

D_{2h}^1
 $P2/m2/m2/m$

No. 47

 $Pmmm$
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	<i>d</i>	1	(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] <i>Pmm2</i> (25)	1; 2; 7; 8				
[2] <i>Pm2m</i> (25, <i>Pmm2</i>)	1; 3; 6; 8				c, a, b
[2] <i>P2mm</i> (25, <i>Pmm2</i>)	1; 4; 6; 7				b, c, a
[2] <i>P222</i> (16)	1; 2; 3; 4				
[2] <i>P112/m</i> (10)	1; 2; 5; 6				
[2] <i>P12/m1</i> (10)	1; 3; 5; 7				
[2] <i>P2/m11</i> (10, <i>P12/m1</i>)	1; 4; 5; 8				c, a, b

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $a' = 2a$					
<i>Pmma</i> (51)	⟨3; 5; 2 + (1,0,0)⟩				2a, b, c
<i>Pmma</i> (51)	⟨2; (3; 5) + (1,0,0)⟩				1/2, 0, 0
<i>Pmam</i> (51, <i>Pmma</i>)	⟨2; 5; 3 + (1,0,0)⟩				2a, -c, b
<i>Pmam</i> (51, <i>Pmma</i>)	⟨3; (2; 5) + (1,0,0)⟩				2a, -c, b
<i>Pmaa</i> (49, <i>Pccm</i>)	⟨5; (2; 3) + (1,0,0)⟩				1/2, 0, 0
<i>Pmaa</i> (49, <i>Pccm</i>)	⟨2; 3; 5 + (1,0,0)⟩				b, c, 2a
<i>Pmmm</i> (47)	⟨2; 3; 5⟩				b, c, 2a
<i>Pmmm</i> (47)	⟨(2; 3; 5) + (1,0,0)⟩				1/2, 0, 0
[2] $b' = 2b$					
<i>Pbmm</i> (51, <i>Pmma</i>)	⟨2; 5; 3 + (0,1,0)⟩				2b, c, a
<i>Pbmm</i> (51, <i>Pmma</i>)	⟨(2; 3; 5) + (0,1,0)⟩				2b, c, a
<i>Pmmb</i> (51, <i>Pmma</i>)	⟨5; (2; 3) + (0,1,0)⟩				0, 1/2, 0
<i>Pmmb</i> (51, <i>Pmma</i>)	⟨2; (3; 5) + (0,1,0)⟩				-2b, a, c
<i>Pmbb</i> (49, <i>Pccm</i>)	⟨3; 5; 2 + (0,1,0)⟩				-2b, a, c
<i>Pmbb</i> (49, <i>Pccm</i>)	⟨2; 3; 5 + (0,1,0)⟩				0, 1/2, 0
<i>Pmmm</i> (47)	⟨2; 3; 5⟩				c, a, 2b
<i>Pmmm</i> (47)	⟨3; (2; 5) + (0,1,0)⟩				c, a, 2b
<i>Pmmm</i> (47)	⟨2; 3; 5⟩				a, 2b, c
<i>Pmmm</i> (47)	⟨3; (2; 5) + (0,1,0)⟩				a, 2b, c
[2] $c' = 2c$					
<i>Pcmm</i> (51, <i>Pmma</i>)	⟨3; 5; 2 + (0,0,1)⟩				2c, b, -a
<i>Pcmm</i> (51, <i>Pmma</i>)	⟨(2; 3; 5) + (0,0,1)⟩				2c, b, -a
<i>Pmcm</i> (51, <i>Pmma</i>)	⟨5; (2; 3) + (0,0,1)⟩				0, 0, 1/2
<i>Pmcm</i> (51, <i>Pmma</i>)	⟨3; (2; 5) + (0,0,1)⟩				2c, a, b
<i>Pccm</i> (49)	⟨2; 5; 3 + (0,0,1)⟩				2c, a, b
<i>Pccm</i> (49)	⟨2; 3; 5 + (0,0,1)⟩				0, 0, 1/2
<i>Pmmm</i> (47)	⟨2; 3; 5⟩				a, b, 2c
<i>Pmmm</i> (47)	⟨2; (3; 5) + (0,0,1)⟩				a, b, 2c
<i>Pmmm</i> (47)	⟨2; 3; 5⟩				a, b, 2c
<i>Pmmm</i> (47)	⟨2; (3; 5) + (0,0,1)⟩				0, 0, 1/2
[2] $b' = 2b, c' = 2c$					
<i>Aemm</i> (67, <i>Cmme</i>)	⟨3; 5; 2 + (0,0,1)⟩				2b, 2c, a
<i>Aemm</i> (67, <i>Cmme</i>)	⟨(2; 3; 5) + (0,0,1)⟩				2b, 2c, a
<i>Aemm</i> (67, <i>Cmme</i>)	⟨2; 5; 3 + (0,0,1)⟩				0, 0, 1/2
<i>Aemm</i> (67, <i>Cmme</i>)	⟨2; 3; 5 + (0,0,1)⟩				2b, 2c, a
<i>Ammm</i> (65, <i>Cmmm</i>)	⟨2; 3; 5⟩				2b, 2c, a
<i>Ammm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (0,0,1)⟩				2b, 2c, a
<i>Ammm</i> (65, <i>Cmmm</i>)	⟨5; (2; 3) + (0,0,1)⟩				0, 0, 1/2
<i>Ammm</i> (65, <i>Cmmm</i>)	⟨3; (2; 5) + (0,0,1)⟩				2b, 2c, a
<i>Ammm</i> (65, <i>Cmmm</i>)	⟨3; (2; 5) + (0,0,1)⟩				2b, 2c, a
[2] $a' = 2a, c' = 2c$					
<i>Bmem</i> (67, <i>Cmme</i>)	⟨2; 5; 3 + (1,0,0)⟩				2c, 2a, b
<i>Bmem</i> (67, <i>Cmme</i>)	⟨3; (2; 5) + (1,0,0)⟩				2c, 2a, b
<i>Bmem</i> (67, <i>Cmme</i>)	⟨5; (2; 3) + (1,0,0)⟩				1/2, 0, 0
<i>Bmem</i> (67, <i>Cmme</i>)	⟨2; 3; 5 + (1,0,0)⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; 3; 5⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨(2; 3; 5) + (1,0,0)⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨3; 5; 2 + (1,0,0)⟩				1/2, 0, 0
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (1,0,0)⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (1,0,0)⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (1,0,0)⟩				1/2, 0, 1/2
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (1,0,0)⟩				2c, 2a, b
<i>Bmmm</i> (65, <i>Cmmm</i>)	⟨2; (3; 5) + (1,0,0)⟩				0, 0, 1/2

[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$			
<i>Cmme</i> (67)	$\langle 3; 5; 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 1/2, 0$
<i>Cmme</i> (67)	$\langle 2; (3; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0, 1/2, 0$
<i>Cmme</i> (67)	$\langle 5; (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
<i>Cmme</i> (67)	$\langle 2; 3; 5 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 0, 0$
<i>Cmmm</i> (65)	$\langle 2; 3; 5 \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
<i>Cmmm</i> (65)	$\langle (2; 3; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 0, 0$
<i>Cmmm</i> (65)	$\langle 2; 5; 3 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 1/2, 0$
<i>Cmmm</i> (65)	$\langle 3; (2; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0, 1/2, 0$
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$			
<i>Fmmm</i> (69)	$\langle 2; 3; 5 \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
<i>Fmmm</i> (69)	$\langle (2; 3; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 0, 0$
<i>Fmmm</i> (69)	$\langle 3; 5; 2 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 0, 1/2$
<i>Fmmm</i> (69)	$\langle 2; (3; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 0, 1/2$
<i>Fmmm</i> (69)	$\langle 2; 5; 3 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 1/2, 0$
<i>Fmmm</i> (69)	$\langle 3; (2; 5) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 1/2, 0$
<i>Fmmm</i> (69)	$\langle 5; (2; 3) + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 1/2, 1/2$
<i>Fmmm</i> (69)	$\langle 2; 3; 5 + (1, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 1/2, 1/2$
[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} Pmmm (47) \\ Pmmm (47) \\ Pmmm (47) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle (2; 3; 5) + (2, 0, 0) \rangle$ $\langle (2; 3; 5) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$ $2, 0, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} Pmmm (47) \\ Pmmm (47) \\ Pmmm (47) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle 3; (2; 5) + (0, 2, 0) \rangle$ $\langle 3; (2; 5) + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$ $0, 2, 0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} Pmmm (47) \\ Pmmm (47) \\ Pmmm (47) \end{array} \right.$	$\langle 2; 3; 5 \rangle$ $\langle 2; (3; 5) + (0, 0, 2) \rangle$ $\langle 2; (3; 5) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$ $0, 0, 2$
• Series of maximal isomorphic subgroups			
[<i>p</i>] $\mathbf{a}' = p\mathbf{a}$			
<i>Pmmm</i> (47)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$ prime $p > 2; 0 \leq u < p$ p conjugate subgroups	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
[<i>p</i>] $\mathbf{b}' = p\mathbf{b}$			
<i>Pmmm</i> (47)	$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ prime $p > 2; 0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
[<i>p</i>] $\mathbf{c}' = p\mathbf{c}$			
<i>Pmmm</i> (47)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$ prime $p > 2; 0 \leq u < p$ p conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal translationengleiche supergroups

[2] $P4/mmm$ (123); [2] $P4_2/mmc$ (131); [3] $Pm\bar{3}$ (200)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $Ammm$ (65, $Cmmm$); [2] $Bmmm$ (65, $Cmmm$); [2] $Cmmm$ (65); [2] $Immm$ (71)

• Decreased unit cell

none