

D_{2h}^{15} $P2_1/b2_1/c2_1/a$

No. 61

 $Pbca$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	c	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$

I Maximal *translationengleiche* subgroups

[2] $Pbc2_1$ (29, $Pca2_1$)	1; 2; 7; 8	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	$1/4, 0, 0$
[2] $Pb2_1a$ (29, $Pca2_1$)	1; 3; 6; 8	$\mathbf{a}, -\mathbf{c}, \mathbf{b}$	$0, 0, 1/4$
[2] $P2_1ca$ (29, $Pca2_1$)	1; 4; 6; 7	$\mathbf{c}, \mathbf{b}, -\mathbf{a}$	$0, 1/4, 0$
[2] $P2_12_12_1$ (19)	1; 2; 3; 4		
[2] $P112_1/a$ (14)	1; 2; 5; 6		
[2] $P12_1/c1$ (14)	1; 3; 5; 7		
[2] $P2_1/b11$ (14, $P12_1/c1$)	1; 4; 5; 8	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	

II Maximal *klassengleiche* subgroups

• Enlarged unit cell

[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} Pbca (61) \\ Pbca (61) \\ Pbca (61) \end{array} \right.$	$\langle 3; 5; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$ $2, 0, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} Pbca (61) \\ Pbca (61) \\ Pbca (61) \end{array} \right.$	$\langle 2; 5; 3 + (0, 1, 0) \rangle$ $\langle (2; 5) + (0, 2, 0); 3 + (0, 1, 0) \rangle$ $\langle (2; 5) + (0, 4, 0); 3 + (0, 1, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$ $0, 2, 0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} Pbca (61) \\ Pbca (61) \\ Pbca (61) \end{array} \right.$	$\langle 5; (2; 3) + (0, 0, 1) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$ $0, 0, 2$

• Series of maximal isomorphic subgroups

[p] $\mathbf{a}' = p\mathbf{a}$			
$Pbca (61)$	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$Pbca (61)$	$\langle (2; 5) + (0, 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
[p] $\mathbf{c}' = p\mathbf{c}$			
$Pbca (61)$	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal *translationengleiche* supergroups[3] $Pa\bar{3}$ (205)II Minimal non-isomorphic *klassengleiche* supergroups

• Additional centring translations

[2] $Aema$ (64, $Cmce$); [2] $Bbem$ (64, $Cmce$); [2] $Cmce$ (64); [2] $Ibca$ (73)

• Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pbcm$ (57); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmca$ (57, $Pbcm$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pbma$ (57, $Pbcm$)