

$Pn\bar{3}$

No. 201

 $P2/n\bar{3}$ T_h^2

Axes	Coordinates		Wyckoff positions				
	origin 1	origin 2	2a	4b	4c	6d	8e
I Maximal translationengleiche subgroups							
[2] $P23$ (195)		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	1a; 1b	4e	4e	3c; 3d	$2 \times 4e$ 6g; 6h
[4] $R\bar{3}$ (148) (rhombohedral axes)	$x-\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$		2c	1a; 3e	1b; 3d	6f	$2c; 6f$ $2 \times 6f$ $2 \times 6f$
a - b , b - c , a + b + c (hex. axes)	$\frac{1}{3}(2x-y-z),$ $\frac{1}{3}(x+y-2z),$ $\frac{1}{3}(x+y+z)-\frac{1}{4}$	$\frac{1}{3}(2x-y-z),$ $\frac{1}{3}(x+y-2z),$ $\frac{1}{3}(x+y+z)$	6c	3a; 9e	3b; 9d	18f	$6c; 18f$ $2 \times 18f$ $2 \times 18f$
conjugate: - a - b , b + c , - a + b - c (hex. axes)	$\frac{1}{3}(-2x-y+z),$ $\frac{1}{3}(-x+y+2z),$ $\frac{1}{3}(-x+y-z)-\frac{1}{4}$	$\frac{1}{3}(-2x-y+z)+\frac{1}{2},$ $\frac{1}{3}(-x+y+2z)+\frac{1}{2},$ $\frac{1}{3}(-x+y-z)$					
conjugate: a + b , - b + c , a - b - c (hex. axes)	$\frac{1}{3}(2x+y+z),$ $\frac{1}{3}(x-y+2z),$ $\frac{1}{3}(x-y-z)-\frac{1}{4}$	$\frac{1}{3}(2x+y+z),$ $\frac{1}{3}(x-y+2z)+\frac{1}{2},$ $\frac{1}{3}(x-y-z)$					
conjugate: - a + b , - b - c , - a - b + c (hex. axes)	$\frac{1}{3}(-2x+y-z),$ $\frac{1}{3}(-x-y-2z),$ $\frac{1}{3}(-x-y+z)-\frac{1}{4}$	$\frac{1}{3}(-2x+y-z)+\frac{1}{2},$ $\frac{1}{3}(-x-y-2z),$ $\frac{1}{3}(-x-y+z)$					
[3] $Pnnn$ (48)			2a	4e(f^*)	4f(e^*)	2b; 2c; 2d	8m 4h; 4j; 4l $3 \times 8m$

* origin 2

II Maximal klassengleiche subgroups

Enlarged unit cell, non-isomorphic

[2] $Fd\bar{3}$ (203)	2a, 2b, 2c	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z;$ $+(\frac{1}{2}, 0, 0)$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z;$ $+(\frac{1}{2}, 0, 0)$	8a; 8b	16c; 16d	32e	48f	$2 \times 32e$ 96g	$2 \times 48f$ $2 \times 96g$
[2] $Fd\bar{3}$ (203)	2a, 2b, 2c	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4},$ $\frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4},$ $\frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$	8a; 8b	32e	16c; 16d	48f	$2 \times 32e$ 96g	$2 \times 48f$ $2 \times 96g$

Enlarged unit cell, isomorphic

[27] $Pn\bar{3}$	3a, 3b, 3c	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z;$ $\pm(\frac{1}{3}, 0, 0); \pm(0, \frac{1}{3}, 0); \pm(0, 0, \frac{1}{3});$ $\pm(0, \frac{1}{3}, \frac{1}{3}); \pm(\frac{1}{3}, 0, \frac{1}{3}); \pm(\frac{1}{3}, \frac{1}{3}, 0);$ $\pm(0, \frac{1}{3}, \frac{2}{3}); \pm(\frac{1}{3}, 0, \frac{2}{3}); \pm(\frac{1}{3}, \frac{2}{3}, 0);$ $\pm(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}); \pm(\frac{1}{3}, \frac{1}{3}, \frac{2}{3}); \pm(\frac{1}{3}, \frac{2}{3}, \frac{1}{3}); \pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$	2a; 2 \times 8e; 12f; 24h	4b(c^\dagger); 8e; 4 \times 24h	4c(b^\dagger); 8e; 4 \times 24h	6d; 12f; 2 \times 12g; 5 \times 24h	3 \times 8e; 8 \times 24h	3 \times 12f; 12 \times 24h	
[p^3] $Pn\bar{3}$	p \mathbf{a} , p \mathbf{b} , p \mathbf{c}	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	2a; $(p-1) \times 8e;$ $\frac{p-1}{2} \times 12f;$ $\frac{p^3-7p+6}{12} \times 24h$	4b(c^\ddagger); $\frac{p-1}{2} \times 8e;$ $\frac{p(p^2-1)}{6} \times 24h$	4c(b^\ddagger); $\frac{p-1}{2} \times 8e;$ $\frac{p(p^2-1)}{6} \times 24h$	6d; $\frac{p-1}{2} \times 12f$; $(p-1) \times 12g;$ $\frac{(p-1)^2(p+2)}{4} \times 24h$	$p \times 8e;$ $\frac{p(p^2-1)}{3} \times 24h$	$p \times 12f;$ $\frac{p(p^2-1)}{2} \times 24h$

† origin 1

‡ origin 1 and $p = 4n-1$