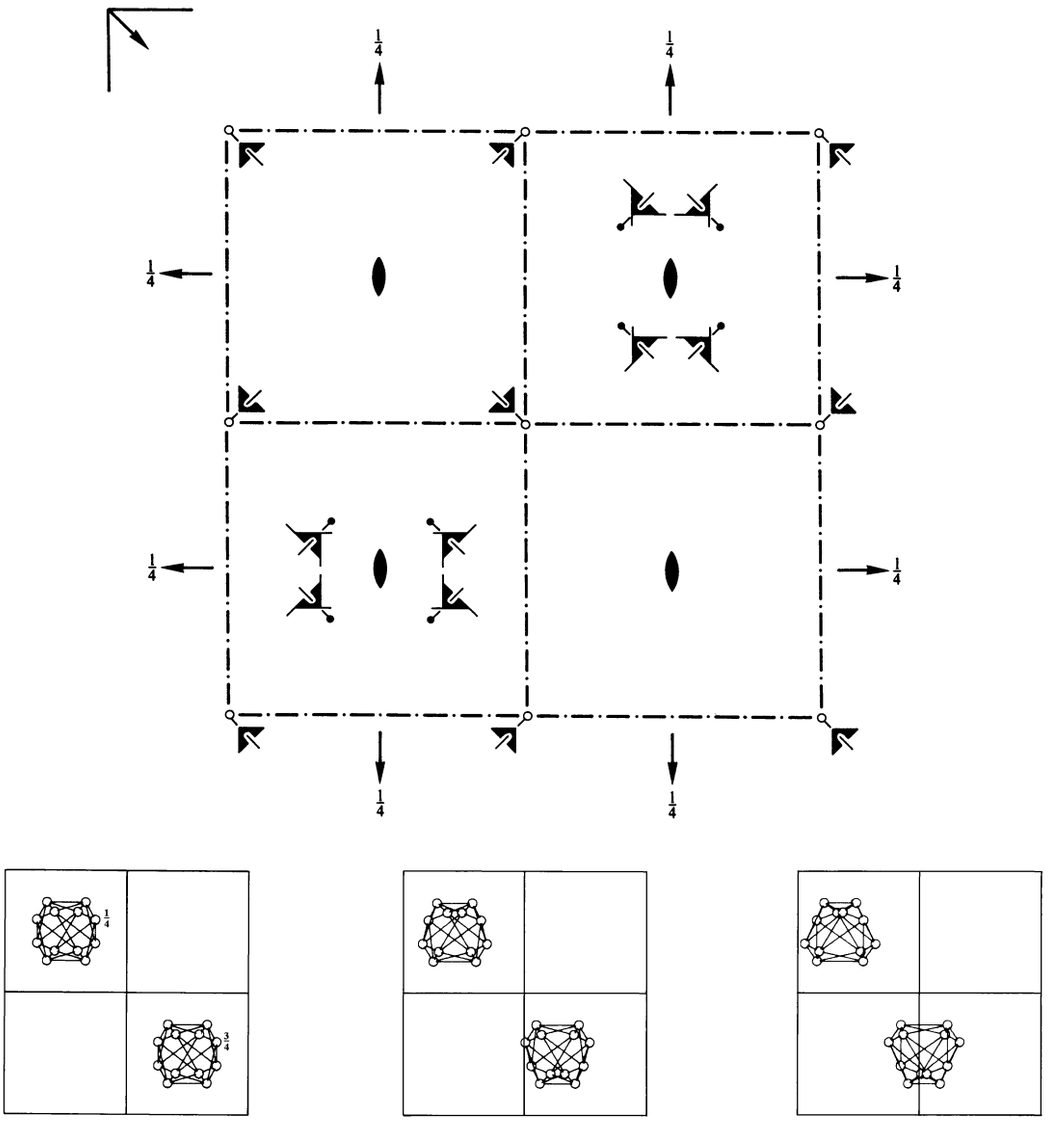
$Pn\bar{3}$ T_h^2 $m\bar{3}$ Cubic

No. 201 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 2



Origin at centre $(\bar{3})$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 23

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

Vertices $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ $\frac{3}{4},-\frac{1}{4},-\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

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

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

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

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P23$ (195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $Pn1$ ($Pnnn$, 48) 1; 2; 3; 4; 13; 14; 15; 16
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 5; 9; 13; 17; 21
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 6; 12; 13; 18; 24
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 7; 10; 13; 19; 22
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 8; 11; 13; 20; 23

IIa none

IIb [2] $Fd\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (203)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (201)

Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)