

$D_{2h}^{18}$ 
 $C2/m2/c2_1/e$ 

No. 64

 $Cmce$ 

 Former space-group symbol  $Cmca$ 
**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 g 1

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

[2] $C2ce$ (41, $Aea2$ )	(1; 4; 6; 7)+	<b>c, b, -a</b>	
[2] $Cm2e$ (39, $Aem2$ )	(1; 3; 6; 8)+	<b>c, a, b</b>	1/4, 0, 1/4
[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $C222_1$ (20)	(1; 2; 3; 4)+		1/4, 0, 0
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		1/4, 1/4, 0
[2] $C112_1/e$ (14, $P112_1/a$ )	(1; 2; 5; 6)+	<b>a, 1/2(-a+b), c</b>	
[2] $C2/m11$ (12, $C12/m1$ )	(1; 4; 5; 8)+	<b>-b, a, c</b>	

**II Maximal klassengleiche subgroups**

## • Loss of centring translations

[2] $Pmnb$ (62, $Pnma$ )	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>-b, a, c</b>	1/4, 1/4, 0
[2] $Pbca$ (61)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		
[2] $Pbna$ (60, $Pbcn$ )	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	1/4, 1/4, 0
[2] $Pmca$ (57, $Pbcm$ )	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	1/4, 1/4, 0
[2] $Pbnb$ (56, $Pccn$ )	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	
[2] $Pmcb$ (55, $Pbam$ )	1; 2; 3; 4; 5; 6; 7; 8	<b>b, c, a</b>	
[2] $Pbcb$ (54, $Pcca$ )	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	1/4, 1/4, 0
[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$		

## • Enlarged unit cell

[3] $a' = 3a$			
$\left\{ \begin{array}{l} Cmce (64) \\ Cmce (64) \\ Cmce (64) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle (2; 3; 5) + (2, 0, 0) \rangle$ $\langle (2; 3; 5) + (4, 0, 0) \rangle$	<b>3a, b, c</b> <b>3a, b, c</b> <b>3a, b, c</b>	1, 0, 0 2, 0, 0
[3] $b' = 3b$			
$\left\{ \begin{array}{l} Cmce (64) \\ Cmce (64) \\ Cmce (64) \end{array} \right.$	$\langle 5; (2; 3) + (0, 1, 0) \rangle$ $\langle 2 + (0, 3, 0); 3 + (0, 1, 0); 5 + (0, 2, 0) \rangle$ $\langle 2 + (0, 5, 0); 3 + (0, 1, 0); 5 + (0, 4, 0) \rangle$	<b>a, 3b, c</b> <b>a, 3b, c</b> <b>a, 3b, c</b>	0, 1, 0 0, 2, 0
[3] $c' = 3c$			
$\left\{ \begin{array}{l} Cmce (64) \\ Cmce (64) \\ Cmce (64) \end{array} \right.$	$\langle 5; (2; 3) + (0, 0, 1) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	<b>a, b, 3c</b> <b>a, b, 3c</b> <b>a, b, 3c</b>	0, 0, 1 0, 0, 2

## • Series of maximal isomorphic subgroups

[p] $a' = pa$			
$Cmce$ (64)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>pa, b, c</b>	$u, 0, 0$
[p] $b' = pb$			
$Cmce$ (64)	$\langle 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0); 5 + (0, 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>a, pb, c</b>	$0, u, 0$
[p] $c' = pc$			
$Cmce$ (64)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>a, b, pc</b>	$0, 0, u$

(Continued on the facing page)

**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)