

D_{2h}^{13}
 $P2_1/m2_1/m2/n$

No. 59

 $Pmnn$

 ORIGIN CHOICE 1, Origin at $mm2/n$, at $\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

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

I Maximal translationengleiche subgroups

[2] $Pm2_1n$ (31, $Pmn2_1$)	1; 3; 6; 8	a, -c, b	
[2] $P2_1mn$ (31, $Pmn2_1$)	1; 4; 6; 7	b, c, a	
[2] $Pmm2$ (25)	1; 2; 7; 8		
[2] $P2_12_12$ (18)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	-a - b, a, c	1/4, 1/4, 0
[2] $P12_1/m1$ (11)	1; 3; 5; 7		1/4, 1/4, 0
[2] $P2_1/m11$ (11, $P12_1/m1$)	1; 4; 5; 8	c, a, b	1/4, 1/4, 0

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
$Pcmn$ (62, $Pnma$)	$\langle 3; 5; 2 + (0, 0, 1) \rangle$	2c, b, -a	1/4, 1/4, 0
$Pcmn$ (62, $Pnma$)	$\langle (2; 3; 5) + (0, 0, 1) \rangle$	2c, b, -a	1/4, 1/4, 1/2
$Pmcn$ (62, $Pnma$)	$\langle 5; (2; 3) + (0, 0, 1) \rangle$	2c, a, b	1/4, 1/4, 0
$Pmcn$ (62, $Pnma$)	$\langle 3; (2; 5) + (0, 0, 1) \rangle$	2c, a, b	1/4, 1/4, 1/2
$Pmnn$ (59)	$\langle 2; 3; 5 \rangle$	a, b, 2c	
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	a, b, 2c	0, 0, 1/2
$Pccn$ (56)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	a, b, 2c	1/4, 1/4, 0
$Pccn$ (56)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	a, b, 2c	1/4, 1/4, 1/2
[3] $a' = 3a$			
$Pmnn$ (59)	$\langle 2; (3; 5) + (1, 0, 0) \rangle$	3a, b, c	
$Pmnn$ (59)	$\langle 2 + (2, 0, 0); (3; 5) + (3, 0, 0) \rangle$	3a, b, c	1, 0, 0
$Pmnn$ (59)	$\langle 2 + (4, 0, 0); (3; 5) + (5, 0, 0) \rangle$	3a, b, c	2, 0, 0
[3] $b' = 3b$			
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 1, 0) \rangle$	a, 3b, c	
$Pmnn$ (59)	$\langle 2 + (0, 2, 0); 3 + (0, 1, 0); 5 + (0, 3, 0) \rangle$	a, 3b, c	0, 1, 0
$Pmnn$ (59)	$\langle 2 + (0, 4, 0); 3 + (0, 1, 0); 5 + (0, 5, 0) \rangle$	a, 3b, c	0, 2, 0
[3] $c' = 3c$			
$Pmnn$ (59)	$\langle 2; 3; 5 \rangle$	a, b, 3c	
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	a, b, 3c	0, 0, 1
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	a, b, 3c	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $a' = pa$			
$Pmnn$ (59)	$\langle 2 + (2u, 0, 0); (3; 5) + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0) \rangle$	pa, b, c	$u, 0, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $b' = pb$			
$Pmnn$ (59)	$\langle 2 + (0, 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0);$	a, pb, c	$0, u, 0$
	$5 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$		
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $c' = pc$			
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$	a, b, pc	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		

I Minimal translationengleiche supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

[2] $Amma$ (63, $Cmcm$); [2] $Bmmb$ (63, $Cmcm$); [2] $Cmmm$ (65); [2] $Immm$ (71)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pmmb$ (51, $Pmma$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmma$ (51)

I Minimal translationengleiche supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

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• **Additional centring translations**

[2] $Amma$ (63, $Cmcm$); [2] $Bmmb$ (63, $Cmcm$); [2] $Cmmm$ (65); [2] $Immm$ (71)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pmmb$ (51, $Pmma$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmma$ (51)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $2_1 2_1 n$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from $mm2$

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

I Maximal translationengleiche subgroups

[2] $Pm2_1n$ (31, $Pmn2_1$)	1; 3; 6; 8	a, -c, b	1/4, 1/4, 0
[2] $P2_1mn$ (31, $Pmn2_1$)	1; 4; 6; 7	b, c, a	1/4, 1/4, 0
[2] $Pmm2$ (25)	1; 2; 7; 8		1/4, 1/4, 0
[2] $P2_12_12$ (18)	1; 2; 3; 4		1/4, 1/4, 0
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	-a - b, a, c	
[2] $P12_1/m1$ (11)	1; 3; 5; 7		
[2] $P2_1/m11$ (11, $P12_1/m1$)	1; 4; 5; 8	c, a, b	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
$Pcmn$ (62, $Pnma$)	$\langle 3; 5; 2 + (0,0,1) \rangle$	2c, b, -a	
$Pcmn$ (62, $Pnma$)	$\langle (2; 3; 5) + (0,0,1) \rangle$	2c, b, -a	0, 0, 1/2
$Pmcn$ (62, $Pnma$)	$\langle 5; (2; 3) + (0,0,1) \rangle$	2c, a, b	
$Pmcn$ (62, $Pnma$)	$\langle 3; (2; 5) + (0,0,1) \rangle$	2c, a, b	0, 0, 1/2
$Pmnn$ (59)	$\langle 2; 3; 5 \rangle$	a, b, 2c	
$Pmnn$ (59)	$\langle 2; (3; 5) + (0,0,1) \rangle$	a, b, 2c	0, 0, 1/2
$Pccn$ (56)	$\langle 2; 5; 3 + (0,0,1) \rangle$	a, b, 2c	
$Pccn$ (56)	$\langle 2; 3; 5 + (0,0,1) \rangle$	a, b, 2c	0, 0, 1/2
[3] $a' = 3a$			
$Pmnn$ (59)	$\langle 3; 5; 2 + (1,0,0) \rangle$	3a, b, c	
$Pmnn$ (59)	$\langle 2 + (3,0,0); (3; 5) + (2,0,0) \rangle$	3a, b, c	1, 0, 0
$Pmnn$ (59)	$\langle 2 + (5,0,0); (3; 5) + (4,0,0) \rangle$	3a, b, c	2, 0, 0
[3] $b' = 3b$			
$Pmnn$ (59)	$\langle 5; (2; 3) + (0,1,0) \rangle$	a, 3b, c	
$Pmnn$ (59)	$\langle 2 + (0,3,0); 3 + (0,1,0); 5 + (0,2,0) \rangle$	a, 3b, c	0, 1, 0
$Pmnn$ (59)	$\langle 2 + (0,5,0); 3 + (0,1,0); 5 + (0,4,0) \rangle$	a, 3b, c	0, 2, 0
[3] $c' = 3c$			
$Pmnn$ (59)	$\langle 2; 3; 5 \rangle$	a, b, 3c	
$Pmnn$ (59)	$\langle 2; (3; 5) + (0,0,2) \rangle$	a, b, 3c	0, 0, 1
$Pmnn$ (59)	$\langle 2; (3; 5) + (0,0,4) \rangle$	a, b, 3c	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $a' = pa$			
$Pmnn$ (59)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$	pa, b, c	$u, 0, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $b' = pb$			
$Pmnn$ (59)	$\langle 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2}, 0); 5 + (0, 2u, 0) \rangle$	a, pb, c	$0, u, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $c' = pc$			
$Pmnn$ (59)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$	a, b, pc	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		

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I Minimal *translationengleiche* supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[2] $Amma$ (63, $Cmcm$); [2] $Bmmb$ (63, $Cmcm$); [2] $Cmmm$ (65); [2] $Immm$ (71)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pmmb$ (51, $Pmma$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmma$ (51)

I Minimal *translationengleiche* supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[2] $Amma$ (63, $Cmcm$); [2] $Bmmb$ (63, $Cmcm$); [2] $Cmmm$ (65); [2] $Immm$ (71)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pmmb$ (51, $Pmma$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmma$ (51)