

$P4/nnc$

No. 126

 $P4/n2/n2/c$ D_{4h}^4

Axes	Coordinates		Wyckoff positions							
	origin 1	origin 2	2a	2b	4c	4d	4e	8f		
				8g	8h	8i	8j	16k		

I Maximal translationengleiche subgroups

[2] $P\bar{4}n2$ (118)	$x+\frac{1}{2}, y, z$ $z+\frac{1}{4}$	$x+\frac{1}{4}, y-\frac{1}{4}, z$	2d	2c $2 \times 4e$	4e 4f; 4g	2a; 2b 8i	4h 8i	8i $2 \times 8i$		
[2] $P\bar{4}2c$ (112)	$x+\frac{1}{2}, y, z$ $y, z+\frac{1}{4}$	$x+\frac{1}{4}, y-\frac{1}{4}, z$	2b	2d $4k; 4l$	2a; 2c 8n	2e; 2f 4g; 4h	4m 4i; 4j	8n $2 \times 8n$		
[2] $P4nc$ (104)		$x+\frac{1}{4}, y, z$ $y+\frac{1}{4}, z+\frac{1}{4}$	2a	2a $2 \times 4b$	4b 8c	4b 8c	$2 \times 2a$ 8c	8c $2 \times 8c$		
[2] $P422$ (89)		$x+\frac{1}{4}, y, z$ $y+\frac{1}{4}, z+\frac{1}{4}$	1a; 1d	1b; 1c $2 \times 4i$	2e; 2f 4j; 4k	4i 4l; 4m	2g; 2h 4n; 4o	8p $2 \times 8p$		
[2] $P4/n$ (85)	$x+\frac{1}{2}, y, z$ $y, z+\frac{1}{4}$		2c	2c $2 \times 4f$	4f 8g	2a; 2b 8g	$2 \times 2c$ 8g	8g $2 \times 8g$		
[2] $Pnnn$ (48)			2a	2c $2 \times 4l$	2b; 2d 8m	4l 4g; 4i	4k 4h; 4j	4e; 4f $2 \times 8m$		
[2] $Ccce$ (68)	$\mathbf{a}-\mathbf{b}, \frac{1}{2}(x-y), \frac{1}{2}(x-y)$ $\mathbf{a}+\mathbf{b}, \mathbf{c}, \frac{1}{2}(x+y), z, \frac{1}{2}(x+y), z$		4a	4b $2 \times 8h$	8h 8e; 8f	8h 16i	8g 16i	8c; 8d $2 \times 16i$		

II Maximal klassengleiche subgroups

Enlarged unit cell, isomorphic

[3] $P4/nnc$ a, b, 3c	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	2a(b^*); 4e	2b(a^*); 4e $3 \times 8g$	4c; 8g 8h; 16k	4d; 8g 8i(j^*); 16k	3×4e 8j(i^*); 16k	8f; 16k 3×16k		
[p] $P4/nnc$ a, b, pc	$x, y, \frac{1}{p}z; \pm(0, 0, \frac{1}{p})$ $+ (0, 0, \frac{u}{p})$	$x, y, \frac{1}{p}z; \pm(0, 0, \frac{1}{p})$ $+ (0, 0, \frac{u}{p})$	$2a(b^\dagger); \frac{p-1}{2} \times 4e$	$2b(a^\dagger); \frac{p-1}{2} \times 4e$ $p \times 8g$	$4c; \frac{p-1}{2} \times 8g$ $8h; \frac{p-1}{2} \times 16k$	$4d; \frac{p-1}{2} \times 8g$ $8i(j^\dagger); \frac{p-1}{2} \times 16k$	$p \times 4e$ $8j(i^\dagger); \frac{p-1}{2} \times 16k$	$8f; \frac{p-1}{2} \times 16k$ $p \times 16k$		
[9] $P4/nnc$ 3a, 3b, c	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3}, 0, 0); \pm(0, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3}, 0, 0); \pm(0, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{2}{3}, 0)$	2a(b^*); 8h; 8i(j^*)	2b(a^*); 8h; 8j(i^*) $8g; 4 \times 16k$	4c; 8i; 8j; 16k $3 \times 8h; 3 \times 16k$	4d; 2×16k $3 \times 8i(j^*); 3 \times 8j(i^*)$	4e; 2×16k $3 \times 16k$	8f; 4×16k $3 \times 16k$		
[p^2] $P4/nnc$ p a, p b, c	$\frac{1}{p}x, \frac{1}{p}y, z; \pm(\frac{1}{p}, 0, 0); \pm(\frac{u}{p}, \frac{v}{p}, 0)$ $+ (\frac{u}{p}, \frac{v}{p}, 0)$	$\frac{1}{p}x, \frac{1}{p}y, z; \pm(\frac{1}{p}, 0, 0); \pm(\frac{u}{p}, \frac{v}{p}, 0)$	$2a(b^\dagger); \frac{p-1}{2} \times 8h; \frac{p-1}{2} \times 8i(j^\dagger); \frac{(p-1)(p-3)}{8} \times 16k$	$2b(a^\dagger); \frac{p-1}{2} \times 8h; \frac{p-1}{2} \times 8j(i^\dagger); \frac{(p-1)(p-3)}{8} \times 16k$	$4c; \frac{p-1}{2} \times 8i; \frac{(p-1)^2}{4} \times 16k$	$4d; \frac{p-1}{2} \times 8j; \frac{(p-1)^2}{4} \times 16k$	4e; $\frac{p^2-1}{4} \times 16k$	8f; $\frac{p^2-1}{4} \times 16k$		
	$p = \text{prime} > 2;$ $u, v = 1, \dots, p-1$				$8g; \frac{p^2-1}{2} \times 16k$	$p \times 8h; \frac{p(p-1)}{2} \times 16k$	$p \times 8i(j^\dagger); \frac{p(p-1)}{2} \times 16k$	$p \times 8j(i^\dagger); \frac{p(p-1)}{2} \times 16k$	$p^2 \times 16k$	

* origin 2

† origin 2 and $p = 4n-1$