

*Pban*

No. 50

*P2/b2/a2/n**D<sub>2h</sub><sup>4</sup>*

Axes	Coordinates		Wyckoff positions									
	origin 1	origin 2	2a	2b	2c	2d	4e	4f	4g	4h	4i	4j

**I Maximal translationengleiche subgroups**

[2] <i>Pba2</i> (32)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	2a	2b	2b	2a	4c	4c	4c	4c	4c	4c	
[2] <i>P2an</i> (30)		$x, y+\frac{1}{4}, z$	2a	2a	2b	2b	4c	4c	2×2a	2×2b	4c	4c	$2\times 4c$
$\cong Pnc2$	<b>c, b, -a</b>	$z, y, -x$		$z, y+\frac{1}{4}, -x$						4c	4c	4c	$2\times 4c$
[2] <i>Pb2n</i> (30)		$x+\frac{1}{4}, y, z$	2a	2a	2b	2b	4c	4c	4c	2×2a	2×2b	2×2b	$2\times 2b$
$\cong Pnc2$	<b>c, a, b</b>	$z, x, y$		$z, x+\frac{1}{4}, y$						4c	4c	4c	$2\times 4c$
[2] <i>P222</i> (16)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	1a; 1e	1b; 1c	1f; 1g	1d; 1h	4u	4u	2i; 2k	2j; 2l	2m; 2o	2n; 2p	
										2q; 2t	2r; 2s		$2\times 4u$
[2] <i>P2/b11</i> (13)		$x+\frac{1}{4}, y+\frac{1}{4}, z$					2e	2e	2f	2f	2a; 2c	2b; 2d	$2\times 2e$
$\cong P12/c1$	<b>c, a, b</b>	$z, x+\frac{1}{4}, y+\frac{1}{4}$		$z, x, y$							2a; 2c	2b; 2d	$2\times 2f$
[2] <i>P12/a1</i> (13)		$x+\frac{1}{4}, y+\frac{1}{4}, z$					2e	2e	2f	2f	2a; 2c	2b; 2d	$4g$
$\cong P12/c1$	<b>-c, b, a</b>	$-z, y+\frac{1}{4}, x+\frac{1}{4}$		$-z, y, x$							4g	4g	$2\times 4g$
[2] <i>P112/n</i> (13)		$x+\frac{1}{4}, y+\frac{1}{4}, z$					2e	2f	2f	2e	2a; 2d	2b; 2c	$4g$
											4g	4g	$2\times 2f$
													$2\times 4g$

**II Maximal klassengleiche subgroups**

## Enlarged unit cell, non-isomorphic

[2] <i>Pnan</i> (52)	<b>a, b, 2c</b>	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	4c	4c	4d	4d	4a; 4b	8e	8e	$2\times 4d$	$2\times 4c$	$8e$
$\cong Pnna$	<b>a, -2c, b</b>	$x+\frac{1}{4}, -\frac{1}{2}z, y+\frac{1}{4};$ $+(0, \frac{1}{2}, 0)$	$x, -\frac{1}{2}z, y;$ $+(0, \frac{1}{2}, 0)$								$8e$	$8e$	$2\times 8e$
[2] <i>Pnan</i> (52)	<b>a, b, 2c</b>	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	4d	4d	4c	4c	8e	4a; 4b	$2\times 4d$	8e	8e	$2\times 4c$
$\cong Pnna$	<b>a, -2c, b</b>	$x+\frac{1}{4}, -\frac{1}{2}z-\frac{1}{4}, y+\frac{1}{4};$ $+(0, \frac{1}{2}, 0)$	$x, -\frac{1}{2}z-\frac{1}{4}, y;$ $+(0, \frac{1}{2}, 0)$								$8e$	$8e$	$2\times 8e$
[2] <i>Pbnn</i> (52)	<b>a, b, 2c</b>	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	4c	4c	4d	4d	4a; 4b	8e	$2\times 4c$	8e	8e	$2\times 4d$
$\cong Pnna$	<b>b, 2c, a</b>	$y+\frac{1}{4}, \frac{1}{2}z, x+\frac{1}{4};$ $+(0, \frac{1}{2}, 0)$	$y, \frac{1}{2}z, x;$ $+(0, \frac{1}{2}, 0)$								$8e$	$8e$	$2\times 8e$
[2] <i>Pbnn</i> (52)	<b>a, b, 2c</b>	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	4d	4d	4c	4c	8e	4a; 4b	8e	$2\times 4c$	$2\times 4d$	$8e$
$\cong Pnna$	<b>b, 2c, a</b>	$y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}, x+\frac{1}{4};$ $+(0, \frac{1}{2}, 0)$	$y, \frac{1}{2}z+\frac{1}{4}, x;$ $+(0, \frac{1}{2}, 0)$								$8e$	$8e$	$2\times 8e$
[2] <i>Pnnn</i> (48)	<b>a, b, 2c</b>	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	4k	4l	$2b; 2d$	$2a; 2c$	4e; 4f	8m	8m	4g; 4h	8m	$4i; 4j$
											$2\times 4k$	$2\times 4l$	$2\times 8m$
[2] <i>Pnnn</i> (48)	<b>a, b, 2c</b>	$x, y, \frac{1}{2}z;$ $+(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0, 0, \frac{1}{2})$	2a; 2c	2b; 2d	4l	4k	8m	4e; 4f	4g; 4h	8m	4i; 4j	8m
											$2\times 4k$	$2\times 4l$	$2\times 8m$

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*P2/b2/a2/n*

No. 50

*Pban*

Axes	Coordinates		Wyckoff positions										
	origin 1	origin 2	2a	2b	2c	2d	4e	4f	4g	4h	4i	8m	
<b>Enlarged unit cell, isomorphic</b>													
[3] <i>Pban</i>	<b>3a, b, c</b>	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$2a(b^*); 4g$	$2b(a^*); 4g$	$2c(d^*); 4h$	$2d(c^*); 4h$	$4e; 8m$	$4f; 8m$	$3 \times 4g$	$3 \times 4h$	$4i; 8m$	
[p] <i>Pban</i>	<b>p a, b, c</b>	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$2a(b^\dagger); \frac{p-1}{2} \times 4g$	$2b(a^\dagger); \frac{p-1}{2} \times 4g$	$2c(d^\dagger); \frac{p-1}{2} \times 4h$	$2d(c^\dagger); \frac{p-1}{2} \times 4h$	$4e; \frac{p-1}{2} \times 8m$	$4f; \frac{p-1}{2} \times 8m$	$p \times 4g$	$p \times 4h$	$4i; \frac{p-1}{2} \times 8m$	
		$p = \text{prime} > 2; u = 1, \dots, p-1$								$4j; \frac{p-1}{2} \times 8m$	$4k(l^\dagger); \frac{p-1}{2} \times 8m$	$4l(k^\dagger); \frac{p-1}{2} \times 8m$	
[3] <i>Pban</i>	<b>a, 3b, c</b>	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$2a(b^*); 4i$	$2b(a^*); 4i$	$2c(d^*); 4j$	$2d(c^*); 4j$	$4e; 8m$	$4f; 8m$	$4g; 8m$	$4h; 8m$	$3 \times 4i$	
[p] <i>Pban</i>	<b>a, p b, c</b>	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$2a(b^\dagger); \frac{p-1}{2} \times 4i$	$2b(a^\dagger); \frac{p-1}{2} \times 4i$	$2c(d^\dagger); \frac{p-1}{2} \times 4j$	$2d(c^\dagger); \frac{p-1}{2} \times 4j$	$4e; \frac{p-1}{2} \times 8m$	$4f; \frac{p-1}{2} \times 8m$	$4g; \frac{p-1}{2} \times 8m$	$4h; \frac{p-1}{2} \times 8m$	$p \times 4i$	
		$p = \text{prime} > 2; u = 1, \dots, p-1$								$p \times 4j$	$4k(l^\dagger); \frac{p-1}{2} \times 8m$	$4l(k^\dagger); \frac{p-1}{2} \times 8m$	
[2] <i>Pban</i>	<b>a, b, 2c</b>	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2a; 2d$	$2b; 2c$	$4l$	$4k$	$4e; 4f$	$8m$	$4g; 4h$	$8m$	$4i; 4j$	
									$8m$	$2 \times 4k$	$2 \times 4l$	$2 \times 8m$	
[2] <i>Pban</i>	<b>a, b, 2c</b>	$x, y, \frac{1}{2}z + \frac{1}{4}; +(0, 0, \frac{1}{2})$	$x, y, \frac{1}{2}z + \frac{1}{4}; +(0, 0, \frac{1}{2})$	$4k$	$4l$	$2b; 2c$	$2a; 2d$	$8m$	$4e; 4f$	$8m$	$4g; 4h$	$8m$	
									$4i; 4j$	$2 \times 4k$	$2 \times 4l$	$2 \times 8m$	
[3] <i>Pban</i>	<b>a, b, 3c</b>	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a; 4k$	$2b; 4l$	$2c; 4l$	$2d; 4k$	$4e; 8m$	$4f; 8m$	$4g; 8m$	$4h; 8m$	$4i; 8m$	
[p] <i>Pban</i>	<b>a, b, pc</b>	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$2a; \frac{p-1}{2} \times 4k$	$2b; \frac{p-1}{2} \times 4l$	$2c; \frac{p-1}{2} \times 4l$	$2d; \frac{p-1}{2} \times 4k$	$4e; \frac{p-1}{2} \times 8m$	$4f; \frac{p-1}{2} \times 8m$	$4g; \frac{p-1}{2} \times 8m$	$4h; \frac{p-1}{2} \times 8m$	$4i; \frac{p-1}{2} \times 8m$	
		$p = \text{prime} > 2; u = 1, \dots, p-1$								$4j; \frac{p-1}{2} \times 8m$	$p \times 4k$	$p \times 4l$	$\frac{p-1}{2} \times 8m$

\* origin 2

† origin 2 and  $p = 4n-1$ **Nonconventional settings**

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

*Pncb*    $a \rightarrow b \rightarrow c \rightarrow a$    **a → b → c → a**    $x \rightarrow y \rightarrow z \rightarrow x$ *Pcna*    $a \leftarrow b \leftarrow c \leftarrow a$    **a ← b ← c ← a**    $x \leftarrow y \leftarrow z \leftarrow x$