

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

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

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

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

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

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

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

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

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

## • Series of maximal isomorphic subgroups

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

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

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

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

[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)

ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $nnn$ , at  $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$  from 222

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

I Maximal translationengleiche subgroups

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

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2]  $a' = 2a, b' = 2b, c' = 2c$

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

[3]  $a' = 3a$

$Pnnn$ (48)	$\langle 5; (2; 3) + (1, 0, 0) \rangle$	<b>3a, b, c</b>	
$Pnnn$ (48)	$\langle (2; 3) + (3, 0, 0); 5 + (2, 0, 0) \rangle$	<b>3a, b, c</b>	1, 0, 0
$Pnnn$ (48)	$\langle (2; 3) + (5, 0, 0); 5 + (4, 0, 0) \rangle$	<b>3a, b, c</b>	2, 0, 0

[3]  $b' = 3b$

$Pnnn$ (48)	$\langle 3; 5; 2 + (0, 1, 0) \rangle$	<b>a, 3b, c</b>	
$Pnnn$ (48)	$\langle 3; 2 + (0, 3, 0); 5 + (0, 2, 0) \rangle$	<b>a, 3b, c</b>	0, 1, 0
$Pnnn$ (48)	$\langle 3; 2 + (0, 5, 0); 5 + (0, 4, 0) \rangle$	<b>a, 3b, c</b>	0, 2, 0

[3]  $c' = 3c$

$Pnnn$ (48)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	<b>a, b, 3c</b>	
$Pnnn$ (48)	$\langle 2; 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$	<b>a, b, 3c</b>	0, 0, 1
$Pnnn$ (48)	$\langle 2; 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	<b>a, b, 3c</b>	0, 0, 2

• Series of maximal isomorphic subgroups

[p]  $a' = pa$

$Pnnn$ (48)	$\langle (2; 3) + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 5 + (2u, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>pa, b, c</b>	$u, 0, 0$
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[p]  $b' = pb$

$Pnnn$ (48)	$\langle 3; 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0); 5 + (0, 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>a, pb, c</b>	$0, u, 0$
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[p]  $c' = pc$

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

[2] *P4/nnc* (126); [2] *P4<sub>2</sub>/nnm* (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**

[2] *P4/nnc* (126); [2] *P4<sub>2</sub>/nnm* (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)