

D_{4h}^7 $P4/n2_1/m2/m$ No. 129 $P\bar{4}/nm\bar{m}$

ORIGIN CHOICE 2, Origin at centre ($2/m$) at $n2_1(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

16	k	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x, z$	(4) $y, \bar{x} + \frac{1}{2}, z$
			(5) $\bar{x}, y + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, \bar{y}, \bar{z}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(8) $\bar{y}, \bar{x}, \bar{z}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(11) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(12) $\bar{y}, x + \frac{1}{2}, \bar{z}$
			(13) $x, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x} + \frac{1}{2}, y, z$	(15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(16) y, x, z

I Maximal translationengleiche subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14	1/4, 3/4, 0
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16	1/4, 3/4, 0
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16	1/4, 1/4, 0
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8	1/4, 3/4, 0
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12	
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
[2] $P2/n2_1/m1$ (59, $Pmmn$)	1; 2; 5; 6; 9; 10; 13; 14	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$		
$P4_2/nbm$ (138)	$\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/nbm$ (138)	$\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/nmc$ (137)	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/nmc$ (137)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/ncc$ (130)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/ncc$ (130)	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
[3] $\mathbf{c}' = 3\mathbf{c}$		
$\left\{ \begin{array}{l} P4/nmm (129) \\ P4/nmm (129) \\ P4/nmm (129) \end{array} \right.$	$\begin{array}{l} \langle 2; 3; 5; 9 \rangle \\ \langle 2; 3; (5; 9) + (0, 0, 2) \rangle \\ \langle 2; 3; (5; 9) + (0, 0, 4) \rangle \end{array}$	$\begin{array}{l} \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \end{array}$
		0, 0, 1 0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$		
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 2u) \rangle$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$p > 2; 0 \leq u < p$	
	p conjugate subgroups for the prime p	
[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$		
$P4/nmm$ (129)	$\begin{array}{l} \langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); \\ 3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2}, 0); \\ 9 + (2u, 2v, 0) \rangle \end{array}$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$
	$p > 2; 0 \leq u < p; 0 \leq v < p$	
	p^2 conjugate subgroups for the prime p	

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mmm$ (139)

• Decreased unit cell

none