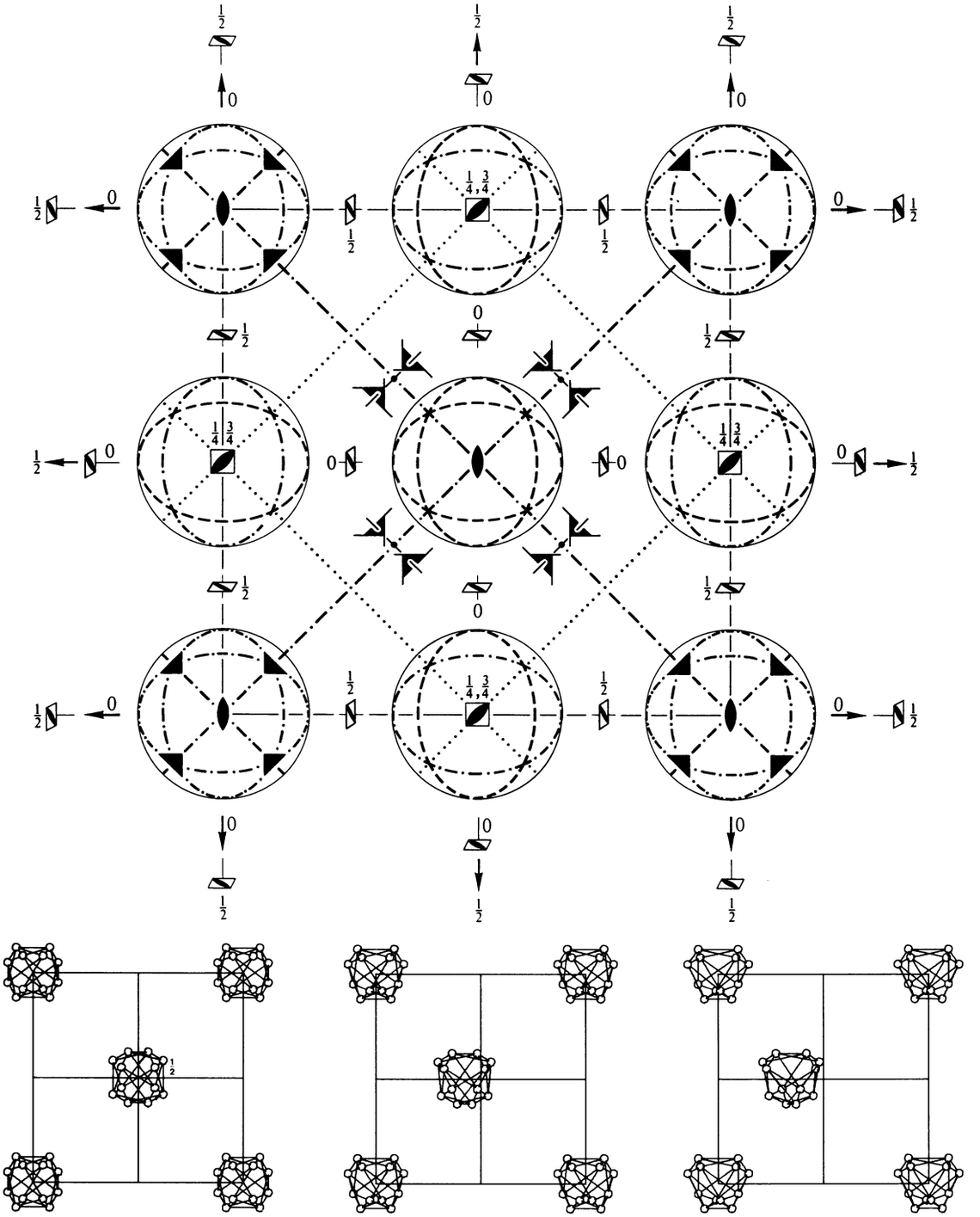
$P\bar{4}3n$ T_d^4 $\bar{4}3m$ Cubic

No. 218 $P\bar{4}3n$ Patterson symmetry $Pm\bar{3}m$



Origin at 2 3

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

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(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) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(14) c $x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(18) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(20) a $x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(22) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$	(23) b $\bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$

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 permutable
							General:
24	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hhl : $l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	
							Special: as above, plus
12	h	2 . .	$x,0,\frac{1}{2}$ $\frac{1}{2},x+\frac{1}{2},0$	$\bar{x},0,\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x,0$ $x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},x$ $0,\frac{1}{2},x+\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h=2n$
12	g	2 . .	$x,\frac{1}{2},0$ $0,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,x$ $\frac{1}{2},0,x+\frac{1}{2}$	$\frac{1}{2},0,\bar{x}$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$	hkl : $h=2n$
12	f	2 . .	$x,0,0$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,x$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	$0,0,\bar{x}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h+k+l=2n$
8	e	. 3 .	x,x,x $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},x$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x,\bar{x}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$			hkl : $h+k+l=2n$
6	d	$\bar{4}$ . .	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$
6	c	$\bar{4}$ . .	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	
6	b	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
2	a	2 3 .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{2},0,z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2\,3\,1$ ($P23$, 195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
- [3] $P\bar{4}\,1\,n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 13; 14; 15; 16
- [3] $P\bar{4}\,1\,n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 17; 18; 19; 20
- [3] $P\bar{4}\,1\,n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 21; 22; 23; 24
- [4] $P\,1\,3\,n$ ($R3c$, 161) 1; 5; 9; 13; 17; 21
- [4] $P\,1\,3\,n$ ($R3c$, 161) 1; 6; 12; 14; 20; 21
- [4] $P\,1\,3\,n$ ($R3c$, 161) 1; 7; 10; 14; 17; 23
- [4] $P\,1\,3\,n$ ($R3c$, 161) 1; 8; 11; 13; 20; 23

IIa none

IIb [4] $I\bar{4}\,3\,d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (220)

Maximal isomorphic subgroups of lowest index

IIc [27] $P\bar{4}\,3\,n$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (218)

Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pm\bar{3}n$ (223)

II [2] $I\bar{4}\,3\,m$ (217); [4] $F\bar{4}\,3\,c$ (219)