

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

II Maximal klassengleiche subgroups

• Enlarged unit cell

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

<i>Pmmm</i> (47)	$\langle 2; 3; 5 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
<i>Pmmm</i> (47)	$\langle (2; 3; 5) + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$
<i>Pmmm</i> (47)	$\langle (2; 3; 5) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2, 0, 0$

[3] $\mathbf{b}' = 3\mathbf{b}$

<i>Pmmm</i> (47)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
<i>Pmmm</i> (47)	$\langle 3; (2; 5) + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$
<i>Pmmm</i> (47)	$\langle 3; (2; 5) + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 2, 0$

[3] $\mathbf{c}' = 3\mathbf{c}$

<i>Pmmm</i> (47)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
<i>Pmmm</i> (47)	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$
<i>Pmmm</i> (47)	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 2$

• Series of maximal isomorphic subgroups

[p] $\mathbf{a}' = p\mathbf{a}$

<i>Pmmm</i> (47)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
------------------	--	---------------------------------------	-----------

[p] $\mathbf{b}' = p\mathbf{b}$

<i>Pmmm</i> (47)	$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
------------------	--	---------------------------------------	-----------

[p] $\mathbf{c}' = p\mathbf{c}$

<i>Pmmm</i> (47)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
------------------	--	---------------------------------------	-----------

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