

$P\bar{3}1c$ 

No. 163

 $P\bar{3}12/c$ 
 $D_{3d}^2$ 
**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 $i$ 1	(1) $x, y, z$	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$
	(4) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	(5) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$	(6) $x, x - y, \bar{z} + \frac{1}{2}$
	(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$
	(10) $y, x, z + \frac{1}{2}$	(11) $x - y, \bar{y}, z + \frac{1}{2}$	(12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$

**I Maximal translationengleiche subgroups**

[2] $P31c$ (159)	1; 2; 3; 10; 11; 12	
[2] $P312$ (149)	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] $P112/c$ (15, $C12/c1$ )	1; 4; 7; 10	$-\mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b}, \mathbf{c}$
[3] $P112/c$ (15, $C12/c1$ )	1; 5; 7; 11	$\mathbf{a}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$
[3] $P112/c$ (15, $C12/c1$ )	1; 6; 7; 12	$\mathbf{b}, -2\mathbf{a} - \mathbf{b}, \mathbf{c}$

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P\bar{3}1c \text{ (163)} \\ P\bar{3}1c \text{ (163)} \\ P\bar{3}1c \text{ (163)} \end{array} \right.$	$\langle 2; 7; 4 + (0, 0, 1) \rangle$ $\langle 2; 4 + (0, 0, 3); 7 + (0, 0, 2) \rangle$ $\langle 2; 4 + (0, 0, 5); 7 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	 0, 0, 1 0, 0, 2
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} H\bar{3}1c \text{ (165, } P\bar{3}c1) \\ H\bar{3}1c \text{ (165, } P\bar{3}c1) \\ H\bar{3}1c \text{ (165, } P\bar{3}c1) \end{array} \right.$	$\langle 2; 4; 7 \rangle$ $\langle 2 + (1, -1, 0); 4 + (1, 1, 0); 7 + (2, 0, 0) \rangle$ $\langle 2 + (2, 1, 0); (4; 7) + (2, 2, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	 1, 0, 0 1, 1, 0
[3] $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} R\bar{3}c \text{ (167)} \\ R\bar{3}c \text{ (167)} \\ R\bar{3}c \text{ (167)} \end{array} \right.$	$\langle 2; 7; 4 + (0, 0, 1) \rangle$ $\langle 2; 4 + (0, 0, 3); 7 + (0, 0, 2) \rangle$ $\langle 2; 4 + (0, 0, 5); 7 + (0, 0, 4) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, 3\mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, 3\mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, 3\mathbf{c}$	 0, 0, 1 0, 0, 2
[3] $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} R\bar{3}c \text{ (167)} \\ R\bar{3}c \text{ (167)} \\ R\bar{3}c \text{ (167)} \end{array} \right.$	$\langle 2; 7; 4 + (0, 0, 1) \rangle$ $\langle 2; 4 + (0, 0, 3); 7 + (0, 0, 2) \rangle$ $\langle 2; 4 + (0, 0, 5); 7 + (0, 0, 4) \rangle$	$2\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, 3\mathbf{c}$ $2\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, 3\mathbf{c}$ $2\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, 3\mathbf{c}$	 0, 0, 1 0, 0, 2
[4] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$			
$\left\{ \begin{array}{l} P\bar{3}1c \text{ (163)} \\ P\bar{3}1c \text{ (163)} \\ P\bar{3}1c \text{ (163)} \\ P\bar{3}1c \text{ (163)} \end{array} \right.$	$\langle 2; 4; 7 \rangle$ $\langle 2 + (1, -1, 0); 4 + (1, 1, 0); 7 + (2, 0, 0) \rangle$ $\langle 2 + (1, 2, 0); 4 + (1, 1, 0); 7 + (0, 2, 0) \rangle$ $\langle 2 + (2, 1, 0); (4; 7) + (2, 2, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	 1, 0, 0 0, 1, 0 1, 1, 0

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P\bar{3}1c$ (163)	$\langle 2; 4 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 7 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, $u$
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P\bar{3}1c$ (163)	$\langle 2 + (u + v, -u + 2v, 0); 4 + (u + v, u + v, 0); 7 + (2u, 2v, 0) \rangle$ $p > 1; p \neq 3; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for the prime $p$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

**I Minimal translationengleiche supergroups**

 [2]  $P6/mcc$  (192); [2]  $P6_3/mmc$  (194)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [3]  $H\bar{3}1c$  (165,  $P\bar{3}c1$ )

## • Decreased unit cell

 [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $P\bar{3}1m$  (162)