Pban No. 50 $P2/b2/a2/n$ D_{2h}^4

ORIGIN CHOICE 1, Origin at $2\,2\,2/n$, 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	*m*	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] *Pba*2 (32)	1; 2; 7; 8		
[2] *Pb*2*n* (30, *Pnc*2)	1; 3; 6; 8	**c**, **a**, **b**	
[2] *P*2*an* (30, *Pnc*2)	1; 4; 6; 7	**c**, **b**, −**a**	
[2] *P*222 (16)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	−**a** − **b**, **a**, **c**	$1/4,1/4,0$
[2] $P12/a1$ (13, $P12/c1$)	1; 3; 5; 7	−**a** − **c**, **b**, **a**	$1/4,1/4,0$
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	**c**, **a**, **b**	$1/4,1/4,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$

Pnan (52, *Pnna*)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	**a**, −2**c**, **b**	$1/4,1/4,0$
Pnan (52, *Pnna*)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	**a**, −2**c**, **b**	$1/4,1/4,1/2$
Pbnn (52, *Pnna*)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	**b**, 2**c**, **a**	$1/4,1/4,0$
Pbnn (52, *Pnna*)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	**b**, 2**c**, **a**	$1/4,1/4,1/2$
Pban (50)	$\langle 2;\ 3;\ 5\rangle$	**a**, **b**, 2**c**	
Pban (50)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	**a**, **b**, 2**c**	$0,0,1/2$
Pnnn (48)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	**a**, **b**, 2**c**	$0,0,1/2$
Pnnn (48)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	**a**, **b**, 2**c**	

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

Pban (50)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	3**a**, **b**, **c**	
Pban (50)	$\langle (2;\ 3)+(2,0,0);\ 5+(3,0,0)\rangle$	3**a**, **b**, **c**	$1,0,0$
Pban (50)	$\langle (2;\ 3)+(4,0,0);\ 5+(5,0,0)\rangle$	3**a**, **b**, **c**	$2,0,0$

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

Pban (50)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	**a**, 3**b**, **c**	
Pban (50)	$\langle 3;\ 2+(0,2,0);\ 5+(0,3,0)\rangle$	**a**, 3**b**, **c**	$0,1,0$
Pban (50)	$\langle 3;\ 2+(0,4,0);\ 5+(0,5,0)\rangle$	**a**, 3**b**, **c**	$0,2,0$

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

Pban (50)	$\langle 2;\ 3;\ 5\rangle$	**a**, **b**, 3**c**	
Pban (50)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	**a**, **b**, 3**c**	$0,0,1$
Pban (50)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	**a**, **b**, 3**c**	$0,0,2$

- **Series of maximal isomorphic subgroups**

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

Pban (50)	$\langle (2;\ 3)+(2u,0,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	p**a**, **b**, **c**	$u,0,0$

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

Pban (50)	$\langle 3;\ 2+(0,2u,0);\ 5+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	**a**, p**b**, **c**	$0,u,0$

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

Pban (50)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	**a**, **b**, p**c**	$0,0,u$

(*Continued on the preceding page*)

- **Series of maximal isomorphic subgroups**

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

Pccm (49)	$\langle (2;\ 3;\ 5) + (2u,0,0) \rangle$ prime $p > 2;\ 0 \le u < p$ p conjugate subgroups	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u,0,0$

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

Pccm (49)	$\langle 3;\ (2;\ 5) + (0,2u,0) \rangle$ prime $p > 2;\ 0 \le u < p$ p conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$

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

Pccm (49)	$\langle 2;\ 3 + (0,0,\frac{p}{2} - \frac{1}{2} + 2u);\ 5 + (0,0,2u) \rangle$ prime $p > 2;\ 0 \le u < p$ p conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4_2/mcm$ (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*) No. 50 ORIGIN CHOICE 1 *Pban*

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Cmmm* (65); [2] *Aeaa* (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	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $P2an$ (30, $Pnc2$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
[2] $P222$ (16)	1; 2; 3; 4		$1/4,1/4,0$
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P12/a1$ (13, $P12/c1$)	1; 3; 5; 7	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

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

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pban$ (50)	$\langle (2;\ 3)+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 5+(2u,0,0)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pban$ (50)	$\langle 3;\ 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 5+(0,2u,0)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pban$ (50)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups
[2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Cmmm* (65); [2] *Aeaa* (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] $\mathbf{a}' = p\mathbf{a}$			
Pmma (51)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ prime $p>2;\ 0\le u<p$ p conjugate subgroups	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}' = p\mathbf{b}$			
Pmma (51)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ prime $p>2;\ 0\le u<p$ p conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}' = p\mathbf{c}$			
Pmma (51)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ prime $p>2;\ 0\le u<p$ p conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

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)