

Pc $P1c1$

No. 7

 $P1n1$ $P1a1$ C_s^2 UNIQUE AXIS b

CELL CHOICE 1

CELL CHOICE 2

CELL CHOICE 3

Axes

Coordinates

Wyckoff
positions
 $|2a|$

Axes

Coordinates

Axes

Coordinates

I Maximal translationengleiche subgroups

[2] $P1(1)$	$ 2 \times 1a $	$P1$	$P1$
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II Maximal klassengleiche subgroups**Enlarged unit cell, non-isomorphic**

[2] $C1c1$ $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $\frac{1}{2}x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0)$ (9)	$2 \times 4a$	$A1n1$ $\mathbf{a}-\mathbf{c},$ $2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}(x+z); + (0, \frac{1}{2}, 0)$	$I1a1$ $\mathbf{a}, 2\mathbf{b},$ $\mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y, \frac{1}{2}z; + (0, \frac{1}{2}, 0)$
[2] $C1c1$ $2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $\frac{1}{2}x, \frac{1}{2}y+\frac{1}{4}, z;$ (9) $+ (0, \frac{1}{2}, 0)$	$2 \times 4a$	$A1n1$ $\mathbf{a}-\mathbf{c},$ $2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}(x+z);$ $+ (0, \frac{1}{2}, 0)$	$I1a1$ $\mathbf{a}, 2\mathbf{b},$ $\mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z;$ $+ (0, \frac{1}{2}, 0)$

Enlarged unit cell, isomorphic

[2] $P1c1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0)$	$2 \times 2a$	$P1n1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0)$	$P1a1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0)$
[2] $P1c1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ $x, \frac{1}{2}y+\frac{1}{4}, z; + (0, \frac{1}{2}, 0)$	$2 \times 2a$	$P1n1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; + (0, \frac{1}{2}, 0)$	$P1a1$ $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; + (0, \frac{1}{2}, 0)$
[3] $P1c1$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0)$	$3 \times 2a$	$P1n1$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0)$	$P1a1$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0)$
[p] $P1c1$ $\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $x, \frac{1}{p}y, z; + (0, \frac{u}{p}, 0)$ $p = \text{prime}; u = 1, \dots, p-1$	$p \times 2a$	$P1n1$ $\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; + (0, \frac{u}{p}, 0)$ $p = \text{prime}; u = 1, \dots, p-1$	$P1a1$ $\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; + (0, \frac{u}{p}, 0)$ $p = \text{prime}; u = 1, \dots, p-1$
[2] $P1c1$ $2\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\frac{1}{2}x, y, z; + (\frac{1}{2}, 0, 0)$	$2 \times 2a$	$P1n1$ $\mathbf{a}-\mathbf{c},$ $\mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z); + (0, 0, \frac{1}{2})$	$P1a1$ $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; + (0, 0, \frac{1}{2})$
[2] $P1n1$ $2\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\frac{1}{2}x, y, z; + (\frac{1}{2}, 0, 0)$	$2 \times 2a$	$P1a1$ $\mathbf{a}-\mathbf{c},$ $\mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z); + (0, 0, \frac{1}{2})$	$P1n1$ $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; + (0, 0, \frac{1}{2})$
[3] $P1c1$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0)$	$3 \times 2a$	$P1n1$ $\mathbf{a}-2\mathbf{c},$ $\mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z);$ $\pm (0, 0, \frac{1}{3})$	$P1a1$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3})$
[3] $P1c1$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3})$	$3 \times 2a$	$P1n1$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0)$	$P1a1$ $3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm (\frac{1}{3}, 0, 0)$
[3] $P1c1$ $\mathbf{a}+\mathbf{c},$ $\mathbf{b}, 3\mathbf{c}$ $x, y, \frac{1}{3}(-x+z);$ $\pm (0, 0, \frac{1}{3})$	$3 \times 2a$	$P1n1$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3})$	$P1a1$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0)$
[3] $P1c1$ $\mathbf{a}-\mathbf{c},$ $\mathbf{b}, 3\mathbf{c}$ $x, y, \frac{1}{3}(x+z);$ $\pm (0, 0, \frac{1}{3})$	$3 \times 2a$	$P1n1$ $2\mathbf{a}+\mathbf{c}, \mathbf{b},$ $\mathbf{a}+2\mathbf{c}$	$\frac{1}{3}(2x-z), y, \frac{1}{3}(-x+2z);$ $\pm (\frac{1}{3}, 0, \frac{1}{3})$	$P1a1$ $3\mathbf{a}, \mathbf{b},$ $-\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z;$ $\pm (\frac{1}{3}, 0, 0)$
[p] $P1c1$ $p\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\frac{1}{p}x, y, z; + (\frac{u}{p}, 0, 0)$ $p = \text{prime}; u = 1, \dots, p-1;$	$p \times 2a$	$P1n1$ $\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$ $p = \text{prime}; u = 1, \dots, p-1;$	$P1a1$ $\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$ $p = \text{prime}; u = 1, \dots, p-1;$
[p] $P1c1$ $\mathbf{a}+q\mathbf{c},$ $\mathbf{b}, p\mathbf{c}$ $x, y, \frac{1}{p}(-qx+z);$ $+ (0, 0, \frac{u}{p})$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$p \times 2a$	$P1n1$ $\mathbf{a}, \mathbf{b},$ $2qa+\mathbf{c}$	$\frac{1}{p}(x-2qz), y, z;$ $+ (\frac{u}{p}, 0, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$P1a1$ $\mathbf{a}, \mathbf{b},$ $qa+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z;$ $+ (\frac{u}{p}, 0, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

*P*11*a*

No. 7

*P*11*n*

*P*11*b*

Pc

CELL CHOICE 1

CELL CHOICE 2

CELL CHOICE 3

UNIQUE AXIS *c*

Axes	Coordinates	Wyckoff positions 2 <i>a</i>
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Axes	Coordinates
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Axes	Coordinates
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I Maximal *translationengleiche* subgroups

$$[2] P1 (1) \quad | 2 \times 1a \quad | \quad P1$$

*P*1

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

$$[2] A11a \text{ } \mathbf{a}, 2\mathbf{b}, 2\mathbf{c} \quad x, \frac{1}{2}y, \frac{1}{2}z; + (0, 0, \frac{1}{2}) \quad | 2 \times 4a \quad B11n \text{ } 2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c} \quad \frac{1}{2}(x+y), y, \frac{1}{2}z; + (0, 0, \frac{1}{2}) \quad I11b \text{ } 2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c} \quad \frac{1}{2}x, -\frac{1}{2}x+y, \frac{1}{2}z; + (0, 0, \frac{1}{2}) \\ (9)$$

$$[2] A11a \text{ } \mathbf{a}, 2\mathbf{b}, 2\mathbf{c} \quad x, \frac{1}{2}y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2}) \quad | 2 \times 4a \quad B11n \text{ } 2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c} \quad \frac{1}{2}(x+y), y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2}) \quad I11b \text{ } 2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c} \quad \frac{1}{2}x, -\frac{1}{2}x+y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2})$$

Enlarged unit cell, isomorphic

$$[2] P11a \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z; + (0, 0, \frac{1}{2}) \quad | 2 \times 2a \quad P11n \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z; + (0, 0, \frac{1}{2}) \quad P11b \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z; + (0, 0, \frac{1}{2})$$

$$[2] P11a \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2}) \quad | 2 \times 2a \quad P11n \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2}) \quad P11b \text{ } \mathbf{a}, \mathbf{b}, 2\mathbf{c} \quad x, y, \frac{1}{2}z + \frac{1}{4}; + (0, 0, \frac{1}{2})$$

$$[3] P11a \text{ } \mathbf{a}, \mathbf{b}, 3\mathbf{c} \quad x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3}) \quad | 3 \times 2a \quad P11n \text{ } \mathbf{a}, \mathbf{b}, 3\mathbf{c} \quad x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3}) \quad P11b \text{ } \mathbf{a}, \mathbf{b}, 3\mathbf{c} \quad x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3})$$

$$[p] P11a \text{ } \mathbf{a}, \mathbf{b}, p\mathbf{c} \quad x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p}) \quad p = \text{prime}; u = 1, \dots, p-1 \quad | p \times 2a \quad P11n \text{ } \mathbf{a}, \mathbf{b}, p\mathbf{c} \quad x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p}) \quad P11b \text{ } \mathbf{a}, \mathbf{b}, p\mathbf{c} \quad x, y, \frac{1}{p}z; + (0, 0, \frac{u}{p})$$

$$[2] P11a \text{ } \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0) \quad | 2 \times 2a \quad P11n \text{ } 2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{2}(x+y), y, z; + (\frac{1}{2}, 0, 0) \quad P11b \text{ } 2\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{2}x, y, z; + (\frac{1}{2}, 0, 0)$$

$$[2] P11n \text{ } \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y, z; + (0, \frac{1}{2}, 0) \quad | 2 \times 2a \quad P11b \text{ } 2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{2}(x+y), y, z; + (\frac{1}{2}, 0, 0) \quad P11n \text{ } 2\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{2}x, y, z; + (\frac{1}{2}, 0, 0)$$

$$[3] P11a \text{ } \mathbf{a}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0) \quad | 3 \times 2a \quad P11n \text{ } 3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{3}(x+2y), y, z; \pm (\frac{1}{3}, 0, 0) \quad P11b \text{ } 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0)$$

$$[3] P11a \text{ } 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0) \quad | 3 \times 2a \quad P11n \text{ } \mathbf{a}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0) \quad P11b \text{ } \mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}(-x+y), z; \pm (0, \frac{1}{3}, 0)$$

$$[3] P11a \text{ } 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}(x-y), y, z; \pm (\frac{1}{3}, 0, 0) \quad | 3 \times 2a \quad P11n \text{ } 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}x, y, z; \pm (\frac{1}{3}, 0, 0) \quad P11b \text{ } \mathbf{a}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}y, z; \pm (0, \frac{1}{3}, 0)$$

$$[3] P11a \text{ } 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}(x+y), y, z; \pm (\frac{1}{3}, 0, 0) \quad | 3 \times 2a \quad P11n \text{ } 2\mathbf{a}+\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c} \quad \frac{1}{3}(2x-y), \frac{1}{3}(-x+2y), z; \pm (\frac{1}{3}, \frac{1}{3}, 0) \quad P11b \text{ } \mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}(x+y), z; \pm (0, \frac{1}{3}, 0)$$

$$[p] P11a \text{ } \mathbf{a}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}y, z; + (0, \frac{u}{p}, 0) \quad p = \text{prime}; u = 1, \dots, p-1; \quad | p \times 2a \quad P11n \text{ } p\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{p}x, y, z; + (\frac{u}{p}, 0, 0) \quad P11b \text{ } p\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{p}x, y, z; + (\frac{u}{p}, 0, 0)$$

$$[p] P11a \text{ } p\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{p}(x-qy), y, z; \pm (\frac{u}{p}, 0, 0) \quad p = \text{prime} > 2; u = 1, \dots, p-1; \quad | p \times 2a \quad P11n \text{ } \mathbf{a}+2q\mathbf{b}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}(-2qx+y), z; \pm (\frac{u}{p}, 0, 0) \quad P11b \text{ } \mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}(-qx+y), z; \pm (\frac{u}{p}, 0, 0)$$

$$[p] P11a \text{ } p\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{p}(x-qy), y, z; \pm (\frac{u}{p}, 0, 0) \quad p = \text{prime} > 2; u = 1, \dots, p-1; \quad | p \times 2a \quad P11n \text{ } \mathbf{a}+2q\mathbf{b}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}(-2qx+y), z; \pm (\frac{u}{p}, 0, 0) \quad P11b \text{ } \mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}(-qx+y), z; \pm (\frac{u}{p}, 0, 0)$$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3