

C_2^3

A112

No. 5

C2

UNIQUE AXIS c , CELL CHOICE 1Generators 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

4 c 1 $(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ (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)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
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[3] $\mathbf{a}' = 3\mathbf{a}$

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

[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$

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

[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -4\mathbf{a} + \mathbf{b}$

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

[3] $\mathbf{b}' = 3\mathbf{b}$

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

• 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);
 [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)