

$D_{2h}^{11}$ 
 $P2/b2_1/c2_1/m$ 

No. 57

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

**I Maximal translationengleiche subgroups**

[2] $Pbc2_1$ (29, $Pca2_1$ )	1; 2; 7; 8				
[2] $P2cm$ (28, $Pma2$ )	1; 4; 6; 7				$-\mathbf{b}, \mathbf{a}, \mathbf{c}$
[2] $Pb2_1m$ (26, $Pmc2_1$ )	1; 3; 6; 8				$\mathbf{c}, \mathbf{b}, -\mathbf{a}$
[2] $P22_12_1$ (18, $P2_12_12$ )	1; 2; 3; 4				$\mathbf{c}, \mathbf{a}, \mathbf{b}$
[2] $P12_1/c1$ (14)	1; 3; 5; 7				$\mathbf{b}, \mathbf{c}, \mathbf{a}$
[2] $P2/b11$ (13, $P12/c1$ )	1; 4; 5; 8				$\mathbf{c}, \mathbf{a}, \mathbf{b}$
[2] $P112_1/m$ (11, $P112_1/m$ )	1; 2; 5; 6				

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$					
$Pbnm$ (62, $Pnma$ )	$\langle 2; 5; 3 + (1, 0, 0) \rangle$				$\mathbf{b}, \mathbf{c}, 2\mathbf{a}$
$Pbnm$ (62, $Pnma$ )	$\langle 3; (2; 5) + (1, 0, 0) \rangle$				$\mathbf{b}, \mathbf{c}, 2\mathbf{a}$
$Pbca$ (61)	$\langle 3; 5; 2 + (1, 0, 0) \rangle$				$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$Pbca$ (61)	$\langle 2; (3; 5) + (1, 0, 0) \rangle$				$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$Pbna$ (60, $Pbcn$ )	$\langle 5; (2; 3) + (1, 0, 0) \rangle$				$\mathbf{c}, 2\mathbf{a}, \mathbf{b}$
$Pbna$ (60, $Pbcn$ )	$\langle 2; 3; 5 + (1, 0, 0) \rangle$				$\mathbf{c}, 2\mathbf{a}, \mathbf{b}$
$Pbcm$ (57)	$\langle 2; 3; 5 \rangle$				$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
$Pbcm$ (57)	$\langle (2; 3; 5) + (1, 0, 0) \rangle$				$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$					
$Pbcm$ (57)	$\langle 2; 3; 5 \rangle$				$3\mathbf{a}, \mathbf{b}, \mathbf{c}$
$Pbcm$ (57)	$\langle (2; 3; 5) + (2, 0, 0) \rangle$				$3\mathbf{a}, \mathbf{b}, \mathbf{c}$
$Pbcm$ (57)	$\langle (2; 3; 5) + (4, 0, 0) \rangle$				$3\mathbf{a}, \mathbf{b}, \mathbf{c}$
[3] $\mathbf{b}' = 3\mathbf{b}$					
$Pbcm$ (57)	$\langle 2; 5; 3 + (0, 1, 0) \rangle$				$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$
$Pbcm$ (57)	$\langle (2; 5) + (0, 2, 0); 3 + (0, 1, 0) \rangle$				$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$
$Pbcm$ (57)	$\langle (2; 5) + (0, 4, 0); 3 + (0, 1, 0) \rangle$				$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$
[3] $\mathbf{c}' = 3\mathbf{c}$					
$Pbcm$ (57)	$\langle 5; (2; 3) + (0, 0, 1) \rangle$				$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$Pbcm$ (57)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$				$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$Pbcm$ (57)	$\langle 2 + (0, 0, 1); 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$				$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{a}' = p\mathbf{a}$					
$Pbcm$ (57)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$				$p\mathbf{a}, \mathbf{b}, \mathbf{c}$
	prime $p > 2$ ; $0 \leq u < p$				$u, 0, 0$
	$p$ conjugate subgroups				
[ $p$ ] $\mathbf{b}' = p\mathbf{b}$					
$Pbcm$ (57)	$\langle (2; 5) + (0, 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0) \rangle$				$\mathbf{a}, p\mathbf{b}, \mathbf{c}$
	prime $p > 2$ ; $0 \leq u < p$				$0, u, 0$
	$p$ conjugate subgroups				
[ $p$ ] $\mathbf{c}' = p\mathbf{c}$					
$Pbcm$ (57)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$				$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	prime $p > 2$ ; $0 \leq u < p$				$0, 0, u$
	$p$ conjugate subgroups				

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $Cmcm$  (63); [2]  $Bbem$  (64,  $Cmce$ ); [2]  $Aemm$  (67,  $Cmme$ ); [2]  $Ibam$  (72)

## • Decreased unit cell

 [2]  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   $Pmcm$  (51,  $Pmma$ ); [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $Pbmm$  (51,  $Pmma$ )