

$D_{2h}^{17}$ 
 $C2/m2/c2_1/m$ 

No. 63

 $Cmcm$ 
**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},0)$ ; (2); (3); (5)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

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

 16 *h* 1

 (1)  $x, y, z$  (2)  $\bar{x}, \bar{y}, z + \frac{1}{2}$  (3)  $\bar{x}, y, \bar{z} + \frac{1}{2}$  (4)  $x, \bar{y}, \bar{z}$   
 (5)  $\bar{x}, \bar{y}, \bar{z}$  (6)  $x, y, \bar{z} + \frac{1}{2}$  (7)  $x, \bar{y}, z + \frac{1}{2}$  (8)  $\bar{x}, y, z$ 
**I Maximal translationengleiche subgroups**

[2] $C2cm$ (40, $Ama2$ )	(1; 4; 6; 7)+	<b>c, b, -a</b>	
[2] $Cm2m$ (38, $Amm2$ )	(1; 3; 6; 8)+	<b>c, a, b</b>	0, 0, 1/4
[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+		
[2] $C222_1$ (20)	(1; 2; 3; 4)+		
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		
[2] $C2/m11$ (12, $C12/m1$ )	(1; 4; 5; 8)+	<b>-b, a, c</b>	
[2] $C112_1/m$ (11, $P112_1/m$ )	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	

**II Maximal klassengleiche subgroups**

## • Loss of centring translations

[2] $Pbnm$ (62, $Pnma$ )	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	
[2] $Pmcn$ (62, $Pnma$ )	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	1/4, 1/4, 0
[2] $Pbcn$ (60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		
[2] $Pmnm$ (59, $Pmnm$ )	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	1/4, 1/4, 0
[2] $Pmnn$ (58, $Pmnm$ )	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	
[2] $Pbcm$ (57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		1/4, 1/4, 0
[2] $Pbnn$ (52, $Pnna$ )	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	1/4, 1/4, 0
[2] $Pmcm$ (51, $Pmma$ )	1; 2; 3; 4; 5; 6; 7; 8	<b>c, a, b</b>	

## • Enlarged unit cell

[3] $\mathbf{a}' = 3\mathbf{a}$			
$Cmcm$ (63)	$\langle 2; 3; 5 \rangle$	<b>3a, b, c</b>	
$Cmcm$ (63)	$\langle \langle 2; 3; 5 \rangle + (2, 0, 0) \rangle$	<b>3a, b, c</b>	1, 0, 0
$Cmcm$ (63)	$\langle \langle 2; 3; 5 \rangle + (4, 0, 0) \rangle$	<b>3a, b, c</b>	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$Cmcm$ (63)	$\langle 2; 3; 5 \rangle$	<b>a, 3b, c</b>	
$Cmcm$ (63)	$\langle \langle 3; (2; 5) + (0, 2, 0) \rangle \rangle$	<b>a, 3b, c</b>	0, 1, 0
$Cmcm$ (63)	$\langle \langle 3; (2; 5) + (0, 4, 0) \rangle \rangle$	<b>a, 3b, c</b>	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Cmcm$ (63)	$\langle \langle 5; (2; 3) + (0, 0, 1) \rangle \rangle$	<b>a, b, 3c</b>	
$Cmcm$ (63)	$\langle \langle 2 + (0, 0, 1); 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle \rangle$	<b>a, b, 3c</b>	0, 0, 1
$Cmcm$ (63)	$\langle \langle 2 + (0, 0, 1); 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle \rangle$	<b>a, b, 3c</b>	0, 0, 2

## • Series of maximal isomorphic subgroups

[ <i>p</i> ] $\mathbf{a}' = p\mathbf{a}$			
$Cmcm$ (63)	$\langle \langle \langle 2; 3; 5 \rangle + (2u, 0, 0) \rangle \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>pa, b, c</b>	<i>u</i> , 0, 0
[ <i>p</i> ] $\mathbf{b}' = p\mathbf{b}$			
$Cmcm$ (63)	$\langle \langle \langle 3; (2; 5) + (0, 2u, 0) \rangle \rangle \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>a, pb, c</b>	0, <i>u</i> , 0
[ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$			
$Cmcm$ (63)	$\langle \langle \langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle \rangle \rangle$ $5 + (0, 0, 2u)$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>a, b, pc</b>	0, 0, <i>u</i>

**I Minimal translationengleiche supergroups**

[3]  $P6_3/mcm$  (193); [3]  $P6_3/mmc$  (194)

**II Minimal non-isomorphic klassengleiche supergroups**

- Additional centring translations

[2]  $Fmmm$  (69)

- Decreased unit cell

[2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   $Pmcm$  (51,  $Pmma$ ); [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $Cmmm$  (65)

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

- Additional centring translations

[2]  $Fmmm$  (69)

- Decreased unit cell

[2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   $Pmcm$  (51,  $Pmma$ ); [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $Cmme$  (67)