

F 23

T^2

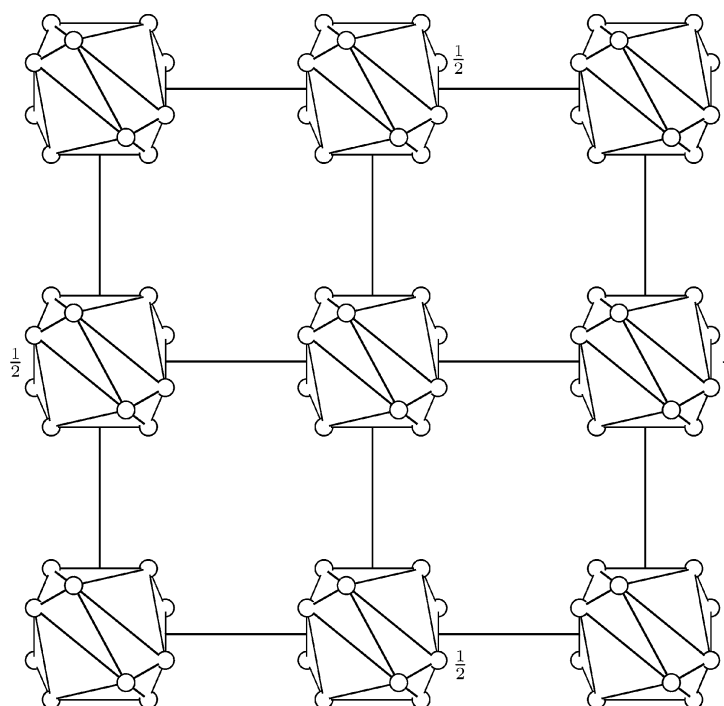
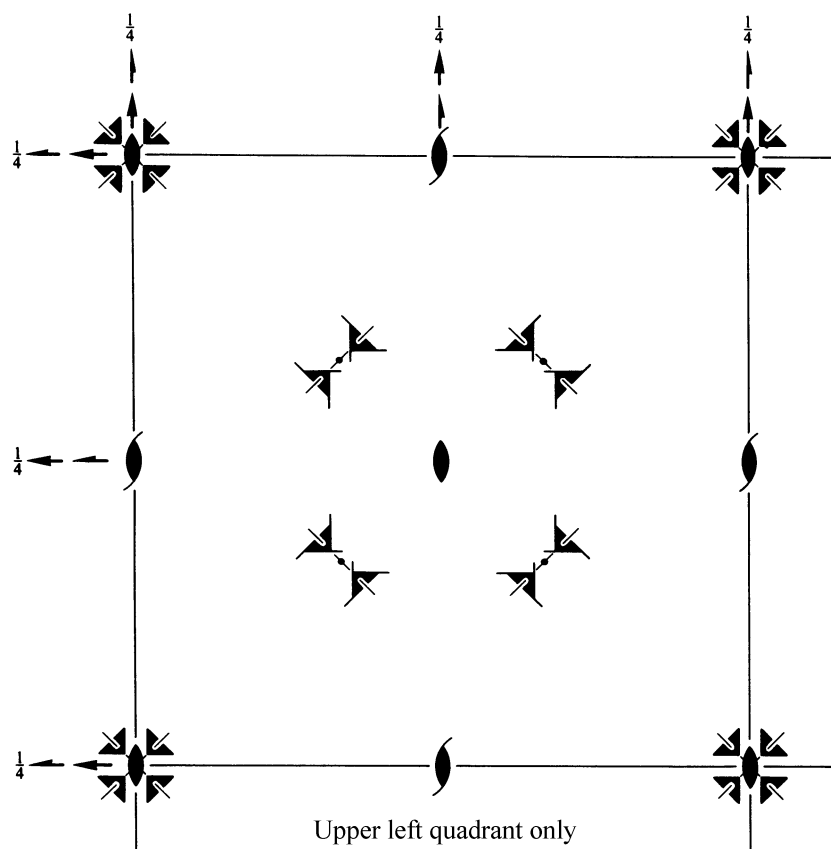
23

Cubic

No. 196

F 23

Patterson symmetry $Fm\bar{3}$



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+ $\frac{1}{6}$,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} |

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				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:	
48 <i>h</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) \bar{x} , \bar{y} ,z (6) z, \bar{x} , \bar{y} (10) \bar{y} ,z, \bar{x}	(3) \bar{x} ,y, \bar{z} (7) \bar{z} , \bar{x} ,y (11) y, \bar{z} , \bar{x}	(4) x, \bar{y} , \bar{z} (8) \bar{z} ,x, \bar{y} (12) \bar{y} , \bar{z} ,x	hkl : $h+k, h+l, k+l = 2n$ $0kl$: $k, l = 2n$ hhl : $h+l = 2n$ $h00$: $h = 2n$	
24 <i>g</i> 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 <i>f</i> 2..	x,0,0	\bar{x} ,0,0	0,x,0	0, \bar{x} ,0	0,0,x	0,0, \bar{x}
16 <i>e</i> .3.	x,x,x	\bar{x} , \bar{x} ,x	\bar{x} ,x, \bar{x}	x, \bar{x} , \bar{x}		
4 <i>d</i> 23.	$\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$					
4 <i>c</i> 23.	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$					
4 <i>b</i> 23.	$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$					
4 <i>a</i> 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