

$D_{2h}^{22}$ 
 $C2/c2/c2/e$ 

No. 68

 $Ccce$ 

 Former space-group symbol  $Ccca$ 

 ORIGIN CHOICE 1, Origin at 222 at  $2/n2/n2$ , at  $0, \frac{1}{4}, \frac{1}{4}$  from  $\bar{1}$ 

 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

Multiplicity, Wyckoff letter, Site symmetry		(0,0,0)+	$(\frac{1}{2}, \frac{1}{2}, 0)+$			
16	<i>i</i>	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x}, y, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$
			(5) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$

**I Maximal translationengleiche subgroups**

[2] $Cc2e$ (41, $Aea2$ )	(1; 3; 6; 8)+	<b>c, a, b</b>	
[2] $C2ce$ (41, $Aea2$ )	(1; 4; 6; 7)+	<b>c, b, -a</b>	
[2] $Ccc2$ (37)	(1; 2; 7; 8)+		1/4, 1/4, 0
[2] $C222$ (21)	(1; 2; 3; 4)+		
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		0, 1/4, 1/4
[2] $C2/c11$ (15, $C12/c1$ )	(1; 4; 5; 8)+	<b>-b, a, c</b>	1/4, 0, 1/4
[2] $C112/e$ (13, $P112/a$ )	(1; 2; 5; 6)+	<b>a, 1/2(-a + b), c</b>	1/4, 0, 1/4

**II Maximal klassengleiche subgroups**

## • Loss of centring translations

[2] $Pcnb$ (60, $Pbcn$ )	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>a, -c, b</b>	0, 1/4, 1/4
[2] $Pnca$ (60, $Pbcn$ )	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	1/4, 0, 1/4
[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8		0, 1/4, 1/4
[2] $Pccb$ (54, $Pcca$ )	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>-b, a, c</b>	1/4, 0, 1/4
[2] $Pn nb$ (52, $Pnna$ )	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>-b, a, c</b>	1/4, 0, 1/4
[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		0, 1/4, 1/4
[2] $Pncb$ (50, $Pban$ )	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	
[2] $Pcna$ (50, $Pban$ )	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>c, a, b</b>	

## • Enlarged unit cell

[3] $a' = 3a$			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 3; 5; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$	<b>3a, b, c</b> <b>3a, b, c</b> <b>3a, b, c</b>	1, 0, 0 2, 0, 0
[3] $b' = 3b$			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 3; (2; 5) + (0, 1, 0) \rangle$ $\langle 3; (2; 5) + (0, 3, 0) \rangle$ $\langle 3; (2; 5) + (0, 5, 0) \rangle$	<b>a, 3b, c</b> <b>a, 3b, c</b> <b>a, 3b, c</b>	0, 1, 0 0, 2, 0
[3] $c' = 3c$			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 2; 3; 5 + (0, 0, 1) \rangle$ $\langle 2; 3 + (0, 0, 2); 5 + (0, 0, 3) \rangle$ $\langle 2; 3 + (0, 0, 4); 5 + (0, 0, 5) \rangle$	<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

[ <i>p</i> ] $a' = pa$			
$Ccce$ (68)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>pa, b, c</b>	$u, 0, 0$
[ <i>p</i> ] $b' = pb$			
$Ccce$ (68)	$\langle 3; (2; 5) + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>a, pb, c</b>	$0, u, 0$
[ <i>p</i> ] $c' = pc$			
$Ccce$ (68)	$\langle 2; 3 + (0, 0, 2u); 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ <i>p</i> conjugate subgroups	<b>a, b, pc</b>	$0, 0, u$

**I Minimal *translationengleiche* supergroups**

[2]  $P4/nnc$  (126); [2]  $P4/ncc$  (130); [2]  $P4_2/nbc$  (133); [2]  $P4_2/nmc$  (137)

**II Minimal non-isomorphic *klassengleiche* supergroups****• Additional centring translations**

[2]  $Fmmm$  (69)

**• Decreased unit cell**

[2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   $Pccm$  (49); [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $Cmme$  (67)

**I Minimal *translationengleiche* supergroups**

[2]  $P4/nnc$  (126); [2]  $P4/ncc$  (130); [2]  $P4_2/nbc$  (133); [2]  $P4_2/nmc$  (137)

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ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $2/nca$ , at  $0, -\frac{1}{4}, -\frac{1}{4}$  from 222

**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,	Coordinates
Wyckoff letter,	$(0,0,0)+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$
Site symmetry	

16	<i>i</i>	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y, \bar{z}$	(7) $x, \bar{y}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$

**I Maximal translationengleiche subgroups**

[2] $Cc2e$ (41, $Aea2$ )	(1; 3; 6; 8)+	<b>c, a, b</b>	0, 1/4, 1/4
[2] $C2ce$ (41, $Aea2$ )	(1; 4; 6; 7)+	<b>c, b, -a</b>	0, 1/4, 1/4
[2] $Ccc2$ (37)	(1; 2; 7; 8)+		1/4, 0, 1/4
[2] $C222$ (21)	(1; 2; 3; 4)+		0, 1/4, 1/4
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		
[2] $C2/c11$ (15, $C12/c1$ )	(1; 4; 5; 8)+	<b>-b, a, c</b>	1/4, 1/4, 0
[2] $C112/e$ (13, $P112/a$ )	(1; 2; 5; 6)+	<b>a, 1/2(-a+b), c</b>	1/4, 1/4, 0

**II Maximal klassengleiche subgroups**
**• Loss of centring translations**

[2] $Pcnb$ (60, $Pbcn$ )	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>a, -c, b</b>	
[2] $Pnca$ (60, $Pbcn$ )	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	1/4, 1/4, 0
[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pccb$ (54, $Pcca$ )	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>-b, a, c</b>	1/4, 1/4, 0
[2] $Pnnb$ (52, $Pnna$ )	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>-b, a, c</b>	1/4, 1/4, 0
[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		
[2] $Pncb$ (50, $Pban$ )	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	<b>b, c, a</b>	
[2] $Pcna$ (50, $Pban$ )	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

**• Enlarged unit cell**

[3] <b>a' = 3a</b>			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 3; 5; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$	<b>3a, b, c</b> <b>3a, b, c</b> <b>3a, b, c</b>	 1, 0, 0 2, 0, 0
[3] <b>b' = 3b</b>			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle 3; (2; 5) + (0, 2, 0) \rangle$ $\langle 3; (2; 5) + (0, 4, 0) \rangle$	<b>a, 3b, c</b> <b>a, 3b, c</b> <b>a, 3b, c</b>	 0, 1, 0 0, 2, 0
[3] <b>c' = 3c</b>			
$\left\{ \begin{array}{l} Ccce (68) \\ Ccce (68) \\ Ccce (68) \end{array} \right.$	$\langle 2; 5; 3 + (0, 0, 1) \rangle$ $\langle 2; 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$ $\langle 2; 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	<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] <b>a' = pa</b>			
$Ccce$ (68)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>pa, b, c</b>	$u, 0, 0$
[p] <b>b' = pb</b>			
$Ccce$ (68)	$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>a, pb, c</b>	$0, u, 0$
[p] <b>c' = pc</b>			
$Ccce$ (68)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	<b>a, b, pc</b>	$0, 0, u$

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**I Minimal translationengleiche supergroups**

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