

$C_{2h}^2$ 
 $P12_1/m1$ 

No. 11

 $P2_1/m$ 

 UNIQUE AXIS  $b$ 
**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  $f$  1

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

[2] $P1m1$ (6)	1; 4		0, 1/4, 0
[2] $P12_11$ (4)	1; 2		
[2] $P\bar{1}$ (2)	1; 3		

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 3; 2 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P12_1/a1$ (14, $P12_1/c1$ )	$\langle 3; 2 + (1, 0, 0) \rangle$	$-2\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{a}$	
$P12_1/a1$ (14, $P12_1/c1$ )	$\langle 2; 3 + (1, 0, 0) \rangle$	$-2\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{a}$	1/2, 0, 0
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	1/2, 0, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$			
$B12_1/e1$ (14, $P12_1/c1$ )	$\langle 3; 2 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B12_1/e1$ (14, $P12_1/c1$ )	$\langle 2; 3 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
$B12_1/m1$ (11, $P12_1/m1$ )	$\langle 2; 3 \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B12_1/m1$ (11, $P12_1/m1$ )	$\langle (2; 3) + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P12_1/m1$ (11)	$\langle 3; 2 + (0, 1, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$P12_1/m1$ (11)	$\langle 2 + (0, 1, 0); 3 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0
$P12_1/m1$ (11)	$\langle 2 + (0, 1, 0); 3 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}' = \mathbf{a} - \mathbf{c}, \mathbf{c}' = 3\mathbf{c}$			
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 2) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 4) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}' = \mathbf{a} - 2\mathbf{c}, \mathbf{c}' = 3\mathbf{c}$			
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a} - 2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 2) \rangle$	$\mathbf{a} - 2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 4) \rangle$	$\mathbf{a} - 2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P12_1/m1$ (11)	$\langle 2; 3 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0
$P12_1/m1$ (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	2, 0, 0

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{b}' = p\mathbf{b}$			
$P12_1/m1$ (11)	$\langle 2 + (0, \frac{p}{2} - \frac{1}{2}, 0); 3 + (0, 2u, 0) \rangle$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	0, $u$ , 0
	prime $p > 2$ ; $0 \leq u < p$		
	$p$ conjugate subgroups		
[ $p$ ] $\mathbf{a}' = \mathbf{a} - q\mathbf{c}, \mathbf{c}' = p\mathbf{c}$			
$P12_1/m1$ (11)	$\langle (2; 3) + (0, 0, 2u) \rangle$	$\mathbf{a} - q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	0, 0, $u$
	prime $p > 2$ ; $0 \leq q < p$ ; $0 \leq u < p$		
	$p$ conjugate subgroups for each pair of $q$ and $p$		
[ $p$ ] $\mathbf{a}' = p\mathbf{a}$			
$P12_1/m1$ (11)	$\langle (2; 3) + (2u, 0, 0) \rangle$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u$ , 0, 0
	prime $p > 2$ ; $0 \leq u < p$		
	$p$ conjugate subgroups		

**I Minimal *translationengleiche* supergroups**

[2]  $Pmma$  (51); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pnma$  (62); [2]  $Cmcm$  (63); [3]  $P6_3/m$  (176)

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

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

**• Decreased unit cell**

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

**I Minimal *translationengleiche* supergroups**

[2]  $Pmma$  (51); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pnma$  (62); [2]  $Cmcm$  (63); [3]  $P6_3/m$  (176)

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

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

**• Decreased unit cell**

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

UNIQUE AXIS *c*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 *f* 1(1) *x, y, z* (2)  $\bar{x}, \bar{y}, z + \frac{1}{2}$  (3)  $\bar{x}, \bar{y}, \bar{z}$  (4) *x, y, z* +  $\frac{1}{2}$ 

## I Maximal translationengleiche subgroups

[2] P11 <i>m</i> (6)	1; 4		0, 0, 1/4
[2] P112 <sub>1</sub> (4)	1; 2		
[2] P $\bar{1}$ (2)	1; 3		

## II Maximal klassengleiche subgroups

## • Enlarged unit cell

[2] <b>a' = 2a</b>			
P112 <sub>1</sub> /a (14)	$\langle 3; 2 + (1, 0, 0) \rangle$	2a, b, c	
P112 <sub>1</sub> /a (14)	$\langle 2; 3 + (1, 0, 0) \rangle$	2a, b, c	1/2, 0, 0
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	2a, b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (1, 0, 0) \rangle$	2a, b, c	1/2, 0, 0
[2] <b>b' = 2b</b>			
P112 <sub>1</sub> /b (14, P112 <sub>1</sub> /a)	$\langle 3; 2 + (0, 1, 0) \rangle$	2b, -a - 2b, c	
P112 <sub>1</sub> /b (14, P112 <sub>1</sub> /a)	$\langle 2; 3 + (0, 1, 0) \rangle$	2b, -a - 2b, c	0, 1/2, 0
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	a, 2b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (0, 1, 0) \rangle$	a, 2b, c	0, 1/2, 0
[2] <b>a' = 2a, b' = 2b</b>			
C112 <sub>1</sub> /e (14, P112 <sub>1</sub> /a)	$\langle 3; 2 + (1, 0, 0) \rangle$	2a, -a + b, c	
C112 <sub>1</sub> /e (14, P112 <sub>1</sub> /a)	$\langle 2; 3 + (1, 0, 0) \rangle$	2a, -a + b, c	1/2, 0, 0
C112 <sub>1</sub> /m (11, P112 <sub>1</sub> /m)	$\langle 2; 3 \rangle$	2a, -a + b, c	
C112 <sub>1</sub> /m (11, P112 <sub>1</sub> /m)	$\langle (2; 3) + (1, 0, 0) \rangle$	2a, -a + b, c	1/2, 0, 0
[3] <b>c' = 3c</b>			
P112 <sub>1</sub> /m (11)	$\langle 3; 2 + (0, 0, 1) \rangle$	a, b, 3c	
P112 <sub>1</sub> /m (11)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 2) \rangle$	a, b, 3c	0, 0, 1
P112 <sub>1</sub> /m (11)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 4) \rangle$	a, b, 3c	0, 0, 2
[3] <b>a' = 3a</b>			
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	3a, b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	3a, b, c	1, 0, 0
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	3a, b, c	2, 0, 0
[3] <b>a' = 3a, b' = -a + b</b>			
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	3a, -a + b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	3a, -a + b, c	1, 0, 0
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	3a, -a + b, c	2, 0, 0
[3] <b>a' = 3a, b' = -2a + b</b>			
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	3a, -2a + b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	3a, -2a + b, c	1, 0, 0
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	3a, -2a + b, c	2, 0, 0
[3] <b>b' = 3b</b>			
P112 <sub>1</sub> /m (11)	$\langle 2; 3 \rangle$	a, 3b, c	
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (0, 2, 0) \rangle$	a, 3b, c	0, 1, 0
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (0, 4, 0) \rangle$	a, 3b, c	0, 2, 0
• Series of maximal isomorphic subgroups			
[ <i>p</i> ] <b>c' = pc</b>			
P112 <sub>1</sub> /m (11)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	a, b, pc	0, 0, <i>u</i>
[ <i>p</i> ] <b>a' = pa, b' = -qa + b</b>			
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (2u, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq q < p$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups for each pair of <i>q</i> and <i>p</i>	pa, -qa + b, c	<i>u</i> , 0, 0
[ <i>p</i> ] <b>b' = pb</b>			
P112 <sub>1</sub> /m (11)	$\langle (2; 3) + (0, 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	a, pb, c	0, <i>u</i> , 0

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**I Minimal *translationengleiche* supergroups**

[2]  $Pmma$  (51); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pnma$  (62); [2]  $Cmcm$  (63); [3]  $P6_3/m$  (176)

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

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

**• Decreased unit cell**

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

**I Minimal *translationengleiche* supergroups**

[2]  $Pmma$  (51); [2]  $Pbcm$  (57); [2]  $Pmnn$  (59); [2]  $Pnma$  (62); [2]  $Cmcm$  (63); [3]  $P6_3/m$  (176)

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

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

**• Decreased unit cell**

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