

C_{2h}^6
 $A112/a$

No. 15

 $C2/c$

 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); (3)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

 8 f 1

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

[2] $A11a$ (9)	(1; 4)+		
[2] $A112$ (5)	(1; 2)+		1/4, 0, 0
[2] $A\bar{1}$ (2, $P\bar{1}$)	(1; 3)+	$\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$	

II Maximal klassengleiche subgroups

• Loss of centring translations

[2] $P112_1/n$ (14, $P112_1/a$)	1; 3; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$	$-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$	
[2] $P112_1/a$ (14)	1; 4; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$		0, 1/4, 1/4
[2] $P112/a$ (13)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$	$-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$	0, 1/4, 1/4

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} A112/a (15) \\ A112/a (15) \\ A112/a (15) \end{array} \right.$	$\langle 2; 3 \rangle$ $\langle 2; 3 + (0, 0, 2) \rangle$ $\langle 2; 3 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1 0, 0, 2
[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} A112/a (15) \\ A112/a (15) \\ A112/a (15) \end{array} \right.$	$\langle 3; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); 3 + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); 3 + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0 2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$			
$\left\{ \begin{array}{l} A112/a (15) \\ A112/a (15) \\ A112/a (15) \end{array} \right.$	$\langle 3; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); 3 + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); 3 + (4, 0, 0) \rangle$	$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$	1, 0, 0 2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = -4\mathbf{a} + \mathbf{b}$			
$\left\{ \begin{array}{l} A112/a (15) \\ A112/a (15) \\ A112/a (15) \end{array} \right.$	$\langle 3; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); 3 + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); 3 + (4, 0, 0) \rangle$	$3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c}$	1, 0, 0 2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} A112/a (15) \\ A112/a (15) \\ A112/a (15) \end{array} \right.$	$\langle 2; 3 \rangle$ $\langle (2; 3) + (0, 2, 0) \rangle$ $\langle (2; 3) + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0 0, 2, 0

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$A112/a$ (15)	$\langle 2; 3 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, u
[p] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = -2q\mathbf{a} + \mathbf{b}$			
$A112/a$ (15)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 3 + (2u, 0, 0) \rangle$ $p > 2; 0 \leq q < p; 0 \leq u < p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a}, -2q\mathbf{a} + \mathbf{b}, \mathbf{c}$	$u, 0, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$A112/a$ (15)	$\langle (2; 3) + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	0, $u, 0$

(Continued on the facing page)

I Minimal translationengleiche supergroups

[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}12/c$ (163, $P\bar{3}1c$); [3] $P\bar{3}2/c1$ (165, $P\bar{3}c1$); [3] $R\bar{3}2/c$ (167, $R\bar{3}c$)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $F12/m1$ (12, $C12/m1$)

• Decreased unit cell

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C12/m1$ (12); [2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P12/c1$ (13)

I Minimal translationengleiche supergroups

[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}12/c$ (163, $P\bar{3}1c$); [3] $P\bar{3}2/c1$ (165, $P\bar{3}c1$); [3] $R\bar{3}2/c$ (167, $R\bar{3}c$)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $F112/m$ (12, $A112/m$)

• Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $A112/m$ (12); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112/a$ (13)