

$P\bar{1}$ 

No. 2

 $P\bar{1}$ 
 $C_i^1$ 
**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2)

**General position**

 Multiplicity,  
 Wyckoff letter,  
 Site symmetry

Coordinates

 2  $i$  1

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

 [2]  $P1$  (1) 1

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	1/2, 0, 0
[2] $\mathbf{b}' = 2\mathbf{b}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	0, 1/2, 0
[2] $\mathbf{c}' = 2\mathbf{c}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
[2] $\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$	$A\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{b} + \mathbf{c}$	
	$A\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 + (0, 1, 0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{b} + \mathbf{c}$	0, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$	$B\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{a} + \mathbf{c}$	
	$B\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{a} + \mathbf{c}$	1/2, 0, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$	$C\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	
	$C\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	1/2, 0, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$	$F\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	
	$F\bar{1}$ (2, $P\bar{1}$ )	$\langle 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	1/2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{a} + \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{a} + \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$	$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	
	$P\bar{1}$ (2)	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	1, 0, 0
	$P\bar{1}$ (2)	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}$	2, 0, 0

[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	1, 0, 0
	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$	$\langle 2 \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (2, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	1, 0, 0
	$\langle 2 + (4, 0, 0) \rangle$	$3\mathbf{a}, 2\mathbf{a} + \mathbf{b}, 2\mathbf{a} + \mathbf{c}$	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0
	$\langle 2 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 2, 0
[3] $\mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = \mathbf{b} + \mathbf{c}$	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b} + \mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b} + \mathbf{c}$	0, 1, 0
	$\langle 2 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b} + \mathbf{c}$	0, 2, 0
[3] $\mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 2\mathbf{b} + \mathbf{c}$	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b} + \mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b} + \mathbf{c}$	0, 1, 0
	$\langle 2 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b} + \mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$\left\{ \begin{array}{l} P\bar{1} (2) \\ P\bar{1} (2) \\ P\bar{1} (2) \end{array} \right.$	$\langle 2 + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
	$\langle 2 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = q\mathbf{a} + \mathbf{b}, \mathbf{c}' = r\mathbf{a} + \mathbf{c}$	$\langle 2 + (2u, 0, 0) \rangle$	$p\mathbf{a}, q\mathbf{a} + \mathbf{b}, r\mathbf{a} + \mathbf{c}$	$u, 0, 0$
	prime $p > 2$ ; $0 \leq q < p$ ; $0 \leq r < p$ ; $0 \leq u < p$		
	$p$ conjugate subgroups for each triplet of $q, r,$ and $p$		
[p] $\mathbf{b}' = p\mathbf{b}, \mathbf{c}' = q\mathbf{b} + \mathbf{c}$	$\langle 2 + (0, 2u, 0) \rangle$	$\mathbf{a}, p\mathbf{b}, q\mathbf{b} + \mathbf{c}$	$0, u, 0$
	prime $p > 2$ ; $0 \leq q < p$ ; $0 \leq u < p$		
	$p$ conjugate subgroups for each pair of $q$ and $p$		
[p] $\mathbf{c}' = p\mathbf{c}$	$\langle 2 + (0, 0, 2u) \rangle$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
	prime $p > 2$ ; $0 \leq u < p$		
	$p$ conjugate subgroups		

I Minimal translationengleiche supergroups

[2]  $P12/m1$  (10); [2]  $P112/m$  (10); [2]  $P12_1/m1$  (11); [2]  $P112_1/m$  (11); [2]  $C12/m1$  (12); [2]  $A112/m$  (12); [2]  $P12/c1$  (13); [2]  $P112/a$  (13); [2]  $P12_1/c1$  (14); [2]  $P112_1/a$  (14); [2]  $C12/c1$  (15); [2]  $A112/a$  (15); [3]  $P\bar{3}$  (147); [3]  $R\bar{3}$  (148)

II Minimal non-isomorphic klassengleiche supergroups

none