

$Fd\bar{3}$

T_h^4

$m\bar{3}$

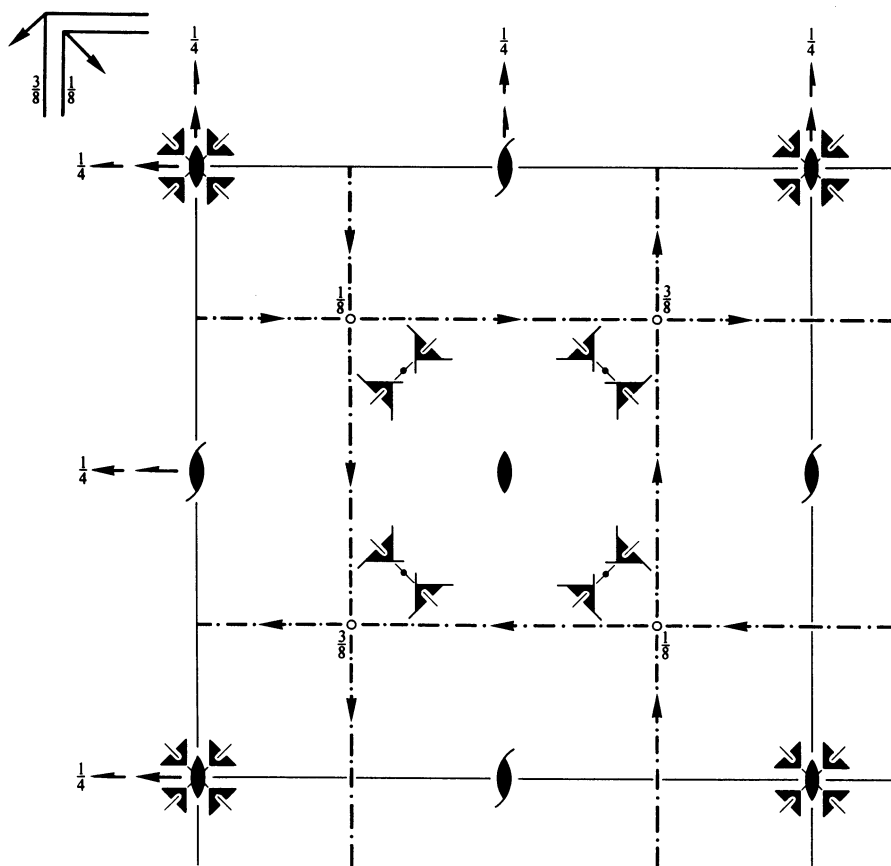
Cubic

No. 203

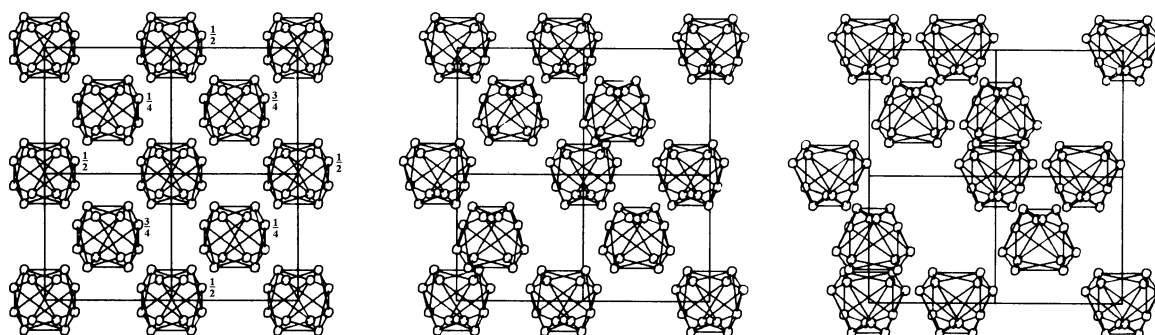
$F2/d\bar{3}$

Patterson symmetry $Fm\bar{3}$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at $2\bar{3}$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}$)

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

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

Symmetry operations

For (0,0,0)+ set

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

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

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

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

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

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

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

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

Positions

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

(Continued on page 623)

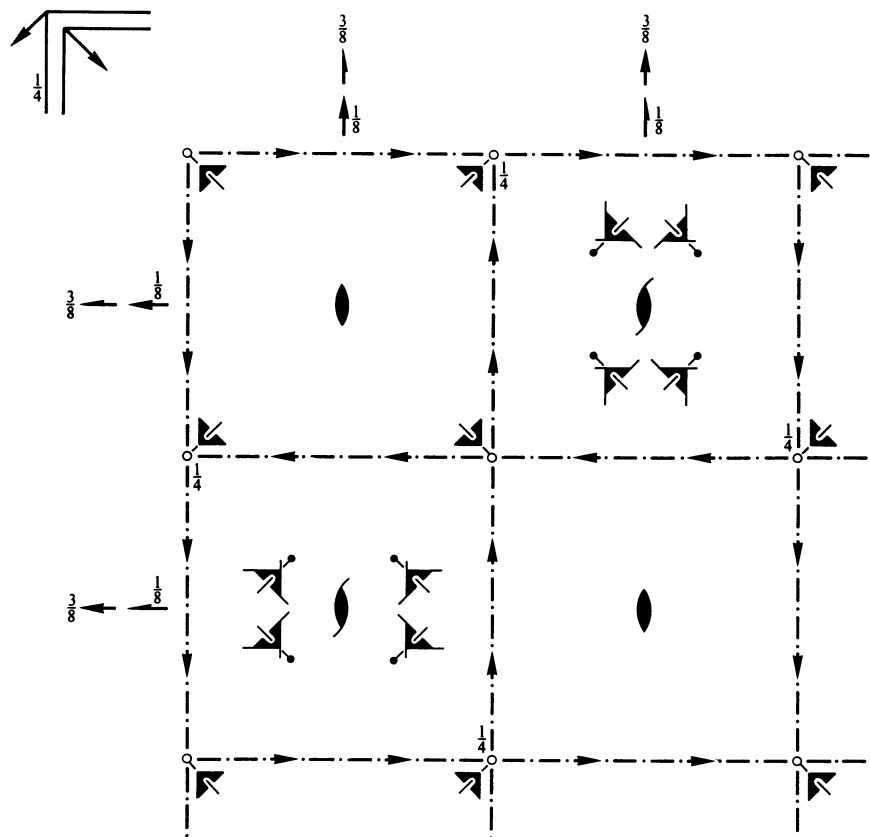
$F d \bar{3}$ T_h^4 $m \bar{3}$

Cubic

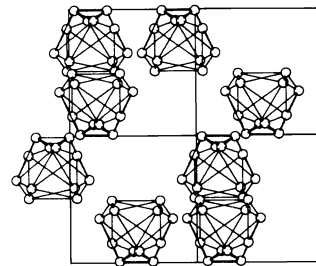
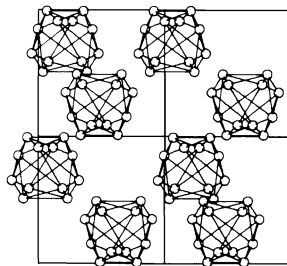
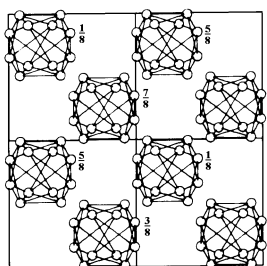
No. 203

 $F 2/d \bar{3}$ Patterson symmetry $F m \bar{3}$

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

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)+	h, k, l cyclicly permutable General:		
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)

