

$Fm\bar{3}m$

No. 69

 $F2/m2/m2/m$ D_{2h}^{23} Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

32	p	1	(0,0,0)+	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$
			(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) x, y, \bar{z}	(7) x, \bar{y}, z	(8) \bar{x}, y, z

I Maximal translationengleiche subgroups

[2] $Fm\bar{3}m$ (42)	(1; 2; 7; 8)+	
[2] $Fm\bar{3}m$ (42, $Fm\bar{3}m$)	(1; 3; 6; 8)+	c, a, b
[2] $Fm\bar{3}m$ (42, $Fm\bar{3}m$)	(1; 4; 6; 7)+	b, c, a
[2] $Fm\bar{3}m$ (22)	(1; 2; 3; 4)+	
[2] $F112/m$ (12, $A112/m$)	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$
[2] $F12/m1$ (12, $C12/m1$)	(1; 3; 5; 7)+	a, b, $1/2(-\mathbf{a}+\mathbf{c})$
[2] $F2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b}, \mathbf{a}, 1/2(\mathbf{b}+\mathbf{c})$

II Maximal klassengleiche subgroups

• Loss of centring translations

[2] $Aaaa$ (68, $Ccce$)	1; 2; 3; 4; (1; 2; 3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, b, $-\mathbf{a}$	1/4, 1/4, 0
[2] $Bbeb$ (68, $Ccce$)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (5; 6; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, a, b	1/4, 1/4, 0
[2] $Ccce$ (68)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (5; 6; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$		0, 1/4, 1/4
[2] $Cmme$ (67)	1; 2; 7; 8; (1; 2; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4; 5; 6) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 5; 6) + $(\frac{1}{2}, 0, \frac{1}{2})$		0, 1/4, 1/4
[2] $Bmem$ (67, $Cmme$)	1; 3; 6; 8; (1; 3; 6; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4; 5; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, a, b	1/4, 1/4, 0
[2] $Aemm$ (67, $Cmme$)	1; 4; 6; 7; (1; 4; 6; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	b, c, a	1/4, 0, 1/4
[2] $Cccm$ (66)	1; 2; 5; 6; (1; 2; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$		1/4, 1/4, 0
[2] $Bbmb$ (66, $Cccm$)	1; 3; 5; 7; (1; 3; 5; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4; 6; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, a, b	1/4, 0, 1/4
[2] $Amaa$ (66, $Cccm$)	1; 4; 5; 8; (1; 4; 5; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	b, c, a	0, 1/4, 1/4
[2] $Ammm$ (65, $Cmmm$)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$	b, c, a	
[2] $Bmmm$ (65, $Cmmm$)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$	c, a, b	
[2] $Cmmm$ (65)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$		
[2] $Aeam$ (64, $Cmce$)	1; 2; 5; 6; (1; 2; 5; 6) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, b, $-\mathbf{a}$	
[2] $Bbem$ (64, $Cmce$)	1; 2; 5; 6; (1; 2; 5; 6) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	c, a, b	
[2] $Aema$ (64, $Cmce$)	1; 3; 5; 7; (1; 3; 5; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	b, c, a	
[2] $Ccme$ (64, $Cmce$)	1; 3; 5; 7; (1; 3; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4; 6; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	
[2] $Bmeb$ (64, $Cmce$)	1; 4; 5; 8; (1; 4; 5; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3; 6; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	a, $-\mathbf{c}, \mathbf{b}$	
[2] $Cmce$ (64)	1; 4; 5; 8; (1; 4; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3; 6; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$		

[2] <i>Amam</i> (63, <i>Cmcm</i>)	1; 3; 6; 8; (1; 3; 6; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)	c, b, -a	1/4, 1/4, 0
[2] <i>Amma</i> (63, <i>Cmcm</i>)	1; 2; 7; 8; (1; 2; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)	b, c, a	1/4, 0, 1/4
[2] <i>Bmmb</i> (63, <i>Cmcm</i>)	1; 2; 7; 8; (1; 2; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 5; 6) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)	a, -c, b	0, 1/4, 1/4
[2] <i>Bbmm</i> (63, <i>Cmcm</i>)	1; 4; 6; 7; (1; 4; 6; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 3; 5; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)	c, a, b	1/4, 1/4, 0
[2] <i>Cmcm</i> (63)	1; 3; 6; 8; (1; 3; 6; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 4; 5; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)		0, 1/4, 1/4
[2] <i>Ccmm</i> (63, <i>Cmcm</i>)	1; 4; 6; 7; (1; 4; 6; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 3; 5; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)	-b, a, c	1/4, 0, 1/4

• **Enlarged unit cell**

[3] a' = 3a			
$\left\{ \begin{array}{l} Fmmm (69) \\ Fmmm (69) \\ Fmmm (69) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle (2; 3; 5) + (2, 0, 0) \rangle$ $\langle (2; 3; 5) + (4, 0, 0) \rangle$	3a, b, c 3a, b, c 3a, b, c	1, 0, 0 2, 0, 0
[3] b' = 3b			
$\left\{ \begin{array}{l} Fmmm (69) \\ Fmmm (69) \\ Fmmm (69) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle 3; (2; 5) + (0, 2, 0) \rangle$ $\langle 3; (2; 5) + (0, 4, 0) \rangle$	a, 3b, c a, 3b, c a, 3b, c	0, 1, 0 0, 2, 0
[3] c' = 3c			
$\left\{ \begin{array}{l} Fmmm (69) \\ Fmmm (69) \\ Fmmm (69) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle 2; (3; 5) + (0, 0, 2) \rangle$ $\langle 2; (3; 5) + (0, 0, 4) \rangle$	a, b, 3c a, b, 3c a, b, 3c	0, 0, 1 0, 0, 2

• **Series of maximal isomorphic subgroups**

[p] a' = pa			
<i>Fmmm</i> (69)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	pa, b, c	$u, 0, 0$
[p] b' = pb			
<i>Fmmm</i> (69)	$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	a, pb, c	$0, u, 0$
[p] c' = pc			
<i>Fmmm</i> (69)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	a, b, pc	$0, 0, u$

I Minimal translationengleiche supergroups

[2] *I4/mmm* (139); [2] *I4/mcm* (140); [3] *Fm $\bar{3}$* (202)

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

none

• **Decreased unit cell**

[2] **a' = $\frac{1}{2}$ a, b' = $\frac{1}{2}$ b, c' = $\frac{1}{2}$ c** *Pmmm* (47)