) $\bar{z} + \frac{3}{4}, x + \frac{1}{4}, y + \frac{3}{4}$</td> <td>(31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{3}{4}$</td> <td>(32) $z + \frac{3}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{4}$</td> </tr> <tr> <td>(33) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$</td> <td>(34) $y + \frac{3}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{4}$</td> <td>(35) $\bar{y} + \frac{3}{4}, z + \frac{1}{4}, x + \frac{3}{4}$</td> <td>(36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{3}{4}$</td> </tr> <tr> <td>(37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$</td> <td>(38) y, x, z</td> <td>(39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$</td> <td>(40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$</td> </tr> <tr> <td>(41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$</td> <td>(42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$</td> <td>(43) x, z, y</td> <td>(44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$</td> </tr> <tr> <td>(45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$</td> <td>(46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$</td> <td>(47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$</td> <td>(48) z, y, x</td> </tr> </table>	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$	(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$	(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$	(14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$	(16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$	(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$	(23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	(25) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(27) $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{4}$	(28) $\bar{x} + \frac{3}{4}, y + \frac{1}{4}, z + \frac{3}{4}$	(29) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(30) $\bar{z} + \frac{3}{4}, x + \frac{1}{4}, y + \frac{3}{4}$	(31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{3}{4}$	(32) $z + \frac{3}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{4}$	(33) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	(34) $y + \frac{3}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{4}$	(35) $\bar{y} + \frac{3}{4}, z + \frac{1}{4}, x + \frac{3}{4}$	(36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{3}{4}$	(37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$	(38) y, x, z	(39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	(41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$	(42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$	(43) x, z, y	(44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$	(48) z, y, x	<p>hkl: $h + k = 2n$ and $h + l, k + l = 2n$ $0kl$: $k + l = 4n$ and $k, l = 2n$ hhl: $h + l = 2n$ $h00$: $h = 4n$</p>
(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$																																															
(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$	(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$																																															
(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$																																															
(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$	(14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$	(16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$																																															
(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$																																															
(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$	(23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$																																															
(25) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(27) $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{4}$	(28) $\bar{x} + \frac{3}{4}, y + \frac{1}{4}, z + \frac{3}{4}$																																															
(29) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(30) $\bar{z} + \frac{3}{4}, x + \frac{1}{4}, y + \frac{3}{4}$	(31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{3}{4}$	(32) $z + \frac{3}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{4}$																																															
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(37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$	(38) y, x, z	(39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$																																															
(41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$	(42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$	(43) x, z, y	(44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$																																															
(45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$	(48) z, y, x																																															
96 h . . 2	<table border="0"> <tr> <td>$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$</td> <td>$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$</td> <td>$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$</td> <td>$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$</td> </tr> <tr> <td>$\bar{y} + \frac{1}{4}, \frac{1}{8}, y$</td> <td>$\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$</td> <td>$y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$</td> <td>$y + \frac{1}{4}, \frac{5}{8}, \bar{y}$</td> </tr> <tr> <td>$y, \bar{y} + \frac{1}{4}, \frac{1}{8}$</td> <td>$\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$</td> <td>$y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$</td> <td>$\bar{y}, y + \frac{1}{4}, \frac{5}{8}$</td> </tr> <tr> <td>$\frac{1}{8}, \bar{y} + \frac{1}{4}, y$</td> <td>$\frac{3}{8}, y + \frac{3}{4}, y + \frac{1}{2}$</td> <td>$\frac{7}{8}, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$</td> <td>$\frac{5}{8}, y + \frac{1}{4}, \bar{y}$</td> </tr> <tr> <td>$y, \frac{1}{8}, \bar{y} + \frac{1}{4}$</td> <td>$y + \frac{1}{2}, \frac{3}{8}, y + \frac{3}{4}$</td> <td>$\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{3}{4}$</td> <td>$\bar{y}, \frac{5}{8}, y + \frac{1}{4}$</td> </tr> <tr> <td>$\bar{y} + \frac{1}{4}, y, \frac{1}{8}$</td> <td>$y + \frac{3}{4}, y + \frac{1}{2}, \frac{3}{8}$</td> <td>$\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{7}{8}$</td> <td>$y + \frac{1}{4}, y, \frac{5}{8}$</td> </tr> </table>	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$	$\bar{y} + \frac{1}{4}, \frac{1}{8}, y$	$\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$	$y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$	$y + \frac{1}{4}, \frac{5}{8}, \bar{y}$	$y, \bar{y} + \frac{1}{4}, \frac{1}{8}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$	$y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$	$\bar{y}, y + \frac{1}{4}, \frac{5}{8}$	$\frac{1}{8}, \bar{y} + \frac{1}{4}, y$	$\frac{3}{8}, y + \frac{3}{4}, y + \frac{1}{2}$	$\frac{7}{8}, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{5}{8}, y + \frac{1}{4}, \bar{y}$	$y, \frac{1}{8}, \bar{y} + \frac{1}{4}$	$y + \frac{1}{2}, \frac{3}{8}, y + \frac{3}{4}$	$\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{3}{4}$	$\bar{y}, \frac{5}{8}, y + \frac{1}{4}$	$\bar{y} + \frac{1}{4}, y, \frac{1}{8}$	$y + \frac{3}{4}, y + \frac{1}{2}, \frac{3}{8}$	$\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{7}{8}$	$y + \frac{1}{4}, y, \frac{5}{8}$	Special: as above, plus no extra conditions																								
$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$																																															
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$y, \frac{1}{8}, \bar{y} + \frac{1}{4}$	$y + \frac{1}{2}, \frac{3}{8}, y + \frac{3}{4}$	$\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{3}{4}$	$\bar{y}, \frac{5}{8}, y + \frac{1}{4}$																																															
$\bar{y} + \frac{1}{4}, y, \frac{1}{8}$	$y + \frac{3}{4}, y + \frac{1}{2}, \frac{3}{8}$	$\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{7}{8}$	$y + \frac{1}{4}, y, \frac{5}{8}$																																															
96 g . . m	<table border="0"> <tr> <td>x, x, z</td> <td>$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$</td> <td>$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$</td> <td>$x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$</td> </tr> <tr> <td>$z, x, x$</td> <td>$z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$</td> <td>$\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$</td> <td>$\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$</td> </tr> <tr> <td>$x, z, x$</td> <td>$\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$</td> <td>$x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$</td> <td>$\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$</td> </tr> <tr> <td>$x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$</td> <td>$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$</td> <td>$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$</td> <td>$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$</td> </tr> <tr> <td>$x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{3}{4}$</td> <td>$\bar{x} + \frac{3}{4}, z + \frac{3}{4}, x + \frac{1}{4}$</td> <td>$\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$</td> <td>$x + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{3}{4}$</td> </tr> <tr> <td>$z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$</td> <td>$z + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$</td> <td>$\bar{z} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$</td> <td>$\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$</td> </tr> </table>	x, x, z	$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	z, x, x	$z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	x, z, x	$\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	$x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	$x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, z + \frac{3}{4}, x + \frac{1}{4}$	$\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{3}{4}$	$z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$z + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{z} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	$\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	no extra conditions																								
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z, x, x	$z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$																																															
x, z, x	$\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$																																															
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48 f 2 . mm	<table border="0"> <tr> <td>$x, 0, 0$</td> <td>$\bar{x}, \frac{1}{2}, \frac{1}{2}$</td> <td>$0, x, 0$</td> <td>$\frac{1}{2}, \bar{x}, \frac{1}{2}$</td> <td>$0, 0, x$</td> <td>$\frac{1}{2}, \frac{1}{2}, \bar{x}$</td> </tr> <tr> <td>$\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$</td> <td>$\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$</td> <td>$x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$</td> <td>$\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$</td> <td>$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$</td> <td>$\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$</td> </tr> </table>	$x, 0, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$0, 0, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$	$\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$	hkl : $h = 2n + 1$ or $h + k + l = 4n$																																				
$x, 0, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$0, 0, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$																																													
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32 e . 3 m	<table border="0"> <tr> <td>x, x, x</td> <td>$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$</td> </tr> <tr> <td>$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$</td> <td>$x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$</td> </tr> <tr> <td>$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$</td> <td>$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$</td> </tr> <tr> <td>$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$</td> <td>$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$</td> </tr> </table>	x, x, x	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	no extra conditions																																								
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16 d . $\bar{3} m$	<table border="0"> <tr> <td>$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$</td> <td>$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$</td> <td>$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$</td> <td>$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$</td> </tr> </table>	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$	<p>hkl: $h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$</p>																																												
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8 b $\bar{4} 3 m$	<table border="0"> <tr> <td>$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$</td> <td>$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$</td> </tr> </table>	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	<p>hkl: $h = 2n + 1$ or $h + k + l = 4n$</p>																																														
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8 a $\bar{4} 3 m$	<table border="0"> <tr> <td>$0, 0, 0$</td> <td>$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$</td> </tr> </table>	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$																																															
$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$																																																	



Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110]$ $c2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, \frac{1}{3}$

$Fd\bar{3}m$

O_h^7

$m\bar{3}m$

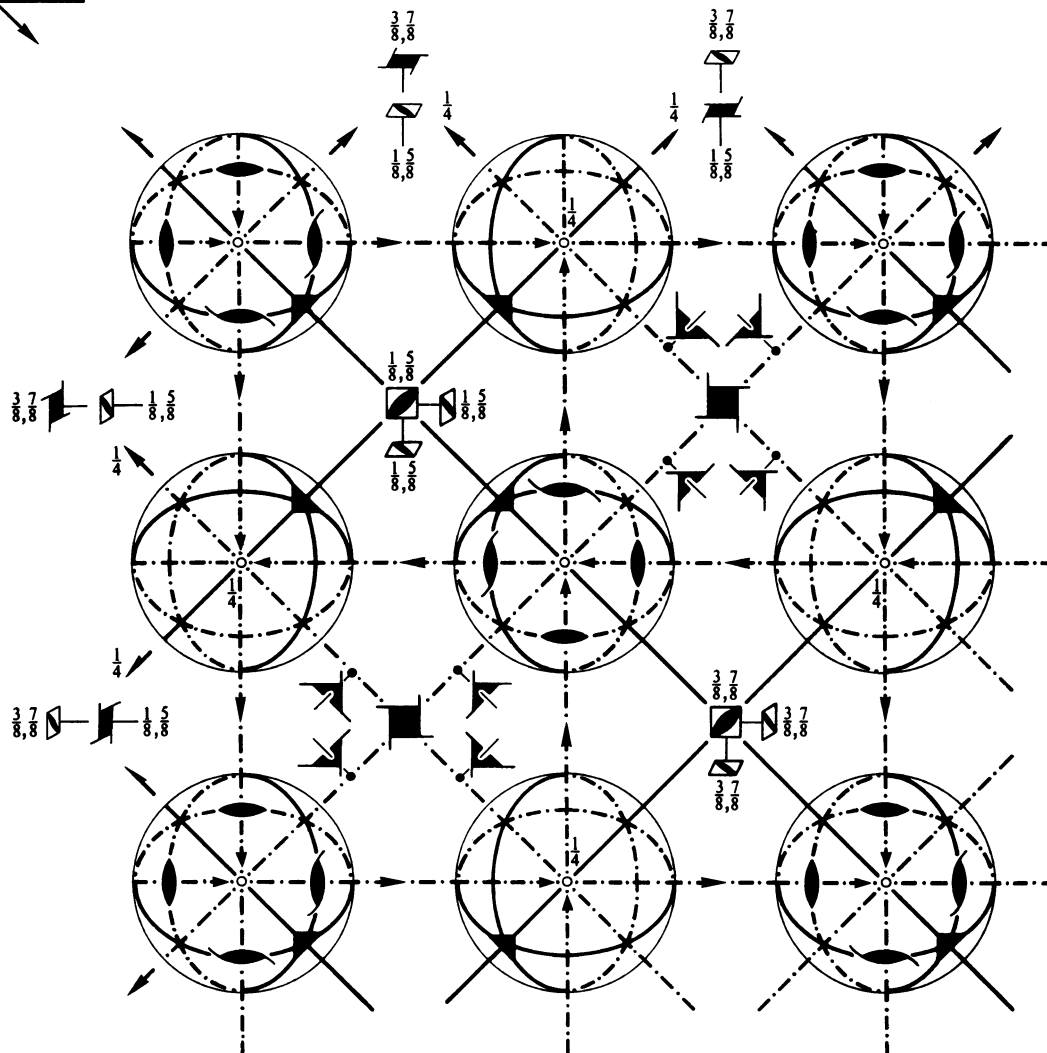
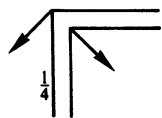
Cubic

No. 227

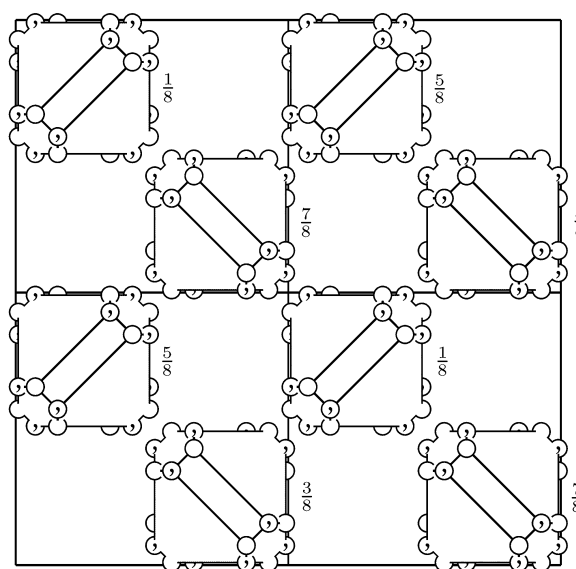
$F4_1/d\bar{3}2/m$

Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 2



Upper left quadrant only



Origin at centre ($\bar{3}m$), at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from $\bar{4}3m$

Asymmetric unit $-\frac{1}{8} \leq x \leq \frac{3}{8}; -\frac{1}{8} \leq y \leq 0; -\frac{1}{4} \leq z \leq 0; y \leq \min(\frac{1}{4} - x, x); -y - \frac{1}{4} \leq z \leq y$
Vertices $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{1}{4}, 0, 0; 0, 0, 0; \frac{1}{4}, 0, -\frac{1}{4}; 0, 0, -\frac{1}{4}$

Symmetry operationsFor $(0,0,0)+$ set

- | | | | |
|---|--|--|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \frac{3}{8}, \frac{1}{8}, z$ | (3) $2(0,\frac{1}{2},0) \frac{1}{8}, y, \frac{3}{8}$ | (4) $2(\frac{1}{2},0,0) x, \frac{3}{8}, \frac{1}{8}$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{5}{12}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \bar{x} + \frac{7}{12}, \bar{x} + \frac{5}{12}, x$ | (12) $3^- (\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} - \frac{1}{6}, x + \frac{7}{12}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{4}, \frac{1}{4}$ | (14) $2 x, \bar{x}, 0$ | (15) $4^-(0,0,\frac{3}{4}) \frac{3}{8}, \frac{1}{8}, z$ | (16) $4^+(0,0,\frac{1}{4}) -\frac{1}{8}, \frac{5}{8}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0) x, \frac{3}{8}, \frac{1}{8}$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4}, y + \frac{1}{4}, y$ | (19) $2 0, y, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0) x, -\frac{1}{8}, \frac{5}{8}$ |
| (21) $4^+(0,\frac{1}{4}, 0) \frac{5}{8}, y, -\frac{1}{8}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x - \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0,\frac{3}{4}, 0) \frac{1}{8}, y, \frac{3}{8}$ | (24) $2 \bar{x}, 0, x$ |
| (25) $\bar{1} 0, 0, 0$ | (26) $d(\frac{1}{4}, \frac{3}{4}, 0) x, y, \frac{1}{4}$ | (27) $d(\frac{3}{4}, 0, \frac{1}{4}) x, \frac{1}{4}, z$ | (28) $d(0, \frac{1}{4}, \frac{3}{4}) \frac{1}{4}, y, z$ |
| (29) $\bar{3}^+ x, x, x; 0, 0, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{3}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{3}{4}$ | (31) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + 1, \bar{x}; 0, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, 0$ |
| (33) $\bar{3}^- x, x, x; 0, 0, 0$ | (34) $\bar{3}^- x + \frac{5}{4}, \bar{x} - 1, \bar{x}; \frac{1}{2}, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{5}{4}, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ | (36) $\bar{3}^- \bar{x} + 1, x + \frac{1}{4}, \bar{x}; \frac{3}{4}, \frac{1}{2}, -\frac{1}{4}$ |
| (37) $g(-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $m x, x, z$ | (39) $\bar{4}^- \frac{1}{8}, \frac{5}{8}, z; \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (40) $\bar{4}^+ \frac{3}{8}, -\frac{1}{8}, z; \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$ |
| (41) $\bar{4}^- x, \frac{1}{8}, \frac{5}{8}; \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (42) $g(\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}) x, y + \frac{1}{2}, \bar{y}$ | (43) $m x, y, y$ | (44) $\bar{4}^+ x, \frac{3}{8}, -\frac{1}{8}; \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ |
| (45) $\bar{4}^+ -\frac{1}{8}, y, \frac{3}{8}; -\frac{1}{8}, \frac{1}{8}, \frac{3}{8}$ | (46) $g(\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{5}{8}, y, \frac{1}{8}; \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (48) $m x, y, x$ |

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

- | | | | |
|--|--|--|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \frac{3}{8}, \frac{3}{8}, z$ | (3) $2 \frac{1}{8}, y, \frac{1}{8}$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{8}, \frac{3}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} + \frac{1}{6}, x + \frac{5}{12}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^- \bar{x}, x + \frac{3}{4}, \bar{x}$ |
| (13) $2(\frac{3}{4}, \frac{3}{4}, 0) x, x, 0$ | (14) $2(-\frac{1}{4}, \frac{1}{4}, 0) x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{4}) \frac{1}{8}, -\frac{1}{8}, z$ | (16) $4^+(0, 0, \frac{3}{4}) \frac{1}{8}, \frac{3}{8}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0) x, \frac{3}{8}, -\frac{3}{8}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{4}, y - \frac{1}{4}, y$ | (19) $2 0, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0) x, -\frac{1}{8}, \frac{1}{8}$ |
| (21) $4^+(0, \frac{3}{4}, 0) \frac{3}{8}, y, -\frac{3}{8}$ | (22) $2(\frac{1}{4}, 0, \frac{1}{4}) x, 0, x$ | (23) $4^-(0, \frac{1}{4}, 0) -\frac{1}{8}, y, \frac{5}{8}$ | (24) $2(-\frac{1}{4}, 0, \frac{1}{4}) \bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |
| (25) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (26) $d(\frac{1}{4}, \frac{1}{4}, 0) x, y, 0$ | (27) $d(\frac{3}{4}, 0, \frac{3}{4}) x, 0, z$ | (28) $d(0, \frac{3}{4}, \frac{1}{4}) \frac{1}{4}, y, z$ |
| (29) $\bar{3}^+ x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{5}{4}, \bar{x}; -\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ | (31) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}; 0, \frac{1}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{3}{4}, x; \frac{3}{4}, -\frac{3}{4}, 0$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (34) $\bar{3}^- x + \frac{3}{4}, \bar{x} - \frac{3}{2}, \bar{x}; 0, -\frac{3}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{4}, \bar{x} + \frac{3}{4}, x; -\frac{1}{4}, \frac{3}{4}, 0$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x - \frac{1}{4}, \bar{x}; \frac{1}{4}, 0, -\frac{1}{4}$ |
| (37) $m x + \frac{1}{4}, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x - \frac{1}{4}, x, z$ | (39) $\bar{4}^- \frac{3}{8}, \frac{3}{8}, z; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (40) $\bar{4}^+ \frac{5}{8}, \frac{1}{8}, z; \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (41) $\bar{4}^- x, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (42) $g(\frac{1}{2}, \frac{1}{4}, -\frac{1}{4}) x, y + \frac{1}{2}, \bar{y}$ | (43) $g(0, \frac{1}{2}, \frac{1}{2}) x, y, y$ | (44) $\bar{4}^+ x, \frac{3}{8}, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8}, y, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (46) $m \bar{x} + \frac{3}{4}, y, x$ | (47) $\bar{4}^- \frac{3}{8}, y, -\frac{1}{8}; \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) x - \frac{1}{4}, y, x$ |

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

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2 \frac{1}{8}, \frac{1}{8}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{3}{8}, y, \frac{1}{8}$ | (4) $2 x, \frac{3}{8}, \frac{3}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+ \bar{x}, x + \frac{3}{4}, \bar{x}$ | (7) $3^+ x + \frac{1}{4}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{5}{12}, \bar{x} + \frac{7}{12}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x - \frac{1}{6}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ | (12) $3^- \bar{x}, x + \frac{1}{4}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0) x, x, 0$ | (14) $2(\frac{1}{4}, -\frac{1}{4}, 0) x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{4}) \frac{3}{8}, -\frac{1}{8}, z$ | (16) $4^+(0, 0, \frac{3}{4}) -\frac{3}{8}, \frac{3}{8}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0) x, \frac{1}{8}, -\frac{1}{8}$ | (18) $2(0, \frac{3}{4}, \frac{3}{4}) 0, y, y$ | (19) $2(0, -\frac{1}{4}, \frac{1}{4}) \frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0) x, \frac{1}{8}, \frac{3}{8}$ |
| (21) $4^+(0, \frac{1}{4}, 0) \frac{1}{8}, y, -\frac{1}{8}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x + \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0, \frac{3}{4}, 0) -\frac{3}{8}, y, \frac{3}{8}$ | (24) $2 \bar{x} + \frac{1}{2}, 0, x$ |
| (25) $\bar{1} \frac{1}{4}, 0, \frac{1}{4}$ | (26) $d(\frac{3}{4}, \frac{3}{4}, 0) x, y, 0$ | (27) $d(\frac{1}{4}, 0, \frac{3}{4}) x, \frac{1}{4}, z$ | (28) $d(0, \frac{1}{4}, \frac{1}{4}) 0, y, z$ |
| (29) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{1}{4}$ | (31) $\bar{3}^+ x - \frac{3}{4}, \bar{x} + \frac{3}{2}, \bar{x}; 0, \frac{3}{4}, -\frac{3}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{5}{4}, \bar{x} + \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{2}$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (34) $\bar{3}^- x + \frac{3}{4}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{4}, \bar{x} + \frac{1}{4}, x; -\frac{1}{4}, \frac{1}{4}, 0$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x - \frac{3}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{3}{4}$ |
| (37) $m x + \frac{3}{4}, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x + \frac{1}{4}, x, z$ | (39) $\bar{4}^- -\frac{1}{8}, \frac{3}{8}, z; -\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (40) $\bar{4}^+ \frac{1}{8}, \frac{3}{8}, z; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (41) $\bar{4}^- x, \frac{3}{8}, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (42) $m x, y + \frac{1}{4}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) x, y - \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{5}{8}, \frac{1}{8}; \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{3}{8}, y, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (46) $g(-\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{8}, y, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) x, y, x$ |

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

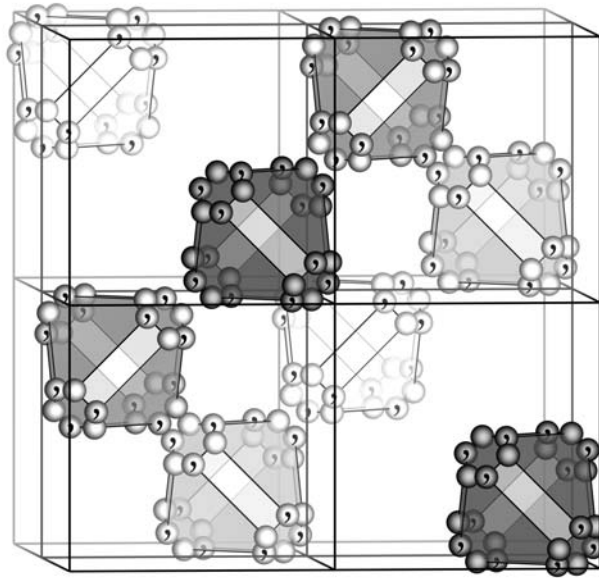
- | | | | |
|---|--|---|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, 0, \frac{1}{2}) \frac{1}{8}, \frac{3}{8}, z$ | (3) $2 \frac{3}{8}, y, \frac{3}{8}$ | (4) $2 x, \frac{1}{8}, \frac{1}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x + \frac{1}{6}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+ (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{7}{12}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^- x + \frac{3}{4}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{3}{4}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{4}, \frac{1}{4}$ | (14) $2 x, \bar{x} + \frac{1}{2}, 0$ | (15) $4^-(0, 0, \frac{3}{4}) \frac{3}{8}, -\frac{3}{8}, z$ | (16) $4^+(0, 0, \frac{1}{4}) -\frac{1}{8}, \frac{1}{8}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0) x, \frac{5}{8}, -\frac{1}{8}$ | (18) $2(0, \frac{1}{4}, \frac{1}{4}) 0, y, y$ | (19) $2(0, \frac{1}{4}, -\frac{1}{4}) \frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0) x, -\frac{3}{8}, \frac{3}{8}$ |
| (21) $4^+(0, \frac{3}{4}, 0) \frac{3}{8}, y, \frac{1}{8}$ | (22) $2(\frac{3}{4}, 0, \frac{3}{4}) x, 0, x$ | (23) $4^-(0, \frac{1}{4}, 0) -\frac{1}{8}, y, \frac{1}{8}$ | (24) $2(\frac{1}{4}, 0, -\frac{1}{4}) \bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |
| (25) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (26) $d(\frac{3}{4}, \frac{1}{4}, 0) x, y, \frac{1}{4}$ | (27) $d(\frac{1}{4}, 0, \frac{1}{4}) x, 0, z$ | (28) $d(0, \frac{3}{4}, \frac{3}{4}) 0, y, z$ |
| (29) $\bar{3}^+ x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (30) $\bar{3}^+ \bar{x} - \frac{3}{2}, x + \frac{3}{4}, \bar{x}; -\frac{3}{4}, 0, \frac{3}{4}$ | (31) $\bar{3}^+ x + \frac{1}{4}, \bar{x} + 1, \bar{x}; \frac{1}{2}, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{4}, \bar{x} - \frac{1}{4}, x; \frac{1}{4}, -\frac{1}{4}, 0$ |
| (33) $\bar{3}^- x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (34) $\bar{3}^- x + \frac{1}{4}, \bar{x} - \frac{1}{2}, \bar{x}; 0, -\frac{1}{4}, \frac{1}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{3}{4}, \bar{x} + \frac{3}{4}, x; -\frac{3}{4}, \frac{3}{4}, 0$ | (36) $\bar{3}^- \bar{x} + 1, x - \frac{1}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{1}{4}$ |
| (37) $g(\frac{1}{4}, -\frac{1}{4}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, 0, 0) x, x, z$ | (39) $\bar{4}^- \frac{1}{8}, \frac{1}{8}, z; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (40) $\bar{4}^+ \frac{3}{8}, \frac{3}{8}, z; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ |
| (41) $\bar{4}^- x, -\frac{1}{8}, \frac{3}{8}; \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$ | (42) $m x, y + \frac{3}{4}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) x, y + \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8}, y, \frac{5}{8}; \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (46) $m \bar{x} + \frac{1}{4}, y, x$ | (47) $\bar{4}^- \frac{3}{8}, y, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) x + \frac{1}{4}, y, x$ |

ORIGIN CHOICE 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); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions		
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	h, k, l permutable General:		
192 <i>i</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{2}$ (17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{1}{2}$ (21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{1}{2}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{1}{2}$	(2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{y} + \frac{1}{4}$ (10) $\bar{y} + \frac{1}{4}, z + \frac{1}{2}, \bar{x} + \frac{3}{4}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{3}{4}, y + \frac{1}{4}$ (22) $z + \frac{1}{4}, \bar{y} + \frac{1}{2}, x + \frac{3}{4}$ (26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{1}{2}$ (30) $\bar{z} + \frac{1}{2}, x + \frac{1}{4}, y + \frac{3}{4}$ (34) $y + \frac{3}{4}, \bar{z} + \frac{1}{2}, x + \frac{1}{4}$ (38) y, x, z	(3) $\bar{x} + \frac{1}{4}, y + \frac{1}{2}, \bar{z} + \frac{3}{4}$ (7) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}$ (15) $y + \frac{1}{4}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$ (19) $\bar{x}, \bar{z}, \bar{y}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{3}{4}, x + \frac{1}{4}$ (27) $x + \frac{3}{4}, \bar{y} + \frac{1}{2}, z + \frac{1}{4}$ (31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{1}{2}$ (35) $\bar{y} + \frac{1}{2}, z + \frac{1}{4}, x + \frac{3}{4}$ (39) $\bar{y} + \frac{3}{4}, x + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (43) x, z, y (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{3}{4}, \bar{z} + \frac{1}{4}$ (8) $\bar{z} + \frac{1}{4}, x + \frac{1}{2}, \bar{y} + \frac{3}{4}$ (12) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{1}{4}, x + \frac{1}{2}$ (16) $\bar{y} + \frac{1}{2}, x + \frac{3}{4}, z + \frac{1}{4}$ (20) $x + \frac{1}{4}, \bar{z} + \frac{1}{2}, y + \frac{3}{4}$ (24) $\bar{z}, \bar{y}, \bar{x}$ (28) $\bar{x} + \frac{1}{2}, y + \frac{1}{4}, z + \frac{3}{4}$ (32) $z + \frac{3}{4}, \bar{x} + \frac{1}{2}, y + \frac{1}{4}$ (36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{1}{2}$ (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (44) $\bar{x} + \frac{3}{4}, z + \frac{1}{2}, \bar{y} + \frac{1}{4}$ (48) z, y, x	hkl : $h + k = 2n$ and $h + l, k + l = 2n$ Ok : $k + l = 4n$ and $k, l = 2n$ hhl : $h + l = 2n$ $h00$: $h = 4n$		
96 <i>h</i> .. 2	$0, y, \bar{y}$ $\bar{y}, 0, y$ $y, \bar{y}, 0$ $0, \bar{y}, y$ $y, 0, \bar{y}$ $\bar{y}, y, 0$	$\frac{3}{4}, \bar{y} + \frac{1}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, y + \frac{3}{4}$ $y + \frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, y + \frac{1}{2}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{1}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{3}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \bar{y} + \frac{3}{4}, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{1}{2}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{4}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{1}{2}, y + \frac{1}{4}$ $y + \frac{1}{4}, \bar{y} + \frac{3}{4}, \frac{1}{2}$	Special: as above, plus no extra conditions		
96 <i>g</i> .. <i>m</i>	x, x, z z, x, x x, z, x $x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{2}$ $x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{2}$ $z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$	$\bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}$ $\bar{x} + \frac{1}{4}, z + \frac{1}{2}, \bar{x} + \frac{3}{4}$ $\bar{x}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, z + \frac{3}{4}, x + \frac{1}{4}$ $z + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, x + \frac{1}{2}, \bar{z} + \frac{3}{4}$ $\bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}$ $x + \frac{1}{4}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$ $\bar{x}, \bar{z}, \bar{x}$ $\bar{z} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{1}{4}$ $\bar{z} + \frac{1}{4}, x + \frac{1}{2}, \bar{x} + \frac{3}{4}$ $\bar{x} + \frac{3}{4}, \bar{z} + \frac{1}{4}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, z + \frac{1}{4}$ $x + \frac{1}{4}, \bar{z} + \frac{1}{2}, x + \frac{3}{4}$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions		
48 <i>f</i> 2. <i>mm</i>	$x, \frac{1}{8}, \frac{1}{8}$ $\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}$	$\bar{x} + \frac{3}{4}, \frac{1}{8}, \frac{5}{8}$ $\frac{7}{8}, \bar{x}, \frac{7}{8}$	$\frac{1}{8}, x, \frac{1}{8}$ $x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}$	$\frac{5}{8}, \bar{x} + \frac{3}{4}, \frac{1}{8}$ $\bar{x} + \frac{1}{2}, \frac{7}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{1}{8}, x$ $\frac{7}{8}, \frac{3}{8}, \bar{x} + \frac{1}{2}$	$\frac{1}{8}, \frac{5}{8}, \bar{x} + \frac{3}{4}$ $\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}$	hkl : $h = 2n + 1$ or $h + k + l = 4n$
32 <i>e</i> . 3 <i>m</i>	x, x, x $\bar{x} + \frac{1}{4}, x + \frac{1}{2}, \bar{x} + \frac{3}{4}$ $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}$ $\bar{x}, \bar{x}, \bar{x}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$				no extra conditions	
16 <i>d</i> . $\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{1}{4}$	$0, \frac{1}{4}, \frac{3}{4}$	} hkl : $h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$		
16 <i>c</i> . $\bar{3}m$	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$			
8 <i>b</i> $\bar{4}3m$	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$			} hkl : $h = 2n + 1$ or $h + k + l = 4n$		
8 <i>a</i> $\bar{4}3m$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{3}{8}$					



Symmetry of special projections

Along $[001]$ $p4mm$
 $\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$
 Origin at $\frac{1}{8}, \frac{3}{8}, z$

Along $[111]$ $p6mm$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

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