

$C_{2h}^4$  $P12/c1$ 

No. 13

 $P2/c$ UNIQUE AXIS  $b$ , CELL CHOICE 1Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4  $g$  1(1)  $x, y, z$  (2)  $\bar{x}, y, \bar{z} + \frac{1}{2}$  (3)  $\bar{x}, \bar{y}, \bar{z}$  (4)  $x, \bar{y}, z + \frac{1}{2}$ I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 4	
[2] $P121$ (3)	1; 2	0, 0, 1/4
[2] $P\bar{1}$ (2)	1; 3	

II Maximal *klassengleiche* subgroups

## • Enlarged unit cell

[2] $\mathbf{b}' = 2\mathbf{b}$			
$P12_1/c1$ (14)	$\langle 3; 2 + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P12_1/c1$ (14)	$\langle (2; 3) + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	0, 1/2, 0
$P12/c1$ (13)	$\langle 2; 3 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P12/c1$ (13)	$\langle 2; 3 + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	0, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P12/c1$ (13)	$\langle 2; 3 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12/c1$ (13)	$\langle (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	1/2, 0, 0
$P12/n1$ (13, $P12/c1$ )	$\langle 3; 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, -2\mathbf{a} + \mathbf{c}$	
$P12/n1$ (13, $P12/c1$ )	$\langle 2 + (2, 0, 0); 3 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, -2\mathbf{a} + \mathbf{c}$	1/2, 0, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$			
$C12/c1$ (15)	$\langle 2; 3 \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$C12/c1$ (15)	$\langle 2; 3 + (0, 1, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	0, 1/2, 0
$C12/c1$ (15)	$\langle (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	1/2, 0, 0
$C12/c1$ (15)	$\langle 2 + (1, 0, 0); 3 + (1, 1, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	1/2, 1/2, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P12/c1$ (13)	$\langle 2; 3 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$P12/c1$ (13)	$\langle 2; 3 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0
$P12/c1$ (13)	$\langle 2; 3 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P12/c1$ (13)	$\langle 3; 2 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P12/c1$ (13)	$\langle 2 + (0, 0, 3); 3 + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P12/c1$ (13)	$\langle 2 + (0, 0, 5); 3 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P12/c1$ (13)	$\langle 2; 3 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12/c1$ (13)	$\langle (2; 3) + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0
$P12/c1$ (13)	$\langle (2; 3) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -2\mathbf{a} + \mathbf{c}$			
$P12/c1$ (13)	$\langle 3; 2 + (-1, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a} + \mathbf{c}$	
$P12/c1$ (13)	$\langle 2 + (1, 0, 0); 3 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a} + \mathbf{c}$	1, 0, 0
$P12/c1$ (13)	$\langle 2 + (3, 0, 0); 3 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -4\mathbf{a} + \mathbf{c}$			
$P12/c1$ (13)	$\langle 3; 2 + (-2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -4\mathbf{a} + \mathbf{c}$	
$P12/c1$ (13)	$\langle 2 + (0, 0, 0); 3 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -4\mathbf{a} + \mathbf{c}$	1, 0, 0
$P12/c1$ (13)	$\langle 2 + (2, 0, 0); 3 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, -4\mathbf{a} + \mathbf{c}$	2, 0, 0

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{b}' = p\mathbf{b}$			
$P12/c1$ (13)	$\langle 2; 3 + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P12/c1$ (13)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 3 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
[ $p$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{c}' = -2q\mathbf{a} + \mathbf{c}$			
$P12/c1$ (13)	$\langle 2 + (-q + 2u, 0, 0); 3 + (2u, 0, 0) \rangle$ $p > 2; 0 \leq q < p; 0 \leq u < p$ $p$ conjugate subgroups for each pair of $q$ and prime $p$	$p\mathbf{a}, \mathbf{b}, -2q\mathbf{a} + \mathbf{c}$	$u, 0, 0$

**I Minimal translationengleiche supergroups**

[2]  $Pnnn$  (48); [2]  $Pccm$  (49); [2]  $Pban$  (50); [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pbcn$  (60); [2]  $Cmme$  (67); [2]  $Ccce$  (68); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86)

**II Minimal non-isomorphic klassengleiche supergroups**• **Additional centring translations**

[2]  $A12/m1$  (12,  $C12/m1$ ); [2]  $C12/c1$  (15); [2]  $I12/c1$  (15,  $C12/c1$ )

• **Decreased unit cell**

[2]  $c' = \frac{1}{2}c$   $P12/m1$  (10)

**I Minimal translationengleiche supergroups**

[2]  $Pnnn$  (48); [2]  $Pccm$  (49); [2]  $Pban$  (50); [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pbcn$  (60); [2]  $Cmme$  (67); [2]  $Ccce$  (68); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86)

**II Minimal non-isomorphic klassengleiche supergroups**• **Additional centring translations**

[2]  $A112/a$  (15); [2]  $B112/m$  (12,  $A112/m$ ); [2]  $I112/a$  (15,  $A112/a$ )

• **Decreased unit cell**

[2]  $a' = \frac{1}{2}a$   $P112/m$  (10)

UNIQUE AXIS *c*, CELL CHOICE 1**Generators selected** (1); *t*(1,0,0); *t*(0,1,0); *t*(0,0,1); (2); (3)**General position**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4 g 1

(1) *x, y, z* (2)  $\bar{x} + \frac{1}{2}, \bar{y}, z$  (3)  $\bar{x}, \bar{y}, \bar{z}$  (4)  $x + \frac{1}{2}, y, \bar{z}$ **I Maximal translationengleiche subgroups**

[2] P11a (7)	1; 4	
[2] P112 (3)	1; 2	1/4, 0, 0
[2] P $\bar{1}$ (2)	1; 3	

**II Maximal klassengleiche subgroups**• **Enlarged unit cell**

[2] <b>c' = 2c</b>			
P112 <sub>1</sub> /a (14)	$\langle 3; 2 + (0, 0, 1) \rangle$	<b>a, b, 2c</b>	
P112 <sub>1</sub> /a (14)	$\langle (2; 3) + (0, 0, 1) \rangle$	<b>a, b, 2c</b>	0, 0, 1/2
P112/a (13)	$\langle 2; 3 \rangle$	<b>a, b, 2c</b>	
P112/a (13)	$\langle 2; 3 + (0, 0, 1) \rangle$	<b>a, b, 2c</b>	0, 0, 1/2
[2] <b>b' = 2b</b>			
P112/a (13)	$\langle 2; 3 \rangle$	<b>a, 2b, c</b>	
P112/a (13)	$\langle (2; 3) + (0, 1, 0) \rangle$	<b>a, 2b, c</b>	0, 1/2, 0
P112/n (13, P112/a)	$\langle 3; 2 + (0, 1, 0) \rangle$	<b>a - 2b, 2b, c</b>	
P112/n (13, P112/a)	$\langle 2 + (0, 2, 0); 3 + (0, 1, 0) \rangle$	<b>a - 2b, 2b, c</b>	0, 1/2, 0
[2] <b>b' = 2b, c' = 2c</b>			
A112/a (15)	$\langle 2; 3 \rangle$	<b>a, 2b, 2c</b>	
A112/a (15)	$\langle 2; 3 + (0, 0, 1) \rangle$	<b>a, 2b, 2c</b>	0, 0, 1/2
A112/a (15)	$\langle (2; 3) + (0, 1, 0) \rangle$	<b>a, 2b, 2c</b>	0, 1/2, 0
A112/a (15)	$\langle 2 + (0, 1, 0); 3 + (0, 1, 1) \rangle$	<b>a, 2b, 2c</b>	0, 1/2, 1/2
[3] <b>c' = 3c</b>			
P112/a (13)	$\langle 2; 3 \rangle$	<b>a, b, 3c</b>	
P112/a (13)	$\langle 2; 3 + (0, 0, 2) \rangle$	<b>a, b, 3c</b>	0, 0, 1
P112/a (13)	$\langle 2; 3 + (0, 0, 4) \rangle$	<b>a, b, 3c</b>	0, 0, 2
[3] <b>a' = 3a</b>			
P112/a (13)	$\langle 3; 2 + (1, 0, 0) \rangle$	<b>3a, b, c</b>	
P112/a (13)	$\langle 2 + (3, 0, 0); 3 + (2, 0, 0) \rangle$	<b>3a, b, c</b>	1, 0, 0
P112/a (13)	$\langle 2 + (5, 0, 0); 3 + (4, 0, 0) \rangle$	<b>3a, b, c</b>	2, 0, 0
[3] <b>b' = 3b</b>			
P112/a (13)	$\langle 2; 3 \rangle$	<b>a, 3b, c</b>	
P112/a (13)	$\langle (2; 3) + (0, 2, 0) \rangle$	<b>a, 3b, c</b>	0, 1, 0
P112/a (13)	$\langle (2; 3) + (0, 4, 0) \rangle$	<b>a, 3b, c</b>	0, 2, 0
[3] <b>a' = a - 2b, b' = 3b</b>			
P112/a (13)	$\langle 3; 2 + (0, -1, 0) \rangle$	<b>a - 2b, 3b, c</b>	
P112/a (13)	$\langle 2 + (0, 1, 0); 3 + (0, 2, 0) \rangle$	<b>a - 2b, 3b, c</b>	0, 1, 0
P112/a (13)	$\langle 2 + (0, 3, 0); 3 + (0, 4, 0) \rangle$	<b>a - 2b, 3b, c</b>	0, 2, 0
[3] <b>a' = a - 4b, b' = 3b</b>			
P112/a (13)	$\langle 3; 2 + (0, -2, 0) \rangle$	<b>a - 4b, 3b, c</b>	
P112/a (13)	$\langle 2 + (0, 0, 0); 3 + (0, 2, 0) \rangle$	<b>a - 4b, 3b, c</b>	0, 1, 0
P112/a (13)	$\langle 2 + (0, 2, 0); 3 + (0, 4, 0) \rangle$	<b>a - 4b, 3b, c</b>	0, 2, 0

• **Series of maximal isomorphic subgroups**

[ <i>p</i> ] <b>c' = pc</b>			
P112/a (13)	$\langle 2; 3 + (0, 0, 2u) \rangle$	<b>a, b, pc</b>	0, 0, <i>u</i>
	$p > 2; 0 \leq u < p$		
	<i>p</i> conjugate subgroups for the prime <i>p</i>		
[ <i>p</i> ] <b>a' = pa</b>			
P112/a (13)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 3 + (2u, 0, 0) \rangle$	<b>pa, b, c</b>	<i>u</i> , 0, 0
	$p > 2; 0 \leq u < p$		
	<i>p</i> conjugate subgroups for the prime <i>p</i>		
[ <i>p</i> ] <b>a' = a - 2qb, b' = pb</b>			
P112/a (13)	$\langle 2 + (0, -q + 2u, 0); 3 + (0, 2u, 0) \rangle$	<b>a - 2qb, pb, c</b>	0, <i>u</i> , 0
	$p > 2; 0 \leq q < p; 0 \leq u < p$		
	<i>p</i> conjugate subgroups for each pair of <i>q</i> and prime <i>p</i>		

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**I Minimal translationengleiche supergroups**

[2]  $Pnnn$  (48); [2]  $Pccm$  (49); [2]  $Pban$  (50); [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pbcn$  (60); [2]  $Cmme$  (67); [2]  $Ccce$  (68); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86)

**II Minimal non-isomorphic klassengleiche supergroups**• **Additional centring translations**

[2]  $A12/m1$  (12,  $C12/m1$ ); [2]  $C12/c1$  (15); [2]  $I12/c1$  (15,  $C12/c1$ )

• **Decreased unit cell**

[2]  $c' = \frac{1}{2}c$   $P12/m1$  (10)

**I Minimal translationengleiche supergroups**

[2]  $Pnnn$  (48); [2]  $Pccm$  (49); [2]  $Pban$  (50); [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pbcn$  (60); [2]  $Cmme$  (67); [2]  $Ccce$  (68); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86)

**II Minimal non-isomorphic klassengleiche supergroups**• **Additional centring translations**

[2]  $A112/a$  (15); [2]  $B112/m$  (12,  $A112/m$ ); [2]  $I112/a$  (15,  $A112/a$ )

• **Decreased unit cell**

[2]  $a' = \frac{1}{2}a$   $P112/m$  (10)