

$P4_2/n$ 

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

## • Series of maximal isomorphic subgroups

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

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

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

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

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

$P4_2/n$ (86)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + u, \frac{q}{2} - \frac{1}{2} - u, 0); 5 + (2u, 0, 0) \rangle$ $q > 0; q$ odd; $r > 1; r$ even; $p > 4; 0 \leq u < p$ $p$ 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)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} + \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + \frac{1}{2} + u, \frac{q}{2} - 1 - u, 0); 5 + (1 + 2u, 0, 0) \rangle$ $q > 1; q$ even; $r > 0; r$ odd; $p > 4; 0 \leq u < p$ $p$ 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

[2] P4<sub>2</sub>/nbc (133); [2] P4<sub>2</sub>/nnm (134); [2] P4<sub>2</sub>/nmc (137); [2] P4<sub>2</sub>/ncm (138)

### II Minimal non-isomorphic klassengleiche supergroups

#### • Additional centring translations

[2] C4<sub>2</sub>/m (84, P4<sub>2</sub>/m); [2] I4/m (87)

#### • Decreased unit cell

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