

$D_{3d}^2$  $P\bar{3}12/c$ 

No. 163

 $P\bar{3}1c$ 

Axes	Coordinates	2a	2b	2c	2d 6g	Wyckoff positions	4e 6h	4f 12i
<b>I Maximal translationengleiche subgroups</b>								
[2] $P31c$ (159)		2a	2a	2b	2b 6c	2×2a 6c	2×2b 2×6c	
[2] $P312$ (149)	$x, y, z + \frac{1}{4}$	1a; 1b	2g	1d; 1e	1c; 1f 6l	2×2g 3j; 3k	2h; 2i	$2\times 6l$
[2] $P\bar{3}$ (147)		2c	1a; 1b	2d	2d 3e; 3f	2×2c 6g	2×2d 2×6g	
[3] $C12/c1$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x - \frac{1}{2}y, \frac{1}{2}y, z$	4e	4a	4e	4e	8f	8f
(15)						4b; 4c; 4d	4e; 8f	$3\times 8f$
conjugate: $\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$							
conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-(x+y), \frac{1}{2}(x-y), z$							

**II Maximal klassengleiche subgroups****Enlarged unit cell, non-isomorphic**

[3] $P\bar{3}c1$ (165)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	2a; 4d	2b; 4d	6f	6f	4c; 2×4d	12g
[3] $R\bar{3}c$ (167)	$\mathbf{a}-\mathbf{b},$ $\mathbf{a}+2\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$ (hexagonal axes)	6a; 12c	6b; 12c	18e	18e	$3\times 12c$	$36f$
[3] $R\bar{3}c$ (167)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z;$ $\pm(0, 0, \frac{1}{3})$ (hexagonal axes)	6a; 12c	6b; 12c	18e	18e	$3\times 12c$	$36f$

**Enlarged unit cell, isomorphic**

[3] $P\bar{3}1c$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	2a; 4e	2b; 4e	2d; 4f	2c; 4f 6g; 12i	3×4e 6h; 12i	3×4f 3×12i
[p] $P\bar{3}1c$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ $p = \text{prime} > 2; u = 1, \dots, p-1$	$2a; \frac{p-1}{2} \times 4e$	$2b; \frac{p-1}{2} \times 4e$	$2c(d^*); \frac{p-1}{2} \times 4f$	$2d(c^*); \frac{p-1}{2} \times 4f$ $6g; \frac{p-1}{2} \times 12i$	$p \times 4e$ $6h; \frac{p-1}{2} \times 12i$	$p \times 4f$ $p \times 12i$
[4] $P\bar{3}1c$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0);$ $+ (0, \frac{1}{2}, 0); + (\frac{1}{2}, \frac{1}{2}, 0)$	2a; 6h	2b; 6g	2d; 6h	2c; 6h 2×12i	4e; 12i 2×6h; 12i	4f; 12i 4×12i
[ $p^2$ ] $P\bar{3}1c$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$ $p = \text{prime} > 4;$ $u, v = 1, \dots, p-1$	2a; $\frac{(p-1)(p-2)}{6} \times 6h;$ $\frac{(p-1)(p-2)}{6} \times 12i$	2b; $\frac{p^2-1}{6} \times 12i$	$2c(d^\dagger);$ $\frac{(p-1) \times 6h}{6};$ $\frac{(p-1)(p-2)}{6} \times 12i$	$2d(c^\dagger);$ $\frac{(p-1) \times 6h}{6};$ $\frac{(p-1)(p-2)}{6} \times 12i$	4e; $6g; \frac{p^2-1}{2} \times 12i$ $p \times 6h;$ $\frac{p(p-1)}{2} \times 12i$	4f; $p^2 \times 12i$

<sup>\*</sup>  $p = 4n-1$ <sup>†</sup>  $p = 6n-1$