

D_{2h}^{27}
 $I2_1/b2_1/c2_1/a$

No. 73

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

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

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

 16 *f* 1

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

[2] $Ibc2$ (45, $Iba2$)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $Ib2a$ (45, $Iba2$)	(1; 3; 6; 8)+	c, a, b	1/4, 0, 0
[2] $I2ca$ (45, $Iba2$)	(1; 4; 6; 7)+	b, c, a	0, 0, 1/4
[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+		
[2] $I112/a$ (15, $A112/a$)	(1; 2; 5; 6)+	b, -a - b, c	
[2] $I12/c1$ (15, $C12/c1$)	(1; 3; 5; 7)+	-a - c, b, a	
[2] $I2/b11$ (15, $C12/c1$)	(1; 4; 5; 8)+	-b - c, a, c	

II Maximal klassengleiche subgroups
• Loss of centring translations

[2] $Pbca$ (61)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pcab$ (61, $Pbca$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	-b, a, c	1/4, 1/4, 1/4
[2] $Pcaa$ (54, $Pcca$)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	c, b, -a	
[2] $Pccb$ (54, $Pcca$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	-b, a, c	
[2] $Pbab$ (54, $Pcca$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	a, -c, b	
[2] $Pbcb$ (54, $Pcca$)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	c, a, b	1/4, 1/4, 1/4
[2] $Pbaa$ (54, $Pcca$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	b, c, a	1/4, 1/4, 1/4
[2] $Pcca$ (54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		1/4, 1/4, 1/4

• Enlarged unit cell

[3] $a' = 3a$			
$\left\{ \begin{array}{l} Ibca (73) \\ Ibca (73) \\ Ibca (73) \end{array} \right.$	$\langle 3; 5; 2 + (1, 0, 0) \rangle$ $\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$ $\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$	3a, b, c 3a, b, c 3a, b, c	1, 0, 0 2, 0, 0
[3] $b' = 3b$			
$\left\{ \begin{array}{l} Ibca (73) \\ Ibca (73) \\ Ibca (73) \end{array} \right.$	$\langle 2; 5; 3 + (0, 1, 0) \rangle$ $\langle (2; 5) + (0, 2, 0); 3 + (0, 1, 0) \rangle$ $\langle (2; 5) + (0, 4, 0); 3 + (0, 1, 0) \rangle$	a, 3b, c a, 3b, c a, 3b, c	0, 1, 0 0, 2, 0
[3] $c' = 3c$			
$\left\{ \begin{array}{l} Ibca (73) \\ Ibca (73) \\ Ibca (73) \end{array} \right.$	$\langle 5; (2; 3) + (0, 0, 1) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$ $\langle 2 + (0, 0, 1); 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$	a, b, 3c a, b, 3c a, b, 3c	0, 0, 1 0, 0, 2

• Series of maximal isomorphic subgroups

[<i>p</i>] $a' = pa$			
$Ibca (73)$	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups	pa, b, c	<i>u</i> , 0, 0
[<i>p</i>] $b' = pb$			
$Ibca (73)$	$\langle (2; 5) + (0, 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups	a, pb, c	0, <i>u</i> , 0
[<i>p</i>] $c' = pc$			
$Ibca (73)$	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups	a, b, pc	0, 0, <i>u</i>

I Minimal translationengleiche supergroups[2] $I4_1/acd$ (142); [3] $Ia\bar{3}$ (206)**II Minimal non-isomorphic klassengleiche supergroups**

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Aemm$ (67, $Cmme$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Bmem$ (67, $Cmme$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmme$ (67)**I Minimal translationengleiche supergroups**[2] $I4_1/amd$ (141)**II Minimal non-isomorphic klassengleiche supergroups**

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Ammm$ (65, $Cmmm$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Bmmm$ (65, $Cmmm$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmme$ (67)