

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

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 symmetry4     $f$     1(1)  $x,y,z$     (2)  $\bar{x},y+\frac{1}{2},\bar{z}$     (3)  $\bar{x},\bar{y},\bar{z}$     (4)  $x,\bar{y}+\frac{1}{2},z$ 

## Coordinates

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

## • Series of maximal isomorphic subgroups

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

**I Minimal *translationengleiche* supergroups**

[2] *Pmma* (51); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] *P6<sub>3</sub>/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] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] *P6<sub>3</sub>/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)

$C_{2h}^2$  $P112_1/m$ 

No. 11

 $P2_1/m$ 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

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

[2] $P11m$ (6)	1; 4	0, 0, 1/4
[2] $P112_1$ (4)	1; 2	
[2] $P\bar{1}$ (2)	1; 3	

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

[2] $\mathbf{a}' = 2\mathbf{a}$		
$P112_1/a$ (14)	$\langle 3; 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$P112_1/a$ (14)	$\langle 2; 3 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$P112_1/m$ (11)	$\langle 2; 3 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$P112_1/m$ (11)	$\langle (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
[2] $\mathbf{b}' = 2\mathbf{b}$		
$P112_1/b$ (14, $P112_1/a$ )	$\langle 3; 2 + (0, 1, 0) \rangle$	$2\mathbf{b}, -\mathbf{a} - 2\mathbf{b}, \mathbf{c}$
$P112_1/b$ (14, $P112_1/a$ )	$\langle 2; 3 + (0, 1, 0) \rangle$	$2\mathbf{b}, -\mathbf{a} - 2\mathbf{b}, \mathbf{c}$
$P112_1/m$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$
$P112_1/m$ (11)	$\langle (2; 3) + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$		
$C112_1/e$ (14, $P112_1/a$ )	$\langle 3; 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
$C112_1/e$ (14, $P112_1/a$ )	$\langle 2; 3 + (1, 0, 0) \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
$C112_1/m$ (11, $P112_1/m$ )	$\langle 2; 3 \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
$C112_1/m$ (11, $P112_1/m$ )	$\langle (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
[3] $\mathbf{c}' = 3\mathbf{c}$		
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 3; 2 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 2) \rangle$	$0, 0, 1$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 4) \rangle$	$0, 0, 2$
[3] $\mathbf{a}' = 3\mathbf{a}$		
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2; 3 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	$1, 0, 0$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	$2, 0, 0$
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}$		
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2; 3 \rangle$	$3\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	$3\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	$3\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$		
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2; 3 \rangle$	$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (2, 0, 0) \rangle$	$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (4, 0, 0) \rangle$	$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$
[3] $\mathbf{b}' = 3\mathbf{b}$		
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle 2; 3 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (0, 2, 0) \rangle$	$0, 1, 0$
$\begin{cases} P112_1/m \\ P112_1/m \\ P112_1/m \end{cases}$ (11)	$\langle (2; 3) + (0, 4, 0) \rangle$	$0, 2, 0$

**• Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$		
$P112_1/m$ (11)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$p$ conjugate subgroups for the prime $p$	
[p] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = -q\mathbf{a} + \mathbf{b}$		
$P112_1/m$ (11)	$\langle (2; 3) + (2u, 0, 0) \rangle$ $p > 2; 0 \leq q < p; 0 \leq u < p$	$p\mathbf{a}, -q\mathbf{a} + \mathbf{b}, \mathbf{c}$
	$p$ conjugate subgroups for each pair of $q$ and prime $p$	
[p] $\mathbf{b}' = p\mathbf{b}$		
$P112_1/m$ (11)	$\langle (2; 3) + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$
	$p$ conjugate subgroups for the prime $p$	

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**I Minimal *translationengleiche* supergroups**

[2] *Pmma* (51); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] *P6<sub>3</sub>/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] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] *P6<sub>3</sub>/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)