

C_2^3

C121

No. 5

C2

UNIQUE AXIS b , CELL CHOICE 1Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4 c 1 $(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$ (1) x,y,z (2) \bar{x},y,\bar{z} I Maximal *translationengleiche* subgroups[2] C1 (1, P1) 1+ $1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$ II Maximal *klassengleiche* subgroups

• Loss of centring translations

[2] $P12_11$ (4) $1; 2+(\frac{1}{2},\frac{1}{2},0)$ $1/4,0,0$
[2] $P121$ (3) $1; 2$

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$
 C121 (5) $\langle 2 \rangle$ $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
 C121 (5) $\langle 2+(0,0,1) \rangle$ $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $0,0,1/2$
 I121 (5, C121) $\langle 2 \rangle$ $\mathbf{a}-2\mathbf{c}, \mathbf{b}, 2\mathbf{c}$
 I121 (5, C121) $\langle 2+(0,0,1) \rangle$ $\mathbf{a}-2\mathbf{c}, \mathbf{b}, 2\mathbf{c}$ $0,0,1/2$

[3] $\mathbf{b}' = 3\mathbf{b}$
 C121 (5) $\langle 2 \rangle$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$

[3] $\mathbf{c}' = 3\mathbf{c}$
 $\left\{ \begin{array}{l} \text{C121 (5)} \\ \text{C121 (5)} \\ \text{C121 (5)} \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2+(0,0,2) \rangle \\ \langle 2+(0,0,4) \rangle \end{array} \right. \left\{ \begin{array}{l} \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}, \mathbf{b}, 3\mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 0,0,1 \\ 0,0,2 \end{array} \right.$

[3] $\mathbf{a}' = \mathbf{a}-2\mathbf{c}, \mathbf{c}' = 3\mathbf{c}$
 $\left\{ \begin{array}{l} \text{C121 (5)} \\ \text{C121 (5)} \\ \text{C121 (5)} \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2+(0,0,2) \rangle \\ \langle 2+(0,0,4) \rangle \end{array} \right. \left\{ \begin{array}{l} \mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 0,0,1 \\ 0,0,2 \end{array} \right.$

[3] $\mathbf{a}' = \mathbf{a}-4\mathbf{c}, \mathbf{c}' = 3\mathbf{c}$
 $\left\{ \begin{array}{l} \text{C121 (5)} \\ \text{C121 (5)} \\ \text{C121 (5)} \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2+(0,0,2) \rangle \\ \langle 2+(0,0,4) \rangle \end{array} \right. \left\{ \begin{array}{l} \mathbf{a}-4\mathbf{c}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}-4\mathbf{c}, \mathbf{b}, 3\mathbf{c} \\ \mathbf{a}-4\mathbf{c}, \mathbf{b}, 3\mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 0,0,1 \\ 0,0,2 \end{array} \right.$

[3] $\mathbf{a}' = 3\mathbf{a}$
 $\left\{ \begin{array}{l} \text{C121 (5)} \\ \text{C121 (5)} \\ \text{C121 (5)} \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2+(2,0,0) \rangle \\ \langle 2+(4,0,0) \rangle \end{array} \right. \left\{ \begin{array}{l} 3\mathbf{a}, \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, \mathbf{b}, \mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 1,0,0 \\ 2,0,0 \end{array} \right.$

• Series of maximal isomorphic subgroups

[p] $\mathbf{b}' = p\mathbf{b}$
 C121 (5) $\langle 2 \rangle$ $\mathbf{a}, p\mathbf{b}, \mathbf{c}$
 prime $p > 2$
 no conjugate subgroups

[p] $\mathbf{a}' = \mathbf{a}-2q\mathbf{c}, \mathbf{c}' = p\mathbf{c}$
 C121 (5) $\langle 2+(0,0,2u) \rangle$ $\mathbf{a}-2q\mathbf{c}, \mathbf{b}, p\mathbf{c}$ $0,0,u$
 prime $p > 2; 0 \leq q < p; 0 \leq u < p$
 p conjugate subgroups for each pair of q and p

[p] $\mathbf{a}' = p\mathbf{a}$
 C121 (5) $\langle 2+(2u,0,0) \rangle$ $p\mathbf{a}, \mathbf{b}, \mathbf{c}$ $u,0,0$
 prime $p > 2; 0 \leq u < p$
 p conjugate subgroups

I Minimal translationengleiche supergroups

[2] C_{12}/m_1 (12); [2] C_{12}/c_1 (15); [2] C_{222}_1 (20); [2] C_{222} (21); [2] F_{222} (22); [2] I_{222} (23); [2] $I_{2_1 2_1 2_1}$ (24); [2] $A_{mm}2$ (38);
 [2] $A_{em}2$ (39); [2] $A_{ma}2$ (40); [2] $A_{ea}2$ (41); [2] $F_{mm}2$ (42); [2] $F_{dd}2$ (43); [2] $I_{mm}2$ (44); [2] $I_{ba}2$ (45); [2] $I_{ma}2$ (46); [2] I_4 (79);
 [2] I_{4_1} (80); [2] I_4^* (82); [3] P_{312} (149); [3] P_{321} (150); [3] $P_{3_1 12}$ (151); [3] $P_{3_1 21}$ (152); [3] $P_{3_2 12}$ (153); [3] $P_{3_2 21}$ (154);
 [3] R_{32} (155)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ P_{121} (3)

I Minimal translationengleiche supergroups

[2] A_{112}/m (12); [2] A_{112}/a (15); [2] C_{222}_1 (20); [2] C_{222} (21); [2] F_{222} (22); [2] I_{222} (23); [2] $I_{2_1 2_1 2_1}$ (24); [2] $A_{mm}2$ (38);
 [2] $A_{em}2$ (39); [2] $A_{ma}2$ (40); [2] $A_{ea}2$ (41); [2] $F_{mm}2$ (42); [2] $F_{dd}2$ (43); [2] $I_{mm}2$ (44); [2] $I_{ba}2$ (45); [2] $I_{ma}2$ (46); [2] I_4 (79);
 [2] I_{4_1} (80); [2] I_4^* (82); [3] P_{312} (149); [3] P_{321} (150); [3] $P_{3_1 12}$ (151); [3] $P_{3_1 21}$ (152); [3] $P_{3_2 12}$ (153); [3] $P_{3_2 21}$ (154);
 [3] R_{32} (155)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ P_{112} (3)

UNIQUE AXIS *c*, CELL CHOICE 1**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**General position**Multiplicity,
Wyckoff letter,
Site symmetry**Coordinates** $(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ 4 *c* 1(1) x, y, z (2) \bar{x}, \bar{y}, z **I Maximal translationengleiche subgroups**[2] A1 (1, P1) 1+ **a, 1/2(b - c), 1/2(b + c)****II Maximal klassengleiche subgroups**• **Loss of centring translations**[2] P112₁ (4) 1; 2 + $(0, \frac{1}{2}, \frac{1}{2})$ 0, 1/4, 0

[2] P112 (3) 1; 2

• **Enlarged unit cell**[2] **a' = 2a**

A112 (5)	$\langle 2 \rangle$	2a, b, c	
A112 (5)	$\langle 2 + (1, 0, 0) \rangle$	2a, b, c	1/2, 0, 0
I112 (5, A112)	$\langle 2 \rangle$	2a, -2a + b, c	
I112 (5, A112)	$\langle 2 + (1, 0, 0) \rangle$	2a, -2a + b, c	1/2, 0, 0

[3] **c' = 3c**A112 (5) $\langle 2 \rangle$ **a, b, 3c**[3] **a' = 3a**

A112 (5)	$\langle 2 \rangle$	3a, b, c	
A112 (5)	$\langle 2 + (2, 0, 0) \rangle$	3a, b, c	1, 0, 0
A112 (5)	$\langle 2 + (4, 0, 0) \rangle$	3a, b, c	2, 0, 0

[3] **a' = 3a, b' = -2a + b**

A112 (5)	$\langle 2 \rangle$	3a, -2a + b, c	
A112 (5)	$\langle 2 + (2, 0, 0) \rangle$	3a, -2a + b, c	1, 0, 0
A112 (5)	$\langle 2 + (4, 0, 0) \rangle$	3a, -2a + b, c	2, 0, 0

[3] **a' = 3a, b' = -4a + b**

A112 (5)	$\langle 2 \rangle$	3a, -4a + b, c	
A112 (5)	$\langle 2 + (2, 0, 0) \rangle$	3a, -4a + b, c	1, 0, 0
A112 (5)	$\langle 2 + (4, 0, 0) \rangle$	3a, -4a + b, c	2, 0, 0

[3] **b' = 3b**

A112 (5)	$\langle 2 \rangle$	a, 3b, c	
A112 (5)	$\langle 2 + (0, 2, 0) \rangle$	a, 3b, c	0, 1, 0
A112 (5)	$\langle 2 + (0, 4, 0) \rangle$	a, 3b, c	0, 2, 0

• **Series of maximal isomorphic subgroups**[*p*] **c' = pc**A112 (5) $\langle 2 \rangle$ **a, b, pc**
prime $p > 2$
no conjugate subgroups[*p*] **a' = pa, b' = -2qa + b**A112 (5) $\langle 2 + (2u, 0, 0) \rangle$ **pa, -2qa + b, c** $u, 0, 0$
prime $p > 2$; $0 \leq q < p$; $0 \leq u < p$
 p conjugate subgroups for each pair of q and p [*p*] **b' = pb**A112 (5) $\langle 2 + (0, 2u, 0) \rangle$ **a, pb, c** $0, u, 0$
prime $p > 2$; $0 \leq u < p$
 p conjugate subgroups

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I Minimal *translationengleiche* supergroups

[2] *C*12/*m*1 (12); [2] *C*12/*c*1 (15); [2] *C*222₁ (20); [2] *C*222 (21); [2] *F*222 (22); [2] *I*222 (23); [2] *I*2₁2₁2₁ (24); [2] *Amm*2 (38);
 [2] *Aem*2 (39); [2] *Ama*2 (40); [2] *Aea*2 (41); [2] *Fmm*2 (42); [2] *Fdd*2 (43); [2] *Imm*2 (44); [2] *Iba*2 (45); [2] *Ima*2 (46); [2] *I*4 (79);
 [2] *I*4₁ (80); [2] *I*4̄ (82); [3] *P*312 (149); [3] *P*321 (150); [3] *P*3₁12 (151); [3] *P*3₁21 (152); [3] *P*3₂12 (153); [3] *P*3₂21 (154);
 [3] *R*32 (155)

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *P*121 (3)

I Minimal *translationengleiche* supergroups

[2] *A*112/*m* (12); [2] *A*112/*a* (15); [2] *C*222₁ (20); [2] *C*222 (21); [2] *F*222 (22); [2] *I*222 (23); [2] *I*2₁2₁2₁ (24); [2] *Amm*2 (38);
 [2] *Aem*2 (39); [2] *Ama*2 (40); [2] *Aea*2 (41); [2] *Fmm*2 (42); [2] *Fdd*2 (43); [2] *Imm*2 (44); [2] *Iba*2 (45); [2] *Ima*2 (46); [2] *I*4 (79);
 [2] *I*4₁ (80); [2] *I*4̄ (82); [3] *P*312 (149); [3] *P*321 (150); [3] *P*3₁12 (151); [3] *P*3₁21 (152); [3] *P*3₂12 (153); [3] *P*3₂21 (154);
 [3] *R*32 (155)

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *P*112 (3)