

$Pccn$

No. 56

 $P2_1/c2_1/c2/n$ D_{2h}^{10} **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

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

I Maximal translationengleiche subgroups

[2] $Pc2_1n$ (33, $Pna2_1$)	1; 3; 6; 8	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	0, 0, 1/4
[2] $P2_1cn$ (33, $Pna2_1$)	1; 4; 6; 7	$\mathbf{c}, \mathbf{b}, -\mathbf{a}$	0, 0, 1/4
[2] $Pcc2$ (27)	1; 2; 7; 8		1/4, 1/4, 0
[2] $P2_12_12$ (18)	1; 2; 3; 4		1/4, 1/4, 1/4
[2] $P12_1/c1$ (14)	1; 3; 5; 7		
[2] $P2_1/c11$ (14, $P12_1/c1$)	1; 4; 5; 8	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a} - \mathbf{b}, \mathbf{a}, \mathbf{c}$	

II Maximal klassengleiche subgroups**• Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} Pccn \text{ (56)} \\ Pccn \text{ (56)} \\ Pccn \text{ (56)} \end{array} \right.$	$\langle 3; 5; 2 + (1, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
	$\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0
	$\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} Pccn \text{ (56)} \\ Pccn \text{ (56)} \\ Pccn \text{ (56)} \end{array} \right.$	$\langle 5; (2; 3) + (0, 1, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
	$\langle 2 + (0, 3, 0); 3 + (0, 1, 0); 5 + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0
	$\langle 2 + (0, 5, 0); 3 + (0, 1, 0); 5 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} Pccn \text{ (56)} \\ Pccn \text{ (56)} \\ Pccn \text{ (56)} \end{array} \right.$	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
	$\langle 2; 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
	$\langle 2; 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{a}' = p\mathbf{a}$			
$Pccn$ (56)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $\mathbf{b}' = p\mathbf{b}$			
$Pccn$ (56)	$\langle 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0); 5 + (0, 2u, 0) \rangle$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, 2u, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $\mathbf{c}' = p\mathbf{c}$			
$Pccn$ (56)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$	$\mathbf{a}, \mathbf{b}, pc$	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		

I Minimal translationengleiche supergroups[2] $P4/ncc$ (130); [2] $P4_2(ncm$ (138)**II Minimal non-isomorphic klassengleiche supergroups****• Additional centring translations**[2] $Aema$ (64, $Cmce$); [2] $Bmcb$ (64, $Cmce$); [2] $Cccm$ (66); [2] $Ibam$ (72)**• Decreased unit cell**[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pccb$ (54, $Pcca$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pcca$ (54); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pmmn$ (59)