

$P\bar{3}c1$

No. 165

 $P\bar{3}2/c1$
 D_{3d}^4
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

| | | | | | |
|----|---|---|--|---|---|
| 12 | g | 1 | (1) x, y, z | (2) $\bar{y}, x - y, z$ | (3) $\bar{x} + y, \bar{x}, z$ |
| | | | (4) $y, x, \bar{z} + \frac{1}{2}$ | (5) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$ | (6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$ |
| | | | (7) $\bar{x}, \bar{y}, \bar{z}$ | (8) $y, \bar{x} + y, \bar{z}$ | (9) $x - y, x, \bar{z}$ |
| | | | (10) $\bar{y}, \bar{x}, z + \frac{1}{2}$ | (11) $\bar{x} + y, y, z + \frac{1}{2}$ | (12) $x, x - y, z + \frac{1}{2}$ |

I Maximal translationengleiche subgroups

| | | |
|-------------------------------------|---------------------|--|
| [2] $P3c1$ (158) | 1; 2; 3; 10; 11; 12 | |
| [2] $P321$ (150) | 1; 2; 3; 4; 5; 6 | 0, 0, 1/4 |
| [2] $P\bar{3}11$ (147, $P\bar{3}$) | 1; 2; 3; 7; 8; 9 | |
| { [3] $P12/c1$ (15, $C12/c1$) | 1; 4; 7; 10 | $-\mathbf{a} + \mathbf{b}, -\mathbf{a} - \mathbf{b}, \mathbf{c}$ |
| { [3] $P12/c1$ (15, $C12/c1$) | 1; 5; 7; 11 | $-\mathbf{a} - 2\mathbf{b}, \mathbf{a}, \mathbf{c}$ |
| { [3] $P12/c1$ (15, $C12/c1$) | 1; 6; 7; 12 | $2\mathbf{a} + \mathbf{b}, \mathbf{b}, \mathbf{c}$ |

II Maximal klassengleiche subgroups

• Enlarged unit cell

| | | | |
|--|--|---|---------|
| [3] $\mathbf{c}' = 3\mathbf{c}$ | | | |
| { $P\bar{3}c1$ (165) | $\langle 2; 7; 4 + (0, 0, 1) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | |
| { $P\bar{3}c1$ (165) | $\langle 2; 4 + (0, 0, 3); 7 + (0, 0, 2) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | 0, 0, 1 |
| { $P\bar{3}c1$ (165) | $\langle 2; 4 + (0, 0, 5); 7 + (0, 0, 4) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | 0, 0, 2 |
| [3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ | | | |
| { $H\bar{3}c1$ (163, $P\bar{3}1c$) | $\langle 2; 4; 7 \rangle$ | $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | |
| { $H\bar{3}c1$ (163, $P\bar{3}1c$) | $\langle (2; 4) + (1, -1, 0); 7 + (2, 0, 0) \rangle$ | $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | 1, 0, 0 |
| { $H\bar{3}c1$ (163, $P\bar{3}1c$) | $\langle 4; 2 + (2, 1, 0); 7 + (2, 2, 0) \rangle$ | $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | 1, 1, 0 |
| [4] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ | | | |
| { $P\bar{3}c1$ (165) | $\langle 2; 4; 7 \rangle$ | $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | |
| { $P\bar{3}c1$ (165) | $\langle (2; 4) + (1, -1, 0); 7 + (2, 0, 0) \rangle$ | $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | 1, 0, 0 |
| { $P\bar{3}c1$ (165) | $\langle 2 + (1, 2, 0); 4 + (-1, 1, 0); 7 + (0, 2, 0) \rangle$ | $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | 0, 1, 0 |
| { $P\bar{3}c1$ (165) | $\langle 4; 2 + (2, 1, 0); 7 + (2, 2, 0) \rangle$ | $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | 1, 1, 0 |

• Series of maximal isomorphic subgroups

| | | | |
|--|--|--|-----------|
| [p] $\mathbf{c}' = p\mathbf{c}$ | | | |
| $P\bar{3}c1$ (165) | $\langle 2; 4 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 7 + (0, 0, 2u) \rangle$ | $\mathbf{a}, \mathbf{b}, p\mathbf{c}$ | 0, 0, u |
| | $p > 2; 0 \leq u < p$ | | |
| | p conjugate subgroups for the prime p | | |
| [p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$ | | | |
| $P\bar{3}c1$ (165) | $\langle 2 + (u + v, -u + 2v, 0); 4 + (u - v, -u + v, 0); 7 + (2u, 2v, 0) \rangle$ | $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ | $u, v, 0$ |
| | $p > 1; p \neq 3; 0 \leq u < p; 0 \leq v < p$ | | |
| | p^2 conjugate subgroups for the prime p | | |

I Minimal translationengleiche supergroups

 [2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [3] $H\bar{3}c1$ (163, $P\bar{3}1c$); [3] $R_{\text{obv}}\bar{3}c$ (167, $R\bar{3}c$); [3] $R_{\text{rev}}\bar{3}c$ (167, $R\bar{3}c$)

• Decreased unit cell

 [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P\bar{3}m1$ (164)