

$Fd\bar{3}$

$T_h^4$

$m\bar{3}$

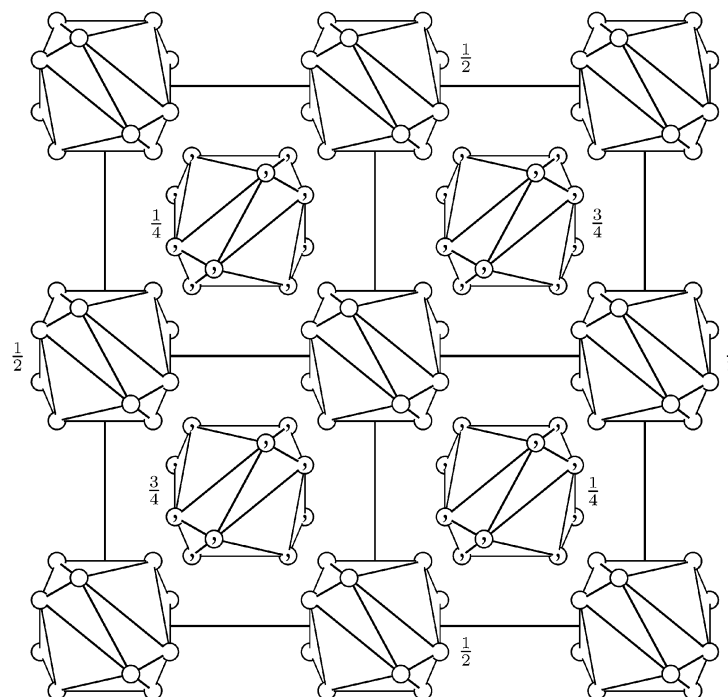
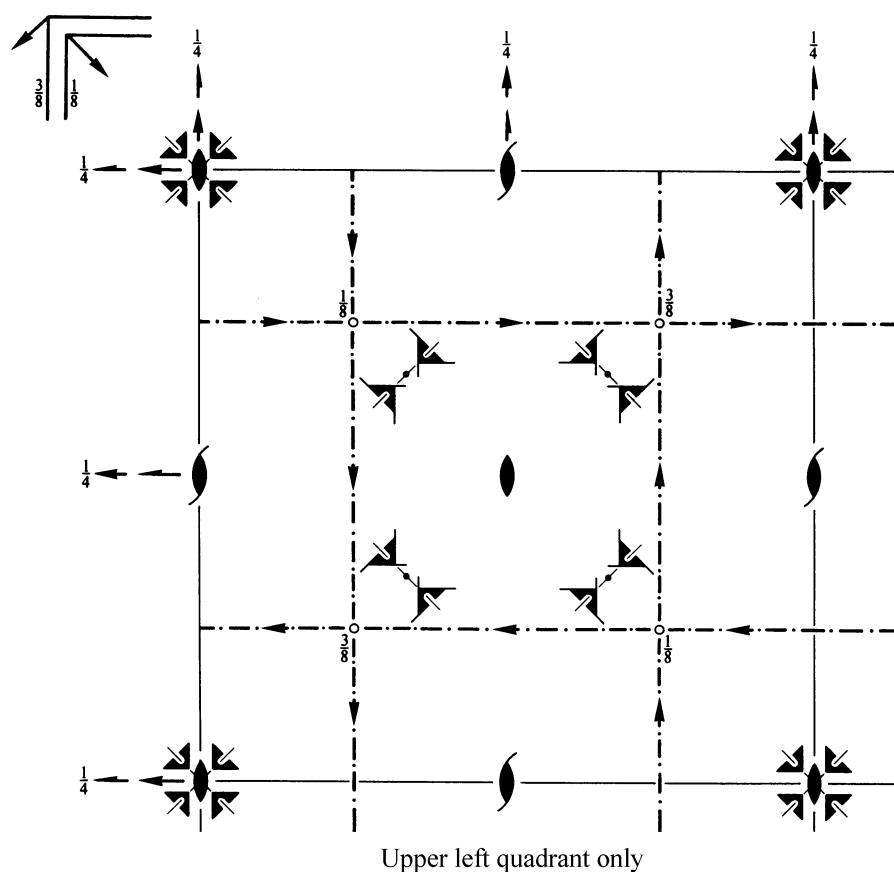
Cubic

No. 203

$F2/d\bar{3}$

Patterson symmetry  $Fm\bar{3}$

ORIGIN CHOICE 1



**Origin** at 23, 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 <sup>+</sup> x,x,x   | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$  | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$  | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x   |
| (9) 3 <sup>-</sup> x,x,x   | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$  | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x   | (12) 3 <sup>-</sup> $\bar{x}$ ,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) 3 <sup>+</sup> x,x,x; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | (18) 3 <sup>+</sup> $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}; -\frac{1}{8},\frac{1}{8},\frac{3}{8}$ | (19) 3 <sup>+</sup> x, $\bar{x}+\frac{1}{2},\bar{x}; \frac{1}{8},\frac{3}{8},-\frac{1}{8}$ | (20) 3 <sup>+</sup> $\bar{x}+\frac{1}{2},\bar{x},x; \frac{3}{8},-\frac{1}{8},\frac{1}{8}$ |
| (21) 3 <sup>-</sup> x,x,x; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | (22) 3 <sup>-</sup> $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}; \frac{1}{8},-\frac{1}{8},\frac{3}{8}$ | (23) 3 <sup>-</sup> $\bar{x},\bar{x}+\frac{1}{2},x; -\frac{1}{8},\frac{3}{8},\frac{1}{8}$  | (24) 3 <sup>-</sup> $\bar{x}+\frac{1}{2},x,\bar{x}; \frac{3}{8},\frac{1}{8},-\frac{1}{8}$ |

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 <sup>+</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) x $-\frac{1}{3},x-\frac{1}{6},x$ | (6) 3 <sup>+</sup> $\bar{x},x+\frac{1}{2},\bar{x}$  | (7) 3 <sup>+</sup> ( $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) x $+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+\frac{1}{2},x$  |
| (9) 3 <sup>-</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) x $-\frac{1}{6},x+\frac{1}{6},x$ | (10) 3 <sup>-</sup> ( $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) x $+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 <sup>-</sup> $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$  | (12) 3 <sup>-</sup> $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$                                       |
| (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) 3 <sup>+</sup> x,x $+\frac{1}{2},x; \frac{1}{8},\frac{5}{8},\frac{1}{8}$                 | (18) 3 <sup>+</sup> $\bar{x}-\frac{3}{2},x+1,\bar{x}; -\frac{5}{8},\frac{7}{8},\frac{7}{8}$                 | (19) 3 <sup>+</sup> x, $\bar{x}+1,\bar{x}; \frac{1}{8},\frac{7}{8},-\frac{1}{8}$                           | (20) 3 <sup>+</sup> $\bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x; \frac{7}{8},-\frac{1}{8},\frac{5}{8}$ |
| (21) 3 <sup>-</sup> x $-\frac{1}{2},x-\frac{1}{2},x; \frac{1}{8},\frac{1}{8},\frac{5}{8}$     | (22) 3 <sup>-</sup> $x+1,\bar{x}-1,\bar{x}; \frac{1}{8},-\frac{1}{8},\frac{7}{8}$                           | (23) 3 <sup>-</sup> $\bar{x}-\frac{1}{2},\bar{x}+1,x; -\frac{5}{8},\frac{7}{8},\frac{1}{8}$                | (24) 3 <sup>-</sup> $\bar{x}+1,x+\frac{1}{2},\bar{x}; \frac{7}{8},\frac{5}{8},-\frac{1}{8}$           |

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

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

**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, $\frac{1}{2},\frac{1}{2}$ )+	( $\frac{1}{2},0,\frac{1}{2}$ )+	( $\frac{1}{2},\frac{1}{2},0$ )+				
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 Okl: k+l=4n and k,l=2n hhl: h+l=2n h00: h=4n  Special: as above, plus			
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	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$						

**Symmetry of special projections**

Along [001] c2mm a' = $\frac{1}{2}$ a    b' = $\frac{1}{2}$ b Origin at 0,0,z	Along [111] p6 a' = $\frac{1}{6}(2a-b-c)$ b' = $\frac{1}{6}(-a+2b-c)$ Origin at x,x,x	Along [110] c2mm a' = $\frac{1}{2}(-a+b)$ b' = c Origin at x,x, $\frac{1}{8}$
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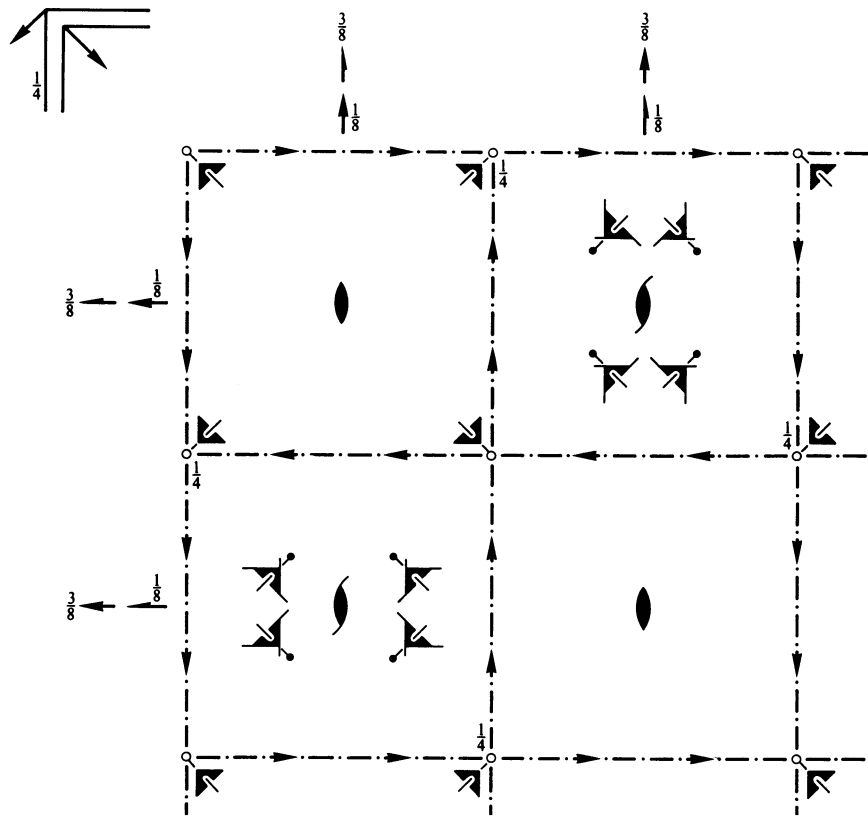
$F d \bar{3}$  $T_h^4$  $m \bar{3}$ 

Cubic

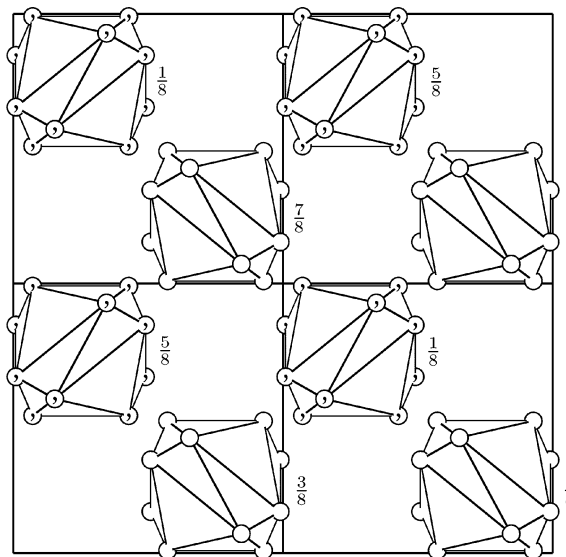
No. 203

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

ORIGIN CHOICE 2



Upper left quadrant only

**Origin** at centre ( $\bar{3}$ ), at  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  from 23

**Asymmetric unit**  $-\frac{1}{2} \leq x \leq \frac{3}{8}$ ;  $-\frac{1}{2} \leq y \leq \frac{1}{8}$ ;  $-\frac{3}{8} \leq z \leq \frac{1}{8}$ ;  $y \leq \min(x, \frac{1}{4} - x)$ ;  $-y - \frac{1}{4} \leq z \leq y$

**Vertices**  $-\frac{1}{2}, -\frac{1}{8}, -\frac{1}{8}$ ;  $\frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}$ ;  $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ ;  $\frac{1}{8}, \frac{1}{8}, -\frac{3}{8}$

**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) $\bar{3}^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{2}$ |
| (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) $\bar{3}^+ \bar{x} + \frac{1}{4}, \bar{x} - \frac{3}{4}, x; \frac{3}{4}, -\frac{3}{4}, 0$ |
| (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)+	$h, k, l$ cyclically 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.	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$						

**Symmetry of special projections**

Along [001] $c2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ Origin at $\frac{1}{8}, \frac{1}{8}, z$	Along [111] $p6$ $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at $x, x, x$	Along [110] $c2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$
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