

$Fd\bar{3}c$

$O_h^8$

$m\bar{3}m$

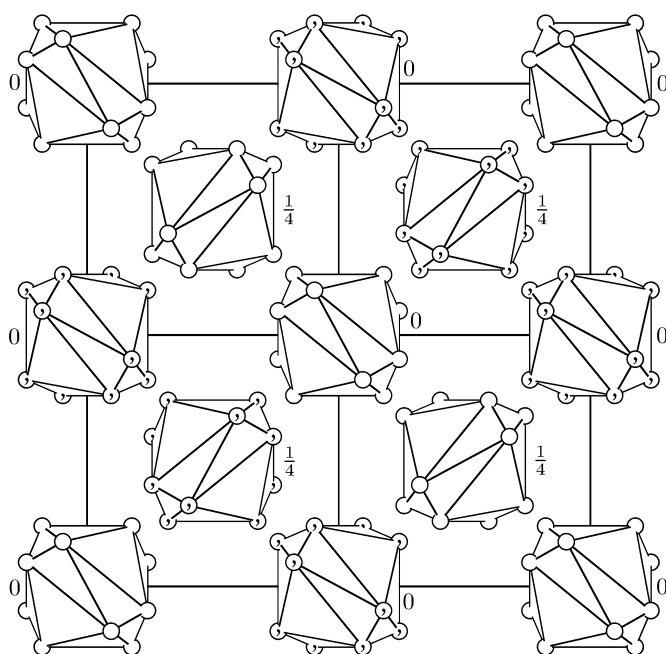
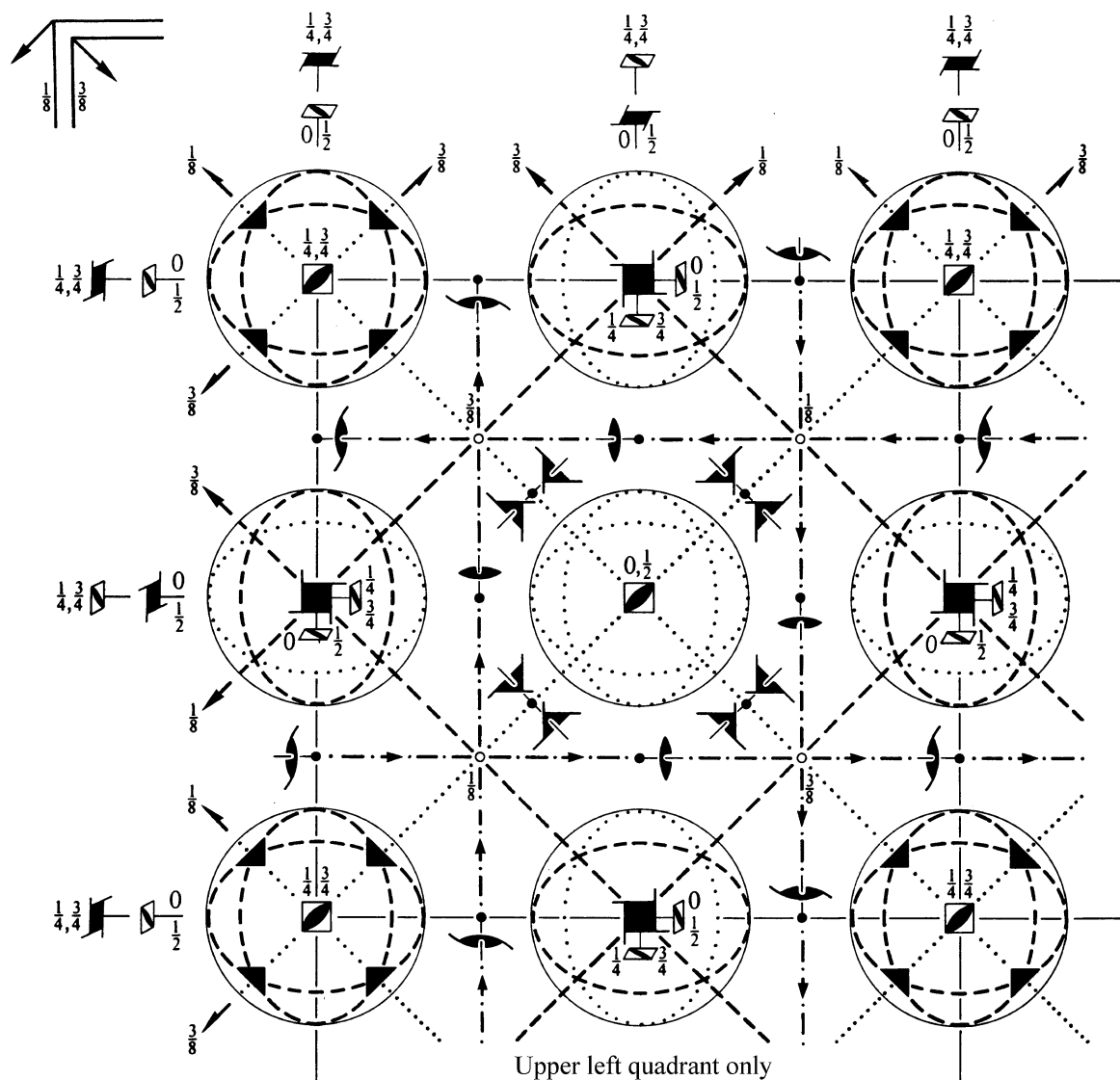
Cubic

No. 228

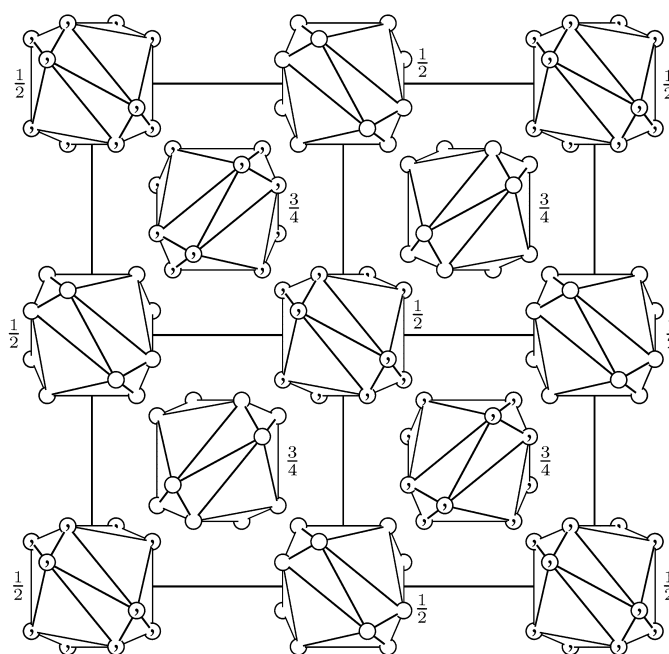
$F 4_1/d \bar{3} 2/c$

Patterson symmetry  $Fm\bar{3}m$

ORIGIN CHOICE 1



Lower half of unit cell



Upper half of unit cell

**Origin** at 23, at  $-\frac{3}{8}, -\frac{3}{8}, -\frac{3}{8}$  from centre ( $\bar{3}$ )

**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) $\bar{1} \quad \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$                      | (26) $d(\frac{3}{4}, \frac{1}{4}, 0) \quad x, y, \frac{1}{8}$   | (27) $d(\frac{1}{4}, 0, \frac{3}{4}) \quad x, \frac{1}{8}, z$   | (28) $d(0, \frac{3}{4}, \frac{1}{4}) \quad \frac{1}{8}, y, z$   |
| (29) $\bar{3}^+ x, x, x; \quad \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$           | (30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; \quad -\frac{3}{8}, \frac{3}{8}, \frac{5}{8}$              | (31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \quad \frac{3}{8}, \frac{5}{8}, -\frac{3}{8}$                          | (32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \quad \frac{5}{8}, -\frac{3}{8}, \frac{3}{8}$                  |
| (33) $\bar{3}^- x, x, x; \quad \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$           | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; \quad -\frac{1}{8}, -\frac{3}{8}, \frac{5}{8}$   | (35) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; \quad -\frac{3}{8}, \frac{5}{8}, -\frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x - \frac{1}{2}, \bar{x}; \quad \frac{5}{8}, -\frac{1}{8}, -\frac{3}{8}$   |
| (37) $g(-\frac{1}{4}, \frac{1}{4}, 0) \quad x + \frac{1}{4}, \bar{x}, z$        | (38) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, x, z$   | (39) $\bar{4}^- \frac{1}{4}, \frac{1}{4}, z; \quad \frac{1}{4}, \frac{1}{4}, 0$                                 | (40) $\bar{4}^+ 0, 0, z; \quad 0, 0, \frac{1}{4}$   |
| (41) $\bar{4}^- x, \frac{1}{4}, \frac{1}{4}; \quad 0, \frac{1}{4}, \frac{1}{4}$ | (42) $g(0, -\frac{1}{4}, \frac{1}{4}) \quad x, y + \frac{1}{4}, \bar{y}$                                | (43) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, y, y$   | (44) $\bar{4}^+ x, 0, 0; \quad \frac{1}{4}, 0, 0$   |
| (45) $\bar{4}^+ 0, y, 0; \quad 0, \frac{1}{4}, 0$                               | (46) $g(\frac{1}{4}, 0, -\frac{1}{4}) \quad \bar{x} + \frac{1}{4}, y, x$                                | (47) $\bar{4}^- \frac{1}{4}, y, \frac{1}{4}; \quad \frac{1}{4}, 0, \frac{1}{4}$                                 | (48) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, y, x$   |

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) $3^+ \quad x, \bar{x}, \bar{x}$  | (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) $3^- \quad x + \frac{1}{2}, \bar{x}, \bar{x}$  | (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) $\bar{1} \quad \frac{3}{8}, \frac{1}{8}, \frac{3}{8}$   | (26) $d(\frac{3}{4}, \frac{3}{4}, 0) \quad x, y, \frac{3}{8}$   | (27) $d(\frac{1}{4}, 0, \frac{1}{4}) \quad x, \frac{3}{8}, z$  | (28) $d(0, \frac{1}{4}, \frac{3}{4}) \quad \frac{1}{8}, y, z$                                       |
| (29) $\bar{3}^+ x, x - \frac{1}{2}, x; \quad \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$               | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{1}{2}, \bar{x}; \quad -\frac{3}{8}, -\frac{1}{8}, \frac{5}{8}$ | (31) $\bar{3}^+ x, \bar{x} + \frac{3}{2}, \bar{x}; \quad \frac{3}{8}, \frac{9}{8}, -\frac{3}{8}$         | (32) $\bar{3}^+ \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \quad \frac{5}{8}, \frac{1}{8}, \frac{3}{8}$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x + \frac{1}{2}, x; \quad \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ | (34) $\bar{3}^- x + 1, \bar{x} - \frac{1}{2}, \bar{x}; \quad \frac{3}{8}, \frac{1}{8}, \frac{5}{8}$   | (35) $\bar{3}^- \bar{x}, \bar{x} + 1, x; \quad -\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$                   | (36) $\bar{3}^- \bar{x} + \frac{3}{2}, x, \bar{x}; \quad \frac{9}{8}, \frac{3}{8}, -\frac{3}{8}$    |
| (37) $c \quad x, \bar{x}, z$   | (38) $g(\frac{1}{4}, \frac{1}{4}, 0) \quad x + \frac{1}{4}, x, z$                                     | (39) $\bar{4}^- 0, \frac{1}{2}, z; \quad 0, \frac{1}{2}, \frac{1}{4}$                                    | (40) $\bar{4}^+ \frac{1}{4}, \frac{1}{4}, z; \quad \frac{1}{4}, \frac{1}{4}, 0$                     |
| (41) $\bar{4}^- x, -\frac{1}{4}, \frac{1}{4}; \quad 0, -\frac{1}{4}, \frac{1}{4}$                  | (42) $g(0, \frac{1}{4}, -\frac{1}{4}) \quad x, y + \frac{1}{4}, \bar{y}$                              | (43) $a \quad x, y, y$   | (44) $\bar{4}^+ x, \frac{1}{2}, 0; \quad \frac{1}{4}, \frac{1}{2}, 0$                               |
| (45) $\bar{4}^+ -\frac{1}{4}, y, \frac{1}{4}; \quad -\frac{1}{4}, 0, \frac{1}{4}$                  | (46) $b \quad \bar{x} + \frac{1}{2}, y, x$  | (47) $\bar{4}^- 0, y, 0; \quad 0, \frac{1}{4}, 0$  | (48) $g(\frac{1}{4}, 0, \frac{1}{4}) \quad x + \frac{1}{4}, y, x$                                   |

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) $3^+ \quad x + \frac{1}{2}, \bar{x}, \bar{x}$   | (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) $3^- \quad (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (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) $\bar{1} \quad \frac{1}{8}, \frac{3}{8}, \frac{1}{8}$   | (26) $d(\frac{1}{4}, \frac{1}{4}, 0) \quad x, y, \frac{3}{8}$   | (27) $d(\frac{3}{4}, 0, \frac{1}{4}) \quad x, \frac{1}{8}, z$   | (28) $d(0, \frac{3}{4}, \frac{3}{4}) \quad \frac{3}{8}, y, z$   |
| (29) $\bar{3}^+ x + \frac{1}{2}, x + \frac{1}{2}, x; \quad \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - \frac{3}{2}, x + \frac{3}{2}, \bar{x}; \quad -\frac{3}{8}, \frac{3}{8}, \frac{9}{8}$  | (31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \quad \frac{3}{8}, \frac{5}{8}, \frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \quad \frac{5}{8}, -\frac{3}{8}, -\frac{1}{8}$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x, x; \quad -\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$               | (34) $\bar{3}^- x + 1, \bar{x} - 1, \bar{x}; \quad \frac{3}{8}, -\frac{3}{8}, \frac{5}{8}$                      | (35) $\bar{3}^- \bar{x}, \bar{x} + \frac{3}{2}, x; \quad -\frac{3}{8}, \frac{9}{8}, \frac{3}{8}$              | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}; \quad \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$   |
| (37) $c \quad x + \frac{1}{2}, \bar{x}, z$   | (38) $g(\frac{1}{4}, \frac{1}{4}, 0) \quad x - \frac{1}{4}, x, z$   | (39) $\bar{4}^- 0, 0, z; \quad 0, 0, \frac{1}{4}$   | (40) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \quad \frac{1}{4}, -\frac{1}{4}, 0$                               |
| (41) $\bar{4}^- x, 0, \frac{1}{2}; \quad \frac{1}{4}, 0, \frac{1}{2}$                              | (42) $a \quad x, y, \bar{y}$  | (43) $g(0, \frac{1}{4}, \frac{1}{4}) \quad x, y + \frac{1}{4}, y$   | (44) $\bar{4}^+ x, \frac{1}{4}, \frac{1}{4}; \quad 0, \frac{1}{4}, \frac{1}{4}$                                 |
| (45) $\bar{4}^+ 0, y, \frac{1}{2}; \quad 0, \frac{1}{4}, \frac{1}{2}$                              | (46) $g(-\frac{1}{4}, 0, \frac{1}{4}) \quad \bar{x} + \frac{1}{4}, y, x$  | (47) $\bar{4}^- \frac{1}{4}, y, -\frac{1}{4}; \quad \frac{1}{4}, 0, -\frac{1}{4}$                             | (48) $b \quad x, y, x$  |

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) $3^+ \quad x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$                                       | (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) $3^- \quad x, \bar{x}, \bar{x}$   | (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) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{3}{8}$                                 | (26) $d(\frac{1}{4}, \frac{3}{4}, 0) \quad x, y, \frac{1}{8}$  | (27) $d(\frac{3}{4}, 0, \frac{3}{4}) \quad x, \frac{3}{8}, z$   | (28) $d(0, \frac{1}{4}, \frac{1}{4}) \quad \frac{3}{8}, y, z$  |
| (29) $\bar{3}^+ x - \frac{1}{2}, x, x; \quad -\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$       | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; \quad \frac{1}{8}, \frac{3}{8}, \frac{5}{8}$            | (31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + 1, \bar{x}; \quad -\frac{1}{8}, \frac{5}{8}, -\frac{3}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{2}, \bar{x}, x; \quad \frac{9}{8}, -\frac{3}{8}, \frac{3}{8}$         |
| (33) $\bar{3}^- x, x - \frac{1}{2}, x; \quad \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$       | (34) $\bar{3}^- x + \frac{3}{2}, \bar{x} - \frac{3}{2}, \bar{x}; \quad \frac{3}{8}, -\frac{3}{8}, \frac{9}{8}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x} + 1, x; \quad \frac{1}{8}, \frac{5}{8}, \frac{3}{8}$   | (36) $\bar{3}^- \bar{x} + 1, x, \bar{x}; \quad \frac{5}{8}, \frac{3}{8}, -\frac{3}{8}$                   |
| (37) $g(\frac{1}{4}, -\frac{1}{4}, 0) \quad x + \frac{1}{4}, \bar{x}, z$                   | (38) $c \quad x, x, z$   | (39) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; \quad -\frac{1}{4}, \frac{1}{4}, 0$                     | (40) $\bar{4}^+ \frac{1}{2}, 0, z; \quad \frac{1}{2}, 0, \frac{1}{4}$                                    |
| (41) $\bar{4}^- x, 0, 0; \quad \frac{1}{4}, 0, 0$  | (42) $a \quad x, y + \frac{1}{2}, \bar{y}$   | (43) $g(0, \frac{1}{4}, \frac{1}{4}) \quad x, y - \frac{1}{4}, y$                                     | (44) $\bar{4}^+ x, \frac{1}{4}, -\frac{1}{4}; \quad 0, \frac{1}{4}, -\frac{1}{4}$                        |
| (45) $\bar{4}^+ \frac{1}{4}, y, \frac{1}{4}; \quad \frac{1}{4}, 0, \frac{1}{4}$            | (46) $b \quad \bar{x}, y, x$   | (47) $\bar{4}^- \frac{1}{2}, y, 0; \quad \frac{1}{2}, \frac{1}{4}, 0$                                 | (48) $g(\frac{1}{4}, 0, \frac{1}{4}) \quad x - \frac{1}{4}, y, x$  |

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

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

Reflection conditions

$h, k, l$  permutable

General:

192	$h$	1	(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) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$	$hkl$ : $h + k = 2n$ and $h + l, k + l = 2n$
			(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) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	$Ok$ : $k + l = 4n$ and $k, l = 2n$
			(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) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	$hhl$ : $h, l = 2n$
			(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) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	$h00$ : $h = 4n$
			(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) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(26) $x + \frac{3}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(27) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{3}{4}$	(28) $\bar{x} + \frac{1}{4}, y + \frac{3}{4}, z + \frac{1}{4}$	
			(29) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}$	(30) $\bar{z} + \frac{1}{4}, x + \frac{3}{4}, y + \frac{1}{4}$	(31) $z + \frac{3}{4}, x + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(32) $z + \frac{1}{4}, \bar{x} + \frac{1}{4}, y + \frac{3}{4}$	
			(33) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	(34) $y + \frac{1}{4}, \bar{z} + \frac{1}{4}, x + \frac{3}{4}$	(35) $\bar{y} + \frac{1}{4}, z + \frac{3}{4}, x + \frac{1}{4}$	(36) $y + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{4}$	
			(37) $\bar{y}, \bar{x} + \frac{1}{2}, z$	(38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(39) $\bar{y} + \frac{1}{2}, x, \bar{z}$	(40) $y, \bar{x}, \bar{z} + \frac{1}{2}$	
			(41) $\bar{x}, \bar{z} + \frac{1}{2}, y$	(42) $x, \bar{z}, \bar{y} + \frac{1}{2}$	(43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(44) $\bar{x} + \frac{1}{2}, z, \bar{y}$	
			(45) $\bar{z}, \bar{y} + \frac{1}{2}, x$	(46) $\bar{z} + \frac{1}{2}, y, \bar{x}$	(47) $z, \bar{y}, \bar{x} + \frac{1}{2}$	(48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	

Special: as above, plus

no extra conditions

96	$g$	. . 2	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$
			$\bar{y} + \frac{1}{4}, \frac{1}{8}, y$	$\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$	$y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$	$y + \frac{1}{4}, \frac{5}{8}, \bar{y}$
			$y, \bar{y} + \frac{1}{4}, \frac{1}{8}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$	$y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$	$\bar{y}, y + \frac{1}{4}, \frac{5}{8}$
			$\frac{5}{8}, \bar{y} + \frac{3}{4}, y + \frac{1}{2}$	$\frac{7}{8}, y + \frac{1}{4}, y$	$\frac{3}{8}, \bar{y} + \frac{1}{4}, \bar{y}$	$\frac{1}{8}, y + \frac{3}{4}, \bar{y} + \frac{1}{2}$
			$y + \frac{1}{2}, \frac{5}{8}, \bar{y} + \frac{3}{4}$	$y, \frac{7}{8}, y + \frac{1}{4}$	$\bar{y}, \frac{3}{8}, \bar{y} + \frac{1}{4}$	$\bar{y} + \frac{1}{2}, \frac{1}{8}, y + \frac{3}{4}$
			$\bar{y} + \frac{3}{4}, y + \frac{1}{2}, \frac{5}{8}$	$y + \frac{1}{4}, y, \frac{7}{8}$	$\bar{y} + \frac{1}{4}, \bar{y}, \frac{3}{8}$	$y + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{8}$

96	$f$	2 . .	$x, 0, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$0, 0, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$	$hkl$ : $h + k + l = 4n$
			$\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$	
			$\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \bar{x} + \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, x + \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x + \frac{3}{4}$	
			$0, \bar{x} + \frac{1}{2}, 0$	$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, 0$	$x, 0, \frac{1}{2}$	$0, \frac{1}{2}, x$	$\frac{1}{2}, 0, \bar{x}$	

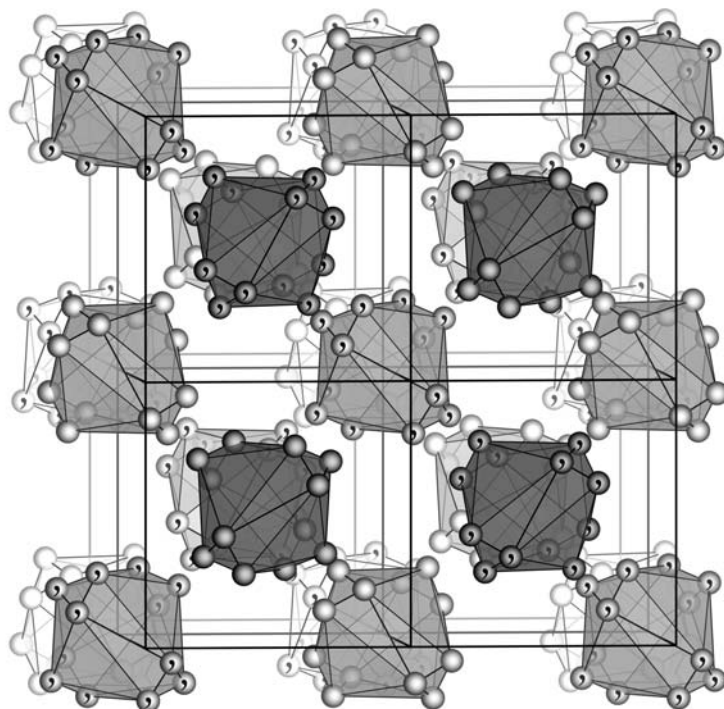
64	$e$	. 3 .	$x, x, x$	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$hkl$ : $h = 2n$
			$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	
			$\bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{x} + \frac{1}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	
			$\bar{x}, \bar{x} + \frac{1}{2}, x$	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, \bar{x}$	$x, \bar{x}, \bar{x} + \frac{1}{2}$	

48	$d$	$\bar{4} . .$	$\frac{1}{4}, 0, 0$	$\frac{3}{4}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{2}$	$0, 0, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl$ : $h + k + l = 4n$
			$\frac{3}{4}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$0, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	

32	$c$	. $\bar{3}$ .	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{5}{8}, \frac{1}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{1}{8}, \frac{5}{8}$	$hkl$ : $h, k, l = 4n + 2$ or $h, k, l = 4n$
----	-----	---------------	---	---	---	---	---	---	---	---	---

32	$b$	. 3 2	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{3}{8}$	$hkl$ : $h, k, l = 4n + 2$ or $h, k, l = 4n$
----	-----	-------	---	---	---	---	---	---	---	---	---

16	$a$	2 3 .	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$0, \frac{1}{2}, 0$					$hkl$ : $h + k + l = 4n$
----	-----	-------	-----------	---	---	---------------------	--	--	--	--	--------------------------



### 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  $[110]$   $p2mm$

$$\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at  $x, x, \frac{1}{8}$

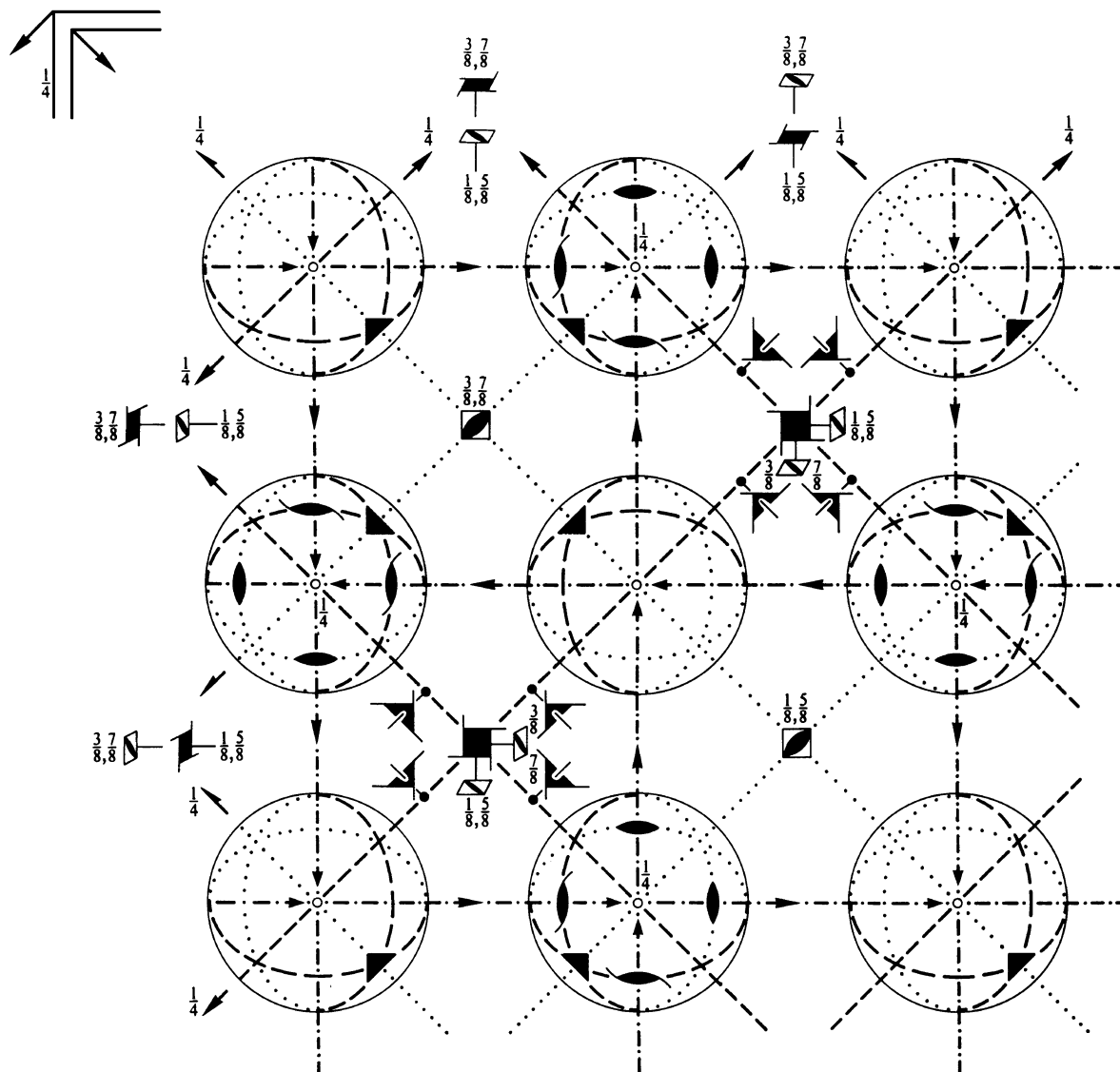
$Fd\bar{3}c$  $O_h^8$  $m\bar{3}m$ 

Cubic

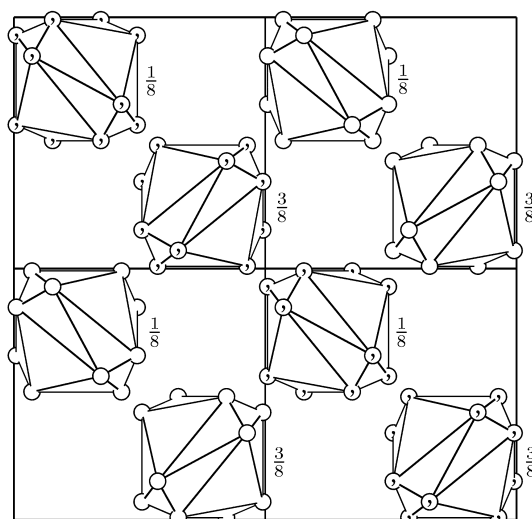
No. 228

 $F4_1/d\bar{3}2/c$ Patterson symmetry  $Fm\bar{3}m$ 

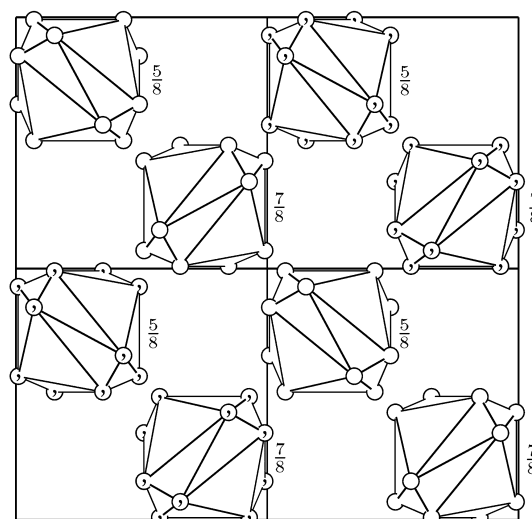
ORIGIN CHOICE 2



Upper left quadrant only



Lower half of unit cell



Upper half of unit cell

**Origin** at centre ( $\bar{3}$ ), at  $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$  from 23

**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 operations

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

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

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

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

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

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

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

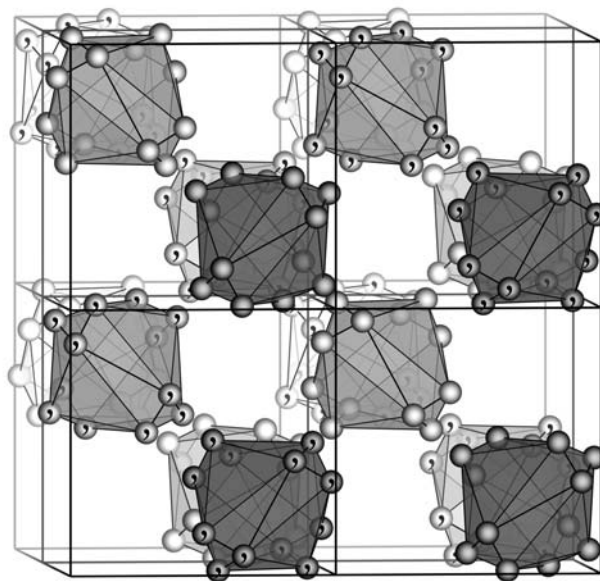
- |  |  |  |   |
|--|--|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$   | (2) $2(0, 0, \frac{1}{2}) \frac{3}{8}, \frac{3}{8}, z$   | (3) $2 \frac{1}{8}, y, \frac{1}{8}$  | (4) $2 x, \frac{3}{8}, \frac{3}{8}$   |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x + \frac{1}{3}, x$ |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

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)+	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$			
192	$h$	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{3}{4}, y + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{3}{4}$	$hkl: h+k=2n$ and $h+l, k+l=2n$	
			(5) $z, x, y$	(6) $z + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(7) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{3}{4}, x + \frac{1}{2}, \bar{y} + \frac{1}{4}$	$Ok: k+l=4n$ and $k, l=2n$	
			(9) $y, z, x$	(10) $\bar{y} + \frac{3}{4}, z + \frac{1}{2}, \bar{x} + \frac{1}{4}$	(11) $y + \frac{1}{2}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(12) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{2}$	$hhl: h, l=2n$	
			(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z}$	(14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(15) $y + \frac{1}{4}, \bar{x}, z + \frac{3}{4}$	(16) $\bar{y}, x + \frac{3}{4}, z + \frac{1}{4}$	$h00: h=4n$	
			(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y}$	(18) $\bar{x}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(20) $x + \frac{1}{4}, \bar{z}, y + \frac{3}{4}$		
			(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x}$	(22) $z + \frac{1}{4}, \bar{y}, x + \frac{3}{4}$	(23) $\bar{z}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$		
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x + \frac{3}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{2}$	(27) $x + \frac{1}{4}, \bar{y} + \frac{1}{2}, z + \frac{3}{4}$	(28) $\bar{x} + \frac{1}{2}, y + \frac{3}{4}, z + \frac{1}{4}$		
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z} + \frac{1}{2}, x + \frac{3}{4}, y + \frac{1}{4}$	(31) $z + \frac{3}{4}, x + \frac{1}{4}, \bar{y} + \frac{1}{2}$	(32) $z + \frac{1}{4}, \bar{x} + \frac{1}{2}, y + \frac{3}{4}$		
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y + \frac{1}{4}, \bar{z} + \frac{1}{2}, x + \frac{3}{4}$	(35) $\bar{y} + \frac{1}{2}, z + \frac{3}{4}, x + \frac{1}{4}$	(36) $y + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{2}$		
			(37) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}, z$	(38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(39) $\bar{y} + \frac{3}{4}, x, \bar{z} + \frac{1}{4}$	(40) $y, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$		
			(41) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}, y$	(42) $x, \bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(44) $\bar{x} + \frac{3}{4}, z, \bar{y} + \frac{1}{4}$		
			(45) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}, x$	(46) $\bar{z} + \frac{3}{4}, y, \bar{x} + \frac{1}{4}$	(47) $z, \bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$		
							Special: as above, plus no extra conditions	
96	$g$	. . 2	$\frac{1}{4}, y, \bar{y}$	$0, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{4}$	$\frac{3}{4}, \bar{y} + \frac{1}{4}, y + \frac{3}{4}$		
			$\bar{y}, \frac{1}{4}, y$	$\bar{y} + \frac{1}{2}, 0, \bar{y} + \frac{3}{4}$	$y + \frac{1}{4}, \frac{1}{2}, y + \frac{1}{2}$	$y + \frac{3}{4}, \frac{3}{4}, \bar{y} + \frac{1}{4}$		
			$y, \bar{y}, \frac{1}{4}$	$\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, 0$	$y + \frac{1}{2}, y + \frac{1}{4}, \frac{1}{2}$	$\bar{y} + \frac{1}{4}, y + \frac{3}{4}, \frac{3}{4}$		
			$\frac{3}{4}, \bar{y}, y$	$0, y + \frac{1}{4}, y + \frac{1}{2}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$\frac{1}{4}, y + \frac{3}{4}, \bar{y} + \frac{1}{4}$		
			$y, \frac{3}{4}, \bar{y}$	$y + \frac{1}{2}, 0, y + \frac{1}{4}$	$\bar{y} + \frac{3}{4}, \frac{1}{2}, \bar{y} + \frac{1}{2}$	$\bar{y} + \frac{1}{4}, \frac{1}{4}, y + \frac{3}{4}$		
			$\bar{y}, y, \frac{3}{4}$	$y + \frac{1}{4}, y + \frac{1}{2}, 0$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{1}{2}$	$y + \frac{3}{4}, \bar{y} + \frac{1}{4}, \frac{1}{4}$		
96	$f$	2 . .	$x, \frac{1}{8}, \frac{1}{8}$	$\bar{x} + \frac{1}{4}, \frac{5}{8}, \frac{5}{8}$	$\frac{1}{8}, x, \frac{1}{8}$	$\frac{5}{8}, \bar{x} + \frac{1}{4}, \frac{5}{8}$	$\frac{1}{8}, \frac{1}{8}, x$	$\frac{5}{8}, \frac{5}{8}, \bar{x} + \frac{1}{4}$
			$\frac{7}{8}, x + \frac{1}{4}, \frac{7}{8}$	$\frac{3}{8}, \bar{x} + \frac{1}{2}, \frac{3}{8}$	$x + \frac{3}{4}, \frac{3}{8}, \frac{7}{8}$	$\bar{x}, \frac{7}{8}, \frac{3}{8}$	$\frac{7}{8}, \frac{3}{8}, \bar{x}$	$\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}$
			$\bar{x}, \frac{7}{8}, \frac{7}{8}$	$x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}$	$\frac{7}{8}, \bar{x}, \frac{7}{8}$	$\frac{3}{8}, x + \frac{3}{4}, \frac{3}{8}$	$\frac{7}{8}, \frac{7}{8}, \bar{x}$	$\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}$
			$\frac{1}{8}, \bar{x} + \frac{3}{4}, \frac{1}{8}$	$\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}$	$\bar{x} + \frac{1}{4}, \frac{5}{8}, \frac{1}{8}$	$x, \frac{1}{8}, \frac{5}{8}$	$\frac{1}{8}, \frac{5}{8}, x$	$\frac{5}{8}, \frac{1}{8}, \bar{x} + \frac{1}{4}$
64	$e$	. 3 .	$x, x, x$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{1}{2}$	$\bar{x} + \frac{3}{4}, x + \frac{1}{2}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$hkl: h=2n$	
			$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$x + \frac{1}{4}, \bar{x}, x + \frac{3}{4}$	$\bar{x}, x + \frac{3}{4}, x + \frac{1}{4}$		
			$\bar{x}, \bar{x}, \bar{x}$	$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$	$x + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$		
			$\bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x$	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{3}{4}, x, \bar{x} + \frac{1}{4}$	$x, \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}$		
48	$d$	$\bar{4} . .$	$\frac{7}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{5}{8}, \frac{1}{8}, \frac{5}{8}$	$\frac{1}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{5}{8}, \frac{3}{8}$
			$\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{3}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{5}{8}$
32	$c$	. $\bar{3}$ .	0,0,0	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
							$\frac{1}{4}, 0, \frac{3}{4}$	$0, \frac{3}{4}, \frac{1}{4}$
								$hkl: h, k, l=4n+2$ or $h, k, l=4n$
32	$b$	. 3 2	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$0, \frac{1}{2}, \frac{1}{4}$
							$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{4}, 0, \frac{1}{2}$
								$hkl: h, k, l=4n+2$ or $h, k, l=4n$
16	$a$	2 3 .	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{7}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$		
								$hkl: h+k+l=4n$



### 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  $\frac{1}{8}, \frac{3}{8}, z$

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  $[110]$   $p2mm$

$$\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at  $x, x, 0$