

$Fd\bar{3}$

T_h^4

$m\bar{3}$

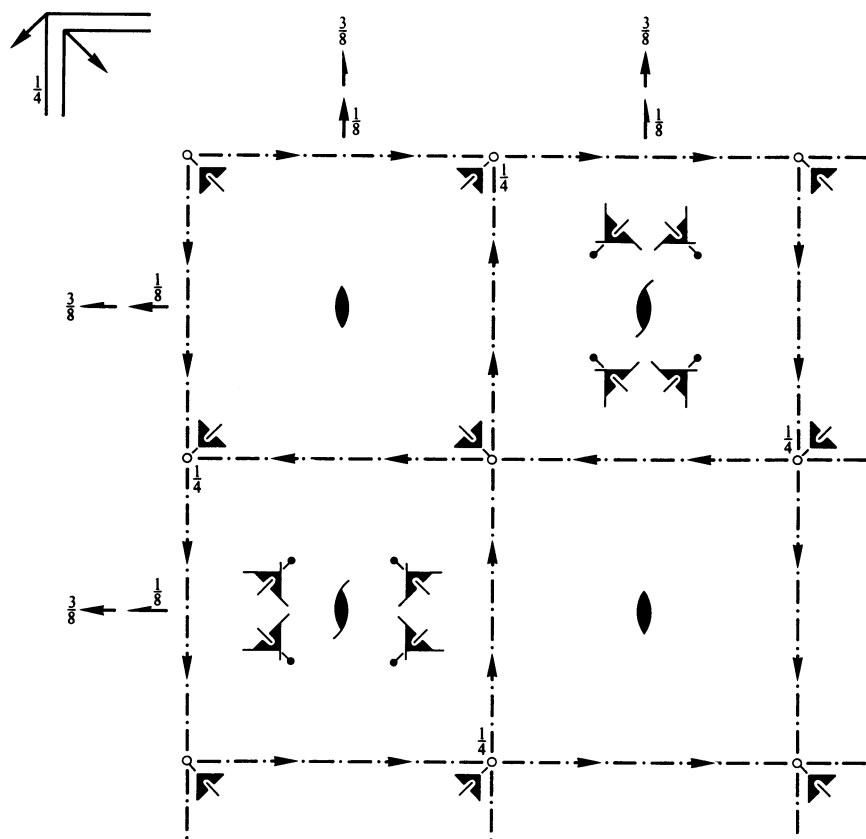
Cubic

No. 203

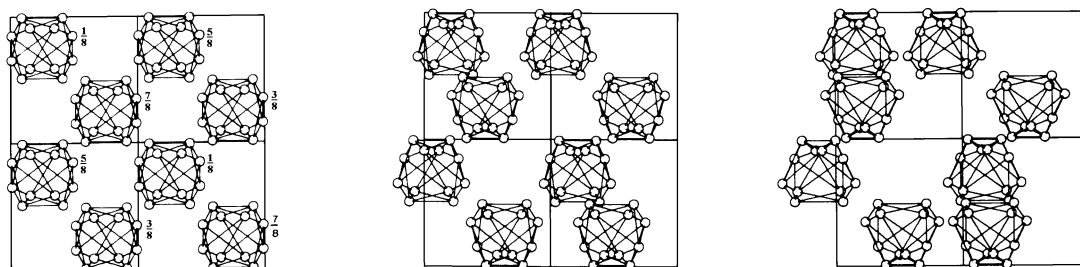
$F2/d\bar{3}$

Patterson symmetry $Fm\bar{3}$

ORIGIN CHOICE 2



Upper left quadrant only



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

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

Vertices $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, -\frac{3}{8}$

Symmetry operations

For (0,0,0)+ set

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

For (0, 1/2, 1/2)+ set

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

For (1/2, 0, 1/2)+ set

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

For (1/2, 1/2, 0)+ set

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

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)

Positions

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

(Continued on page 623)

