

$P4_1 2_1 2$

No. 92

 $P4_1 2_1 2$
 D_4^4

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

I Maximal translationengleiche subgroups

[2] $P4_1 11$ (76, $P4_1$)	1; 2; 3; 4		
[2] $P2_1 12$ (20, $C222_1$)	1; 2; 7; 8	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	0, 1/2, 0
[2] $P2_1 2_1 1$ (19, $P2_1 2_1 2_1$)	1; 2; 5; 6		0, 0, 1/4
			1/4, 0, 3/8

II Maximal klassengleiche subgroups

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4_3 2_1 2 \text{ (96)} \\ P4_3 2_1 2 \text{ (96)} \\ P4_3 2_1 2 \text{ (96)} \end{array} \right.$	$\langle 2 + (0, 0, 1); (3; 5) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
	$\langle 2 + (0, 0, 1); 3 + (0, 0, 2); 5 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
	$\langle 2 + (0, 0, 1); 3 + (0, 0, 2); 5 + (0, 0, 6) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4_3 2_1 2$ (96)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{3p}{4} - \frac{1}{4}); 5 + (0, 0, \frac{3p}{4} - \frac{1}{4} + 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 3 \pmod{4}$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, u
$P4_1 2_1 2$ (92)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); 5 + (0, 0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$ $p > 4; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod{4}$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, u
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_1 2_1 2$ (92)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

I Minimal translationengleiche supergroups

 [3] $P4_1 32$ (213)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $C4_1 22$ (91, $P4_1 22$); [2] $I4_1 22$ (98)

• Decreased unit cell

 [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4_2 2_1 2$ (94)