

$D_3^1$ 

No. 149

 $P312$ 

	Axes	Coordinates	Wyckoff positions									
			1a	1b	1c	1d	1e	1f	2g	2h	2i 3k	3j 6l
<b>I Maximal translationengleiche subgroups</b>												
[2] $P3$ (143)			1a	1a	1b	1b	1c	1c	$2 \times 1a$	$2 \times 1b$	$2 \times 1c$ 3d	3d $2 \times 3d$
[3] $C121$ (5)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	2a	2b	2a	2b	2a	2b	4c	4c	4c 2b;4c	2a;4c $3 \times 4c$
	conjugate: $\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$										
	conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$										
<b>II Maximal klassengleiche subgroups</b>												
<b>Enlarged unit cell, non-isomorphic</b>												
[3] $R32$ (155)	$\mathbf{a}-\mathbf{b},$ $\mathbf{a}+2\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	3a;6c	3b;6c	9d	9e	9d	9e	$3 \times 6c$	18f	18f 9e;18f	9d;18f $3 \times 18f$
[3] $R32$ (155)	$\mathbf{a}-\mathbf{b},$ $\mathbf{a}+2\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(2x-y)-\frac{1}{3}, \frac{1}{3}(x+y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	9d	9e	3a;6c	3b;6c	9d	9e	18f	$3 \times 6c$	18f 9e;18f	9d;18f $3 \times 18f$
[3] $R32$ (155)	$\mathbf{a}-\mathbf{b},$ $\mathbf{a}+2\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(2x-y)+\frac{1}{3}, \frac{1}{3}(x+y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	9d	9e	9d	9e	3a;6c	3b;6c	18f	18f	$3 \times 6c$ 9e;18f	9d;18f $3 \times 18f$
[3] $R32$ (155)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	3a;6c	3b;6c	9d	9e	9d	9e	$3 \times 6c$	18f	18f 9e;18f	9d;18f $3 \times 18f$
[3] $R32$ (155)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	9d	9e	9d	9e	3a;6c	3b;6c	18f	18f	$3 \times 6c$ 9e;18f	9d;18f $3 \times 18f$
[3] $R32$ (155)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$	9d	9e	3a;6c	3b;6c	9d	9e	18f	$3 \times 6c$	18f 9e;18f	9d;18f $3 \times 18f$
[3] $P3_212$ (153)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	3a	3b	3a	3b	3a	3b	6c	6c	6c 3b;6c	3a;6c $3 \times 6c$
[3] $P3_112$ (151)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	3a	3b	3a	3b	3a	3b	6c	6c	6c 3b;6c	3a;6c $3 \times 6c$
[3] $P321$ (150)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	1a;2d	1b;2d	3e	3f	3e	3f	$2c; 2 \times 2d$	6g	6g 3f;6g	3e;6g $3 \times 6g$
[3] $P321$ (150)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	3e	3f	3e	3f	1a;2d	1b;2d	6g	6g	$2c; 2 \times 2d$ 3f;6g	3e;6g $3 \times 6g$
[3] $P321$ (150)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	3e	3f	1a;2d	1b;2d	3e	3f	6g	$2c; 2 \times 2d$	6g 3f;6g	3e;6g $3 \times 6g$
<b>Enlarged unit cell, isomorphic</b>												
[2] $P312$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	1a;1b	2g	1c;1d	2h	1e;1f	2i	$2 \times 2g$	$2 \times 2h$	$2 \times 2i$ 6l	3j;3k $2 \times 6l$
[2] $P312$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	2g	1a;1b	2h	1c;1d	2i	1e;1f	$2 \times 2g$	$2 \times 2h$	$2 \times 2i$ 3j;3k	6l $2 \times 6l$
[3] $P312$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	1a;2g	1b;2g	1c;2h	1d;2h	1e;2i	1f;2i	$3 \times 2g$	$3 \times 2h$	$3 \times 2i$ 3k;6l	3j;6l $3 \times 6l$

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HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions					
			3a	3b	6c	9d	9e	18f
<b>I Maximal translationengleiche subgroups</b>								
[2] $R\bar{3}$ (146)			3a	3a	2×3a	9b	9b	2×9b
[3] $P\bar{1}$	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c}),$	$x+z, -x+y+z, -y+z$	1a	1h	2i	1b; 1c; 1d	1e; 1f; 1g	3×2i
(2)	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),$							
	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$							
	rhombo. axes: $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$x, y, z$						
<b>II Maximal klassengleiche subgroups</b>								
<b>Loss of centring translations</b>								
[3] $P\bar{3}$ (147)			1a; 2d	1b; 2d	2c; 2×2d	3f; 6g	3e; 6g	3×6g
<b>Enlarged unit cell, isomorphic</b>								
[2] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z; + (0, 0, \frac{1}{2})$	3a; 3b	6c	2×6c	18f	9d; 9e	2×18f
[2] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2})$	6c	3a; 3b	2×6c	9d; 9e	18f	2×18f
[p] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$	$-x, -y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$	$3a; \frac{p-1}{2} \times 6c$	$3b; \frac{p-1}{2} \times 6c$	$p \times 6c$	$9d; \frac{p-1}{2} \times 18f$	$9e; \frac{p-1}{2} \times 18f$	$p \times 18f$
	$p = \text{prime} = 6n-1; u = 1, \dots, p-1$							
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$						
	$p = \text{prime} = 6n+1; u = 1, \dots, p-1$							
[7] $R\bar{3}$	$3\mathbf{a}+\mathbf{b},$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z;$	3a; 18f	3b; 18f	6c; 2×18f	9d; 3×18f	9e; 3×18f	7×18f
	$-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\pm(\frac{3}{7}, \frac{3}{7}, 0); \pm(\frac{3}{7}, \frac{1}{7}, 0); \pm(\frac{3}{7}, \frac{2}{7}, 0)$						
[7] $R\bar{3}$	$\mathbf{a}+3\mathbf{b},$	$\frac{1}{7}(-2x+3y), \frac{1}{7}(-3x+y), z;$	3a; 18f	3b; 18f	6c; 2×18f	9d; 3×18f	9e; 3×18f	7×18f
	$-3\mathbf{a}-2\mathbf{b}, \mathbf{c}$	$\pm(\frac{1}{7}, \frac{5}{7}, 0); \pm(\frac{2}{7}, \frac{3}{7}, 0); \pm(\frac{3}{7}, \frac{1}{7}, 0)$						
[p] $R\bar{3}$	$q\mathbf{a}+r\mathbf{b},$	$\frac{1}{p}((q-r)x+ry),$	$3a; \frac{p-1}{6} \times 18f$	$3b; \frac{p-1}{6} \times 18f$	$6c; \frac{p-1}{3} \times 18f$	$9d; \frac{p-1}{2} \times 18f$	$9e; \frac{p-1}{2} \times 18f$	$p \times 18f$
	$-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(-rx+qy), z; + (\frac{ur}{p}, \frac{uq}{p}, 0)$						
	$p = q^2 - qr + r^2 = \text{prime} = 6n+1;$							
	$q, r = 1, 2, \dots; q \neq r; q+r = 3n+1;$							
	$u = 1, \dots, p-1$							
[4] $R\bar{3}$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z; + (\frac{1}{2}, 0, 0);$	3a; 9e	3b; 9d	6c; 18f	2×18f	2×18f	4×18f
		$+ (0, \frac{1}{2}, 0); + (\frac{1}{2}, \frac{1}{2}, 0)$						
[p <sup>2</sup> ] $R\bar{3}$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$	$-\frac{1}{p}x, -\frac{1}{p}y, z; + (\frac{u}{p}, \frac{v}{p}, 0)$	$3a; \frac{p^2-1}{6} \times 18f$	$3b; \frac{p^2-1}{6} \times 18f$	$6c; \frac{p^2-1}{3} \times 18f$	$9d; \frac{p^2-1}{2} \times 18f$	$9e; \frac{p^2-1}{2} \times 18f$	$p^2 \times 18f$
	$p = \text{prime} = 6n-1; u, v = 1, \dots, p-1$							

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	Axes	Coordinates	Wyckoff positions						
			1a	1b	1c	1d	1e	1f	2g
[p] $P312$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$	$1a; \frac{p-1}{2} \times 2g$	$1b; \frac{p-1}{2} \times 2g$	$1c; \frac{p-1}{2} \times 2h$	$1d; \frac{p-1}{2} \times 2h$	$1e; \frac{p-1}{2} \times 2i$	$1f; \frac{p-1}{2} \times 2i$	$p \times 2g$
	$p = \text{prime} > 2; u = 1, \dots, p-1$				$p \times 2h$	$p \times 2i$	$3j; \frac{p-1}{2} \times 6l$	$3k; \frac{p-1}{2} \times 6l$	$p \times 6l$
[4] $P312$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; + (\frac{1}{2}, 0, 0);$	1a; 3j	1b; 3k	1e; 3j	1f; 3k	1c; 3j	1d; 3k	2g; 6l
		$+ (0, \frac{1}{2}, 0); + (\frac{1}{2}, \frac{1}{2}, 0)$			2i; 6l	2h; 6l	2×3j; 6l	2×3k; 6l	4×6l
[p <sup>2</sup> ] $P312$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; + (\frac{u}{p}, \frac{v}{p}, 0)$	1a;	1b;	1c(e*);	1d(f*);	1e(c*);	1f(d*);	2g; $\frac{p^2-1}{3} \times 6l$
	$p = \text{prime} > 4;$		$(p-1) \times 3j;$	$(p-1) \times 3k;$	$(p-1) \times 3j;$	$(p-1) \times 3k;$	$(p-1) \times 3j;$	$(p-1) \times 3k;$	
	$u, v = 1, \dots, p-1$		$\frac{(p-1)(p-2)}{6} \times 6l$						
					2h(i*);	2i(h*);	$p \times 3j;$	$p \times 3k;$	$p^2 \times 6l$
					$\frac{p^2-1}{3} \times 6l$	$\frac{p^2-1}{3} \times 6l$	$\frac{p(p-1)}{2} \times 6l$	$\frac{p(p-1)}{2} \times 6l$	

\*  $p = 6n-1$