

F 23

T^2

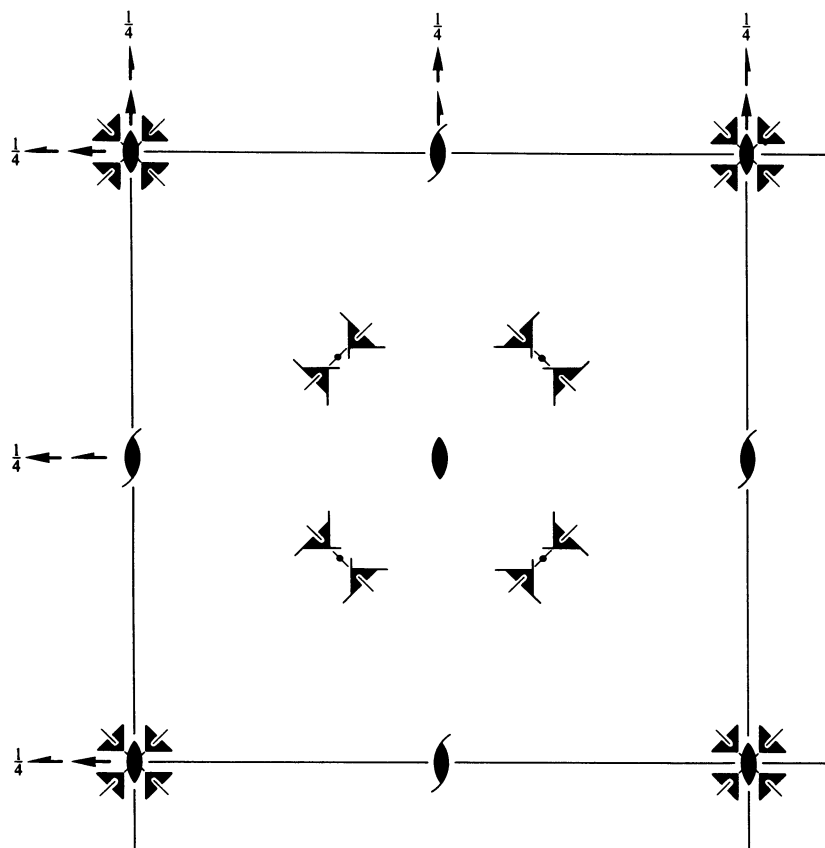
23

Cubic

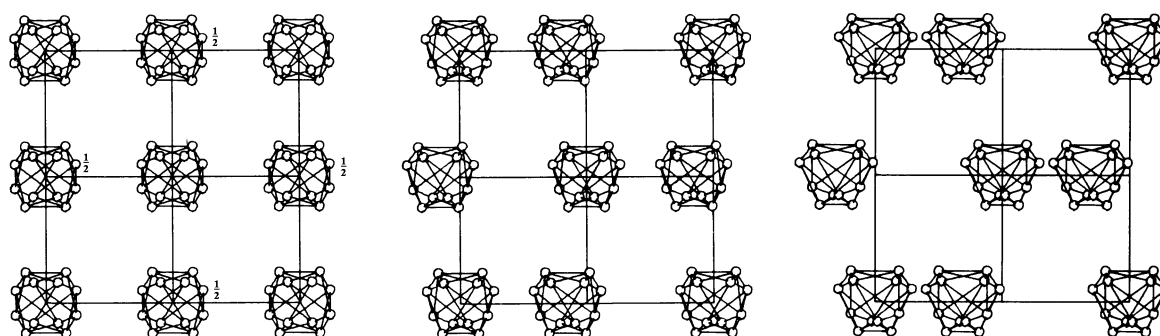
No. 196

F 23

Patterson symmetry $Fm\bar{3}$



Upper left quadrant only



Origin at 23

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

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

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} |

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} |

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- $\frac{1}{3}$,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+ $\frac{1}{3}$, \bar{x} |

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} |

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)**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 cyclically permutable

General:

- | | | | | | | |
|----|-----|---|-----------|------------------------------|-------------------------------|-------------------------------|
| 48 | h | 1 | (1) x,y,z | (2) \bar{x} , \bar{y} ,z | (3) \bar{x} ,y, \bar{z} | (4) x, \bar{y} , \bar{z} |
| | | | (5) z,x,y | (6) z, \bar{x} , \bar{y} | (7) \bar{z} , \bar{x} ,y | (8) \bar{z} ,x, \bar{y} |
| | | | (9) y,z,x | (10) \bar{y} ,z, \bar{x} | (11) y, \bar{z} , \bar{x} | (12) \bar{y} , \bar{z} ,x |

- hkl : $h+k, h+l, k+l = 2n$
 Ok : $k, l = 2n$
 hhl : $h+l = 2n$
 $h00$: $h = 2n$

Special: no extra conditions

- | | | | | | | | | |
|----|-----|-----|---|---|---------------------------------|---|----------------------------------|---|
| 24 | g | 2.. | x, $\frac{1}{4}$, $\frac{1}{4}$ | \bar{x} , $\frac{3}{4}$, $\frac{1}{4}$ | $\frac{1}{4}$,x, $\frac{1}{4}$ | $\frac{1}{4}$, \bar{x} , $\frac{3}{4}$ | $\frac{1}{4}$, $\frac{1}{4}$,x | $\frac{3}{4}$, $\frac{1}{4}$, \bar{x} |
| 24 | f | 2.. | x,0,0 | \bar{x} ,0,0 | 0,x,0 | 0, \bar{x} ,0 | 0,0,x | 0,0, \bar{x} |
| 16 | e | .3. | x,x,x | \bar{x} , \bar{x} ,x | \bar{x} ,x, \bar{x} | x, \bar{x} , \bar{x} | | |
| 4 | d | 23. | $\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$ | | | | | |
| 4 | c | 23. | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$ | | | | | |
| 4 | b | 23. | $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$ | | | | | |
| 4 | a | 23. | 0,0,0 | | | | | |

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [111] $p3$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x,x,x

Along [110] $c1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at x,x,0

Maximal non-isomorphic subgroups

- I** [3] $F 21 (F 222, 22)$ (1; 2; 3; 4)+
 { [4] $F 13 (R3, 146)$ (1; 5; 9)+
 [4] $F 13 (R3, 146)$ (1; 6; 12)+
 [4] $F 13 (R3, 146)$ (1; 7; 10)+
 [4] $F 13 (R3, 146)$ (1; 8; 11)+
- IIa** { [4] $P 2_1 3 (198)$ 1; 5; 9; (2; 7; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 7; 10; (2; 5; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 8; 11; (2; 6; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 6; 12; (2; 8; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 5; 9; (3; 8; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 7; 10; (3; 6; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 8; 11; (3; 5; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 6; 12; (3; 7; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (9; 10; 11; 12) + $(0, \frac{1}{2}, \frac{1}{2})$
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (9; 10; 11; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$
 [4] $P 23 (195)$ 1; 5; 9; (4; 6; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 7; 10; (4; 8; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 8; 11; (4; 7; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 6; 12; (4; 5; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [27] $F 23 (a' = 3a, b' = 3b, c' = 3c)$ (196)

Minimal non-isomorphic supergroups

- I** [2] $F m \bar{3} (202)$; [2] $F d \bar{3} (203)$; [2] $F 432 (209)$; [2] $F 4_1 32 (210)$; [2] $F \bar{4} 3 m (216)$; [2] $F \bar{4} 3 c (219)$
II [2] $P 23 (a' = \frac{1}{2}c, b' = \frac{1}{2}b, c' = \frac{1}{2}c)$ (195)