

$P4_2/n$

No. 86

 $P4_2/n$
 C_{4h}^4

 ORIGIN CHOICE 1, Origin at $\bar{4}$, 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	g	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$
			(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) y, \bar{x}, \bar{z}	(8) \bar{y}, x, \bar{z}

I Maximal translationengleiche subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		
[2] $P4_2$ (77)	1; 2; 3; 4		1/2, 0, 0
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a} - \mathbf{b}, \mathbf{a}, \mathbf{c}$	1/4, 1/4, 1/4

II Maximal klassengleiche subgroups

• Enlarged unit cell

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

$F4_1/d$ (88, $I4_1/a$)	⟨2; 3; 5⟩	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	
$F4_1/d$ (88, $I4_1/a$)	⟨2; 3; 5 + (0, 0, 1)⟩	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
$F4_1/d$ (88, $I4_1/a$)	⟨2; 5; 3 + (0, 0, 1)⟩	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	1/2, 1/2, 0
$F4_1/d$ (88, $I4_1/a$)	⟨2; (3; 5) + (0, 0, 1)⟩	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	1/2, 1/2, 1/2

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

$\left\{ \begin{array}{l} P4_2/n \text{ (86)} \\ P4_2/n \text{ (86)} \\ P4_2/n \text{ (86)} \end{array} \right.$	$\left\{ \begin{array}{l} \langle 2; (3; 5) + (0, 0, 1) \rangle \\ \langle 2; 3 + (0, 0, 1); 5 + (0, 0, 3) \rangle \\ \langle 2; 3 + (0, 0, 1); 5 + (0, 0, 5) \rangle \end{array} \right.$	$\left\{ \begin{array}{l} \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \end{array} \right.$	$\left\{ \begin{array}{l} \\ 0, 0, 1 \\ 0, 0, 2 \end{array} \right.$
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• Series of maximal isomorphic subgroups

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

$P4_2/n$ (86)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, u
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 [p²] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$

$P4_2/n$ (86)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); p\mathbf{a}, p\mathbf{b}, \mathbf{c} \rangle$ $5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups for $p = 4n - 1$		$u, v, 0$
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 [p = q² + r²] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$

$P4_2/n$ (86)	$\langle 2 + (2u, 0, 0); 3 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2} - u, 0); q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c} \rangle$ $5 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0) \rangle$ prime $p > 4$; $q > 0$; $r > 0$; $0 \leq u < p$ p conjugate subgroups for $p = 4n + 1$		$u, 0, 0$
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I Minimal translationengleiche supergroups

 [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $C4_2/m$ (84, $P4_2/m$); [2] $I4/m$ (87)

• Decreased unit cell

 [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4/n$ (85)

ORIGIN CHOICE 2, Origin at $\bar{1}$ on n , at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{4}$

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

I Maximal translationengleiche subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		1/4, 1/4, 1/4
[2] $P4_2$ (77)	1; 2; 3; 4		3/4, 1/4, 0
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	-a - b, a, c	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$			
$F4_1/d$ (88, $I4_1/a$)	$\langle 2; 3; 5 \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	
$F4_1/d$ (88, $I4_1/a$)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
$F4_1/d$ (88, $I4_1/a$)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	1/2, 1/2, 0
$F4_1/d$ (88, $I4_1/a$)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	1/2, 1/2, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P4_2/n$ (86)	$\langle 2; 3 + (0, 0, 1); 5 + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P4_2/n$ (86)	$\langle 2; 3 + (0, 0, 1); 5 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); 5 + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, u
[p ²] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_2/n$ (86)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$ $3 + (u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (2u, 2v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups for $p = 4n - 1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
[p = q ² + r ²] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$			
$P4_2/n$ (86)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0);$ $3 + (\frac{r}{2} + u, \frac{q}{2} - \frac{1}{2} - u, 0); 5 + (2u, 0, 0) \rangle$ prime $p = 4n + 1$; q odd; $r > 1$; r even; $0 \leq u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$u, 0, 0$
$P4_2/n$ (86)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} + \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0);$ $3 + (\frac{r}{2} + \frac{1}{2} + u, \frac{q}{2} - 1 - u, 0); 5 + (1 + 2u, 0, 0) \rangle$ prime $p = 4n + 1$; $q > 1$; q even; r odd; $0 \leq u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$1/2 + u, 0, 0$

I Minimal translationengleiche supergroups

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