

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

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

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

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

• Series of maximal isomorphic subgroups

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

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

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

I Minimal translationengleiche supergroups

[2] $C12/m1$ (12); [2] $C12/c1$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38);
 [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79);
 [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154);
 [3] $R32$ (155)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P121$ (3)

I Minimal translationengleiche supergroups

[2] $A112/m$ (12); [2] $A112/a$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38);
 [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79);
 [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154);
 [3] $R32$ (155)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112$ (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+ $\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$

II Maximal klassengleiche subgroups

• **Loss of centring translations**

[2] $P112_1$ (4) $1; 2 + (0, \frac{1}{2}, \frac{1}{2})$ 0, 1/4, 0
 [2] $P112$ (3) 1; 2

• **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$
 A112 (5) $\langle 2 \rangle$ $2\mathbf{a}, \mathbf{b}, \mathbf{c}$
 A112 (5) $\langle 2 + (1, 0, 0) \rangle$ $2\mathbf{a}, \mathbf{b}, \mathbf{c}$ 1/2, 0, 0
 I112 (5, A112) $\langle 2 \rangle$ $2\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$
 I112 (5, A112) $\langle 2 + (1, 0, 0) \rangle$ $2\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$ 1/2, 0, 0

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

[3] $\mathbf{a}' = 3\mathbf{a}$
 $\left\{ \begin{array}{l} A112 (5) \\ A112 (5) \\ A112 (5) \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2 + (2, 0, 0) \rangle \\ \langle 2 + (4, 0, 0) \rangle \end{array} \right. \left\{ \begin{array}{l} 3\mathbf{a}, \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, \mathbf{b}, \mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 1, 0, 0 \\ 2, 0, 0 \end{array} \right.$

[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$
 $\left\{ \begin{array}{l} A112 (5) \\ A112 (5) \\ A112 (5) \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2 + (2, 0, 0) \rangle \\ \langle 2 + (4, 0, 0) \rangle \end{array} \right. \left\{ \begin{array}{l} 3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 1, 0, 0 \\ 2, 0, 0 \end{array} \right.$

[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -4\mathbf{a} + \mathbf{b}$
 $\left\{ \begin{array}{l} A112 (5) \\ A112 (5) \\ A112 (5) \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2 + (2, 0, 0) \rangle \\ \langle 2 + (4, 0, 0) \rangle \end{array} \right. \left\{ \begin{array}{l} 3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c} \\ 3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 1, 0, 0 \\ 2, 0, 0 \end{array} \right.$

[3] $\mathbf{b}' = 3\mathbf{b}$
 $\left\{ \begin{array}{l} A112 (5) \\ A112 (5) \\ A112 (5) \end{array} \right. \left\{ \begin{array}{l} \langle 2 \rangle \\ \langle 2 + (0, 2, 0) \rangle \\ \langle 2 + (0, 4, 0) \rangle \end{array} \right. \left\{ \begin{array}{l} \mathbf{a}, 3\mathbf{b}, \mathbf{c} \\ \mathbf{a}, 3\mathbf{b}, \mathbf{c} \\ \mathbf{a}, 3\mathbf{b}, \mathbf{c} \end{array} \right. \left\{ \begin{array}{l} \\ 0, 1, 0 \\ 0, 2, 0 \end{array} \right.$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$
 A112 (5) $\langle 2 \rangle$ $\mathbf{a}, \mathbf{b}, p\mathbf{c}$
 $p > 2$
 no conjugate subgroups

[p] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = -2q\mathbf{a} + \mathbf{b}$
 A112 (5) $\langle 2 + (2u, 0, 0) \rangle$ $p\mathbf{a}, -2q\mathbf{a} + \mathbf{b}, \mathbf{c}$ $u, 0, 0$
 $p > 2; 0 \leq q < p; 0 \leq u < p$
 p conjugate subgroups for each pair of q and prime p

[p] $\mathbf{b}' = p\mathbf{b}$
 A112 (5) $\langle 2 + (0, 2u, 0) \rangle$ $\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $0, u, 0$
 $p > 2; 0 \leq u < p$
 p conjugate subgroups for the prime p

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I Minimal translationengleiche supergroups

[2] $C12/m1$ (12); [2] $C12/c1$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38);
 [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79);
 [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154);
 [3] $R32$ (155)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P121$ (3)

I Minimal translationengleiche supergroups

[2] $A112/m$ (12); [2] $A112/a$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38);
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 [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154);
 [3] $R32$ (155)

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- Additional centring translations none

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[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112$ (3)