

$Pn\bar{n}n$

No. 48

 $P2/n\bar{2}/n\bar{2}/n$ D_{2h}^2

Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions							
			2a	2b	2c	2d 4i	4e 4j	4f 4k	4g 4l	4h 8m
I Maximal translationengleiche subgroups										
[2] $P2nn$ (34) $\cong Pnn2$	b, c, a y, z, x	$x, y + \frac{1}{4}, z + \frac{1}{4}$ $y + \frac{1}{4}, z + \frac{1}{4}, x$	2a	2a	2b	2b	4c	4c	$2 \times 2a$	$2 \times 2b$
[2] $Pn2n$ (34) $\cong Pnn2$	c, a, b z, x, y	$x + \frac{1}{4}, y, z + \frac{1}{4}$ $z + \frac{1}{4}, x + \frac{1}{4}, y$	2a	2b	2b	2a	4c	4c	4c	4c
[2] $Pnn2$ (34)		$x + \frac{1}{4}, y + \frac{1}{4}, z$	2a	2b	2a	2b	4c	4c	4c	4c
						4c	4c	$2 \times 2a$	$2 \times 2b$	$2 \times 4c$
[2] $P222$ (16)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	1a; 1h	1b; 1g	1d; 1e	1c; 1f	4u	4u	$2i; 2l$	$2j; 2k$
						2m; 2p	2n; 2o	2q; 2t	2r; 2s	$2 \times 4u$
[2] $P2/n11$ (13) $\cong P12/n1$	c, a, b	$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$ $z + \frac{1}{4}, x + \frac{1}{4}, y + \frac{1}{4}$	2e	2e	2f	2f	2c; 2d	2a; 2b	$2 \times 2e$	$2 \times 2f$
		z, x, y				4g	4g	4g	4g	$2 \times 4g$
[2] $P12/n1$ (13)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	2e	2f	2f	2e	2c; 2d	2a; 2b	4g	4g
						2 $\times 2e$	2 $\times 2f$	4g	4g	$2 \times 4g$
[2] $P112/n$ (13)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	2e	2f	2e	2f	2c; 2d	2a; 2b	4g	4g
						4g	4g	$2 \times 2e$	$2 \times 2f$	$2 \times 4g$

II Maximal klassengleiche subgroups

Enlarged unit cell, non-isomorphic

[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z;$ $\underbrace{\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z + \frac{1}{4};}_{+ (\frac{1}{2}, 0, 0)}$	8a; 8b	16e	16g	16f	16c; 16d	32h	$2 \times 16e$	32h
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y, \frac{1}{2}z;$ $\underbrace{\frac{1}{2}x, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z + \frac{1}{4};}_{+ (\frac{1}{2}, 0, 0)}$	16e	8a; 8b	16f	16g	32h	16c; 16d	$2 \times 16e$	32h
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z;$ $\underbrace{\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y, \frac{1}{2}z + \frac{1}{4};}_{+ (\frac{1}{2}, 0, 0)}$	16f	16g	16e	8a; 8b	32h	16c; 16d	32h	$2 \times 16e$
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z + \frac{1}{4};$ $\underbrace{\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z;}_{+ (\frac{1}{2}, 0, 0)}$	16g	16f	8a; 8b	16e	32h	16c; 16d	32h	$2 \times 16e$
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z + \frac{1}{4};$ $\underbrace{\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y, \frac{1}{2}z;}_{+ (\frac{1}{2}, 0, 0)}$	16e	8a; 8b	16f	16g	32h	16c; 16d	32h	$2 \times 16e$
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y, \frac{1}{2}z + \frac{1}{4};$ $\underbrace{\frac{1}{2}x, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z;}_{+ (\frac{1}{2}, 0, 0)}$	16f	16g	16e	8a; 8b	16c; 16d	32h	$2 \times 16e$	32h
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z;$ $\underbrace{\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z + \frac{1}{4};}_{+ (\frac{1}{2}, 0, 0)}$	16g	16f	8a; 8b	16e	16c; 16d	32h	$2 \times 16e$	32h
[2] $Fddd$ (70)	2a, 2b, 2c	$\frac{1}{2}x + \frac{1}{4}, \frac{1}{2}y + \frac{1}{4}, \frac{1}{2}z;$ $\underbrace{\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z;}_{+ (\frac{1}{2}, 0, 0)}$	8a; 8b	16e	16g	16f	32h	16c; 16d	$2 \times 16e$	32h

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*P*2/*n*2/*n*2/*n*

No. 48

Pnnn

Axes	Coordinates		Wyckoff positions							
	origin 1	origin 2	2 <i>a</i>	2 <i>b</i>	2 <i>c</i>	2 <i>d</i> 4 <i>i</i>	4 <i>e</i> 4 <i>j</i>	4 <i>f</i> 4 <i>k</i>	4 <i>g</i> 4 <i>l</i>	4 <i>h</i> 8 <i>m</i>
Enlarged unit cell, isomorphic										
[3] <i>Pnnn</i>	3a, b, c	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$2a(b^*); 4g$	$2b(a^*); 4g$	$2c(d^*); 4h$	$2d(c^*); 4h$	$4f(e^*); 8m$	$4e(f^*); 8m$	$3 \times 4g$
[<i>p</i>] <i>Pnnn</i>	pa, b, c	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$2a(b^\dagger); \frac{p-1}{2} \times 4g$	$2b(a^\dagger); \frac{p-1}{2} \times 4g$	$2c(d^\dagger); \frac{p-1}{2} \times 4h$	$2d(c^\dagger); \frac{p-1}{2} \times 4h$	$4e(f^\ddagger); \frac{p-1}{2} \times 8m$	$4f(e^\ddagger); \frac{p-1}{2} \times 8m$	$p \times 4g$
		$p = \text{prime} > 2; u = 1, \dots, p-1$						$4i(j^\dagger); \frac{p-1}{2} \times 8m$	$4j(i^\dagger); \frac{p-1}{2} \times 8m$	$4k(l^\dagger); \frac{p-1}{2} \times 8m$
[3] <i>Pnnn</i>	a, 3b, c	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$2a(d^*); 4i$	$2b(c^*); 4j$	$2c(b^*); 4j$	$2d(a^*); 4i$	$4f(e^*); 8m$	$4e(f^*); 8m$	$4g(h^*); 8m$
[<i>p</i>] <i>Pnnn</i>	a, pb, c	$x, \frac{1}{p}y, z; +(\frac{u}{p}, 0, 0)$	$x, \frac{1}{p}y, z; +(\frac{u}{p}, 0, 0)$	$2a(d^\dagger); \frac{p-1}{2} \times 4i$	$2b(c^\dagger); \frac{p-1}{2} \times 4j$	$2c(b^\dagger); \frac{p-1}{2} \times 4j$	$2d(a^\dagger); \frac{p-1}{2} \times 4i$	$4e(f^\ddagger); \frac{p-1}{2} \times 8m$	$4f(e^\ddagger); \frac{p-1}{2} \times 8m$	$4g(h^\dagger); \frac{p-1}{2} \times 8m$
		$p = \text{prime} > 2; u = 1, \dots, p-1$						$p \times 4i$	$p \times 4j$	$4k(l^\dagger); \frac{p-1}{2} \times 8m$
[3] <i>Pnnn</i>	a, b, 3c	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a(c^*); 4k$	$2b(d^*); 4l$	$2c(a^*); 4k$	$2d(b^*); 4l$	$4f(e^*); 8m$	$4e(f^*); 8m$	$4g(h^*); 8m$
[<i>p</i>] <i>Pnnn</i>	a, b, pc	$x, y, \frac{1}{p}z; +(\frac{u}{p}, 0, 0)$	$x, y, \frac{1}{p}z; +(\frac{u}{p}, 0, 0)$	$2a(c^\dagger); \frac{p-1}{2} \times 4k$	$2b(d^\dagger); \frac{p-1}{2} \times 4l$	$2c(a^\dagger); \frac{p-1}{2} \times 4k$	$2d(b^\dagger); \frac{p-1}{2} \times 4l$	$4e(f^\ddagger); \frac{p-1}{2} \times 8m$	$4f(e^\ddagger); \frac{p-1}{2} \times 8m$	$4g(h^\dagger); \frac{p-1}{2} \times 8m$
		$p = \text{prime} > 2; u = 1, \dots, p-1$						$4i(j^\dagger); \frac{p-1}{2} \times 8m$	$4j(i^\dagger); \frac{p-1}{2} \times 8m$	$p \times 4k$

* origin 2

‡ origin 1 and $p = 4n-1$ † origin 2 and $p = 4n-1$

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*P*2/*c*2/*c*2/*m*

No. 49

Pccm

Axes	Coordi-nates		Wyckoff positions									
	2 <i>a</i>	2 <i>b</i>	2 <i>c</i>	2 <i>d</i>	2 <i>e</i> 4 <i>l</i>	2 <i>f</i> 4 <i>m</i>	2 <i>g</i> 4 <i>n</i>	2 <i>h</i> 4 <i>o</i>	2 <i>i</i> 4 <i>p</i>	2 <i>j</i> 4 <i>q</i>	2 <i>k</i> 8 <i>r</i>	
[3] <i>Pccm</i>	a, b, 3c	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a; 4m$	$2b; 4n$	$2c; 4o$	$2d; 4p$	$2e; 4m$	$2f; 4p$	$2g; 4o$	$2h; 4n$	$4i; 8r$	$4j; 8r$
[<i>p</i>] <i>Pccm</i>	a, b, pc	$x, y, \frac{1}{p}z; +(\frac{u}{p}, 0, 0)$	$2a; \frac{p-1}{2} \times 4m$	$2b; \frac{p-1}{2} \times 4n$	$2c; \frac{p-1}{2} \times 4o$	$2d; \frac{p-1}{2} \times 4p$	$2e; \frac{p-1}{2} \times 4m$	$2f; \frac{p-1}{2} \times 4p$	$2g; \frac{p-1}{2} \times 4o$	$2h; \frac{p-1}{2} \times 4n$	$4i; \frac{p-1}{2} \times 8r$	$4j; \frac{p-1}{2} \times 8r$
		$p = \text{prime} > 2;$										
		$u = 1, \dots, p-1$						$4l; \frac{p-1}{2} \times 8r$	$p \times 4m$	$p \times 4n$	$p \times 4o$	$p \times 4p$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Pmaa $C \rightarrow A \quad a \rightarrow b \rightarrow c \rightarrow a \quad \mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a} \quad x \rightarrow y \rightarrow z \rightarrow x$ *Pbmmb* $C \rightarrow B \quad a \leftarrow b \leftarrow c \leftarrow a \quad \mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a} \quad x \leftarrow y \leftarrow z \leftarrow x$