

D_{2h}^2
 $P2/n2/n2/n$

No. 48

 $Pn\bar{1}n$

 ORIGIN CHOICE 1, Origin at 222, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

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

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	<i>m</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$

I Maximal translationengleiche subgroups

[2] $Pnn2$ (34)	1; 2; 7; 8		
[2] $Pn2n$ (34, $Pnn2$)	1; 3; 6; 8	c, a, b	
[2] $P2nn$ (34, $Pnn2$)	1; 4; 6; 7	b, c, a	
[2] $P222$ (16)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	−a − b, a, c	$1/4, 1/4, 1/4$
[2] $P12/n1$ (13, $P12/c1$)	1; 3; 5; 7	c, b, −a − c	$1/4, 1/4, 1/4$
[2] $P2/n11$ (13, $P12/c1$)	1; 4; 5; 8	−b, a, b + c	$1/4, 1/4, 1/4$

II Maximal klassengleiche subgroups

• Enlarged unit cell

 [2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$

$Fddd$ (70)	$\langle 2; 3; 5 \rangle$	2a, 2b, 2c	
$Fddd$ (70)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	2a, 2b, 2c	$0, 0, 1/2$
$Fddd$ (70)	$\langle (2; 3; 5) + (0, 0, 1) \rangle$	2a, 2b, 2c	$1/2, 0, 0$
$Fddd$ (70)	$\langle 3; (2; 5) + (0, 0, 1) \rangle$	2a, 2b, 2c	$0, 1/2, 0$
$Fddd$ (70)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	2a, 2b, 2c	$1/2, 1/2, 0$
$Fddd$ (70)	$\langle 3; 5; 2 + (0, 0, 1) \rangle$	2a, 2b, 2c	$1/2, 0, 1/2$
$Fddd$ (70)	$\langle 5; (2; 3) + (0, 0, 1) \rangle$	2a, 2b, 2c	$0, 1/2, 1/2$
$Fddd$ (70)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	2a, 2b, 2c	$1/2, 1/2, 1/2$

 [3] $\mathbf{a}' = 3\mathbf{a}$

$Pn\bar{1}n$ (48)	$\langle 2; 3; 5 + (1, 0, 0) \rangle$	3a, b, c	
$Pn\bar{1}n$ (48)	$\langle (2; 3) + (2, 0, 0); 5 + (3, 0, 0) \rangle$	3a, b, c	$1, 0, 0$
$Pn\bar{1}n$ (48)	$\langle (2; 3) + (4, 0, 0); 5 + (5, 0, 0) \rangle$	3a, b, c	$2, 0, 0$

 [3] $\mathbf{b}' = 3\mathbf{b}$

$Pn\bar{1}n$ (48)	$\langle 2; 3; 5 + (0, 1, 0) \rangle$	a, 3b, c	
$Pn\bar{1}n$ (48)	$\langle 3; 2 + (0, 2, 0); 5 + (0, 3, 0) \rangle$	a, 3b, c	$0, 1, 0$
$Pn\bar{1}n$ (48)	$\langle 3; 2 + (0, 4, 0); 5 + (0, 5, 0) \rangle$	a, 3b, c	$0, 2, 0$

 [3] $\mathbf{c}' = 3\mathbf{c}$

$Pn\bar{1}n$ (48)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	a, b, 3c	
$Pn\bar{1}n$ (48)	$\langle 2; 3 + (0, 0, 2); 5 + (0, 0, 3) \rangle$	a, b, 3c	$0, 0, 1$
$Pn\bar{1}n$ (48)	$\langle 2; 3 + (0, 0, 4); 5 + (0, 0, 5) \rangle$	a, b, 3c	$0, 0, 2$

• Series of maximal isomorphic subgroups

 [p] $\mathbf{a}' = p\mathbf{a}$

$Pn\bar{1}n$ (48)	$\langle (2; 3) + (2u, 0, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	pa, b, c	$u, 0, 0$
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 [p] $\mathbf{b}' = p\mathbf{b}$

$Pn\bar{1}n$ (48)	$\langle 3; 2 + (0, 2u, 0); 5 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	a, pb, c	$0, u, 0$
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 [p] $\mathbf{c}' = p\mathbf{c}$

$Pn\bar{1}n$ (48)	$\langle 2; 3 + (0, 0, 2u); 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	a, b, pc	$0, 0, u$
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I Minimal translationengleiche supergroups

[2] $P4/nnc$ (126); [2] $P4_2/nm$ (134); [3] $Pn\bar{3}$ (201)

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

[2] $Immm$ (71); [2] $Amaa$ (66, $Cccm$); [2] $Bbmb$ (66, $Cccm$); [2] $Cccm$ (66)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pncb$ (50, $Pban$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pcna$ (50, $Pban$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pban$ (50)

I Minimal translationengleiche supergroups

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