

Pban

No. 50

$P2/b2/a2/n$

D_{2h}^4

 ORIGIN CHOICE 1, Origin at $222/n$, 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	<i>m</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) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$

I Maximal translationengleiche subgroups

[2] <i>Pba2</i> (32)	1; 2; 7; 8		
[2] <i>Pb2n</i> (30, <i>Pnc2</i>)	1; 3; 6; 8	c, a, b	
[2] <i>P2an</i> (30, <i>Pnc2</i>)	1; 4; 6; 7	c, b, -a	
[2] <i>P222</i> (16)	1; 2; 3; 4		
[2] <i>P112/n</i> (13, <i>P112/a</i>)	1; 2; 5; 6	-a - b, a, c	1/4, 1/4, 0
[2] <i>P12/a1</i> (13, <i>P12/c1</i>)	1; 3; 5; 7	-a - c, b, a	1/4, 1/4, 0
[2] <i>P2/b11</i> (13, <i>P12/c1</i>)	1; 4; 5; 8	c, a, b	1/4, 1/4, 0

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
<i>Pnan</i> (52, <i>Pnna</i>)	$\langle 3; 5; 2 + (0, 0, 1) \rangle$	a, -2c, b	1/4, 1/4, 0
<i>Pnan</i> (52, <i>Pnna</i>)	$\langle (2; 3; 5) + (0, 0, 1) \rangle$	a, -2c, b	1/4, 1/4, 1/2
<i>Pbnn</i> (52, <i>Pnna</i>)	$\langle 5; (2; 3) + (0, 0, 1) \rangle$	b, 2c, a	1/4, 1/4, 0
<i>Pbnn</i> (52, <i>Pnna</i>)	$\langle 3; (2; 5) + (0, 0, 1) \rangle$	b, 2c, a	1/4, 1/4, 1/2
<i>Pban</i> (50)	$\langle 2; 3; 5 \rangle$	a, b, 2c	
<i>Pban</i> (50)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	a, b, 2c	0, 0, 1/2
<i>Pnnn</i> (48)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	a, b, 2c	0, 0, 1/2
<i>Pnnn</i> (48)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	a, b, 2c	
[3] $a' = 3a$			
<i>Pban</i> (50)	$\langle 2; 3; 5 + (1, 0, 0) \rangle$	3a, b, c	
<i>Pban</i> (50)	$\langle (2; 3) + (2, 0, 0); 5 + (3, 0, 0) \rangle$	3a, b, c	1, 0, 0
<i>Pban</i> (50)	$\langle (2; 3) + (4, 0, 0); 5 + (5, 0, 0) \rangle$	3a, b, c	2, 0, 0
[3] $b' = 3b$			
<i>Pban</i> (50)	$\langle 2; 3; 5 + (0, 1, 0) \rangle$	a, 3b, c	
<i>Pban</i> (50)	$\langle 3; 2 + (0, 2, 0); 5 + (0, 3, 0) \rangle$	a, 3b, c	0, 1, 0
<i>Pban</i> (50)	$\langle 3; 2 + (0, 4, 0); 5 + (0, 5, 0) \rangle$	a, 3b, c	0, 2, 0
[3] $c' = 3c$			
<i>Pban</i> (50)	$\langle 2; 3; 5 \rangle$	a, b, 3c	
<i>Pban</i> (50)	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	a, b, 3c	0, 0, 1
<i>Pban</i> (50)	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	a, b, 3c	0, 0, 2
• Series of maximal isomorphic subgroups			
[<i>p</i>] $a' = pa$			
<i>Pban</i> (50)	$\langle (2; 3) + (2u, 0, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0) \rangle$	pa, b, c	$u, 0, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[<i>p</i>] $b' = pb$			
<i>Pban</i> (50)	$\langle 3; 2 + (0, 2u, 0); 5 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$	a, pb, c	$0, u, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[<i>p</i>] $c' = pc$			
<i>Pban</i> (50)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$	a, b, pc	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		

(Continued on the preceding page)

- Series of maximal isomorphic subgroups

[<i>p</i>] $\mathbf{a}' = p\mathbf{a}$ <i>Pccm</i> (49)	$\langle (2; 3; 5) + (2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
[<i>p</i>] $\mathbf{b}' = p\mathbf{b}$ <i>Pccm</i> (49)	$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
[<i>p</i>] $\mathbf{c}' = p\mathbf{c}$ <i>Pccm</i> (49)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal translationengleiche supergroups

[2] *P4/mcc* (124); [2] *P4₂/mcm* (132)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

[2] *Cccm* (66); [2] *Aemm* (67, *Cmme*); [2] *Bmem* (67, *Cmme*); [2] *Ibam* (72)

- Decreased unit cell

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

(Continued from the following page)

I Minimal translationengleiche supergroups

[2] *P4/nbm* (125); [2] *P4₂/nbc* (133)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

[2] *Cmmm* (65); [2] *Aaaa* (68, *Ccce*); [2] *Bbeb* (68, *Ccce*); [2] *Ibam* (72)

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pbmb* (49, *Pccm*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmaa* (49, *Pccm*)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at ban , at $-\frac{1}{4}, -\frac{1}{4}, 0$ from 222

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

I Maximal translationengleiche subgroups

[2] $Pba2$ (32)	1; 2; 7; 8		1/4, 1/4, 0
[2] $Pb2n$ (30, $Pnc2$)	1; 3; 6; 8	c, a, b	1/4, 1/4, 0
[2] $P2an$ (30, $Pnc2$)	1; 4; 6; 7	c, b, -a	1/4, 1/4, 0
[2] $P222$ (16)	1; 2; 3; 4		1/4, 1/4, 0
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	-a - b, a, c	
[2] $P12/a1$ (13, $P12/c1$)	1; 3; 5; 7	-a - c, b, a	
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	c, a, b	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
$Pnan$ (52, $Pnna$)	$\langle 3; 5; 2 + (0, 0, 1) \rangle$	a, -2c, b	
$Pnan$ (52, $Pnna$)	$\langle (2; 3; 5) + (0, 0, 1) \rangle$	a, -2c, b	0, 0, 1/2
$Pbnn$ (52, $Pnna$)	$\langle 5; (2; 3) + (0, 0, 1) \rangle$	b, 2c, a	
$Pbnn$ (52, $Pnna$)	$\langle 3; (2; 5) + (0, 0, 1) \rangle$	b, 2c, a	0, 0, 1/2
$Pban$ (50)	$\langle 2; 3; 5 \rangle$	a, b, 2c	
$Pban$ (50)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	a, b, 2c	0, 0, 1/2
$Pnnn$ (48)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	a, b, 2c	
$Pnnn$ (48)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	a, b, 2c	0, 0, 1/2
[3] $a' = 3a$			
$Pban$ (50)	$\langle 5; (2; 3) + (1, 0, 0) \rangle$	3a, b, c	
$Pban$ (50)	$\langle (2; 3) + (3, 0, 0); 5 + (2, 0, 0) \rangle$	3a, b, c	1, 0, 0
$Pban$ (50)	$\langle (2; 3) + (5, 0, 0); 5 + (4, 0, 0) \rangle$	3a, b, c	2, 0, 0
[3] $b' = 3b$			
$Pban$ (50)	$\langle 3; 5; 2 + (0, 1, 0) \rangle$	a, 3b, c	
$Pban$ (50)	$\langle 3; 2 + (0, 3, 0); 5 + (0, 2, 0) \rangle$	a, 3b, c	0, 1, 0
$Pban$ (50)	$\langle 3; 2 + (0, 5, 0); 5 + (0, 4, 0) \rangle$	a, 3b, c	0, 2, 0
[3] $c' = 3c$			
$Pban$ (50)	$\langle 2; 3; 5 \rangle$	a, b, 3c	
$Pban$ (50)	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	a, b, 3c	0, 0, 1
$Pban$ (50)	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	a, b, 3c	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $a' = pa$			
$Pban$ (50)	$\langle (2; 3) + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 5 + (2u, 0, 0) \rangle$	pa, b, c	$u, 0, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $b' = pb$			
$Pban$ (50)	$\langle 3; 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0); 5 + (0, 2u, 0) \rangle$	a, pb, c	$0, u, 0$
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p] $c' = pc$			
$Pban$ (50)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$	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/nbm* (125); [2] *P4₂/nbc* (133)

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

[2] *Cmmm* (65); [2] *Aaaa* (68, *Ccce*); [2] *Bbeb* (68, *Ccce*); [2] *Ibam* (72)

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pbmb* (49, *Pccm*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmaa* (49, *Pccm*)

Pmma

No. 51

(Continued from the facing page)

• **Series of maximal isomorphic subgroups**

<p>[<i>p</i>] $\mathbf{a}' = p\mathbf{a}$ <i>Pmma</i> (51)</p>	<p>$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i></p>	<p>$p\mathbf{a}, \mathbf{b}, \mathbf{c}$</p>	<p>$u, 0, 0$</p>
<p>[<i>p</i>] $\mathbf{b}' = p\mathbf{b}$ <i>Pmma</i> (51)</p>	<p>$\langle 3; (2; 5) + (0, 2u, 0) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i></p>	<p>$\mathbf{a}, p\mathbf{b}, \mathbf{c}$</p>	<p>$0, u, 0$</p>
<p>[<i>p</i>] $\mathbf{c}' = p\mathbf{c}$ <i>Pmma</i> (51)</p>	<p>$\langle 2; (3; 5) + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i></p>	<p>$\mathbf{a}, \mathbf{b}, p\mathbf{c}$</p>	<p>$0, 0, u$</p>

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

[2] *Amma* (63, *Cmcm*); [2] *Bmmm* (65, *Cmmm*); [2] *Cmme* (67); [2] *Imma* (74)

• **Decreased unit cell**

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