

$C_2^3$  $C\bar{1}21$ 

No. 5

 $A\bar{1}21$  $C2$ UNIQUE AXIS  $b$ 

CELL CHOICE 1

CELL CHOICE 2

Axes	Coordinates	Wyckoff positions			Axes	Coordinates
		$ 2a$	$ 2b$	$ 4c$		

**I Maximal translationengleiche subgroups**[2]  $P1(1)$   $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$   $2x, x+y, z$  $|1a| 1a |2 \times 1a| P1 \mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c}) x, x+y, 2z$ **II Maximal klassengleiche subgroups****Loss of centring translations**[2]  $P12_11(4)$   $x+\frac{1}{4}, y, z$  $|2a| 2a |2 \times 2a| P12_11 x, y, z+\frac{1}{4}$ [2]  $P121(3)$  $|1a; 1c| 1b; 1d |2 \times 2e| \Rightarrow P121$ **Enlarged unit cell, isomorphic**[3]  $C121$   $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$   $x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$  $|3 \times 2a| 3 \times 2b |3 \times 4c| A121 \mathbf{a}, 3\mathbf{b}, \mathbf{c} x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$ [p]  $C121$   $\mathbf{a}, p\mathbf{b}, \mathbf{c}$   $x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$   
 $p = \text{prime} > 2; u = 1, \dots, p-1$  $|p \times 2a| p \times 2b |p \times 4c| A121 \mathbf{a}, p\mathbf{b}, \mathbf{c} x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$   
 $p = \text{prime} > 2; u = 1, \dots, p-1$ [2]  $C121$   $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$   $x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$  $|2a; 2b| 4c |2 \times 4c| A121 2\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$ [2]  $C121$   $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$   $x, y, \frac{1}{2}z + \frac{1}{4}; +(0, 0, \frac{1}{2})$  $|4c| 2a; 2b |2 \times 4c| A121 2\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{2}x - \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$ [2]  $I121$   $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$   $x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$  $|2a; 2b| 4c |2 \times 4c| I121 2\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$ [2]  $I121$   $\mathbf{a}, \mathbf{b}, 2\mathbf{c}$   $x, y, \frac{1}{2}z + \frac{1}{4}; +(0, 0, \frac{1}{2})$  $|4c| 2a; 2b |2 \times 4c| I121 2\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{2}x - \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$ [3]  $C121$   $3\mathbf{a}, \mathbf{b}, \mathbf{c}$   $\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$  $|2a; 4c| 2b; 4c |3 \times 4c| A121 \mathbf{a}+\mathbf{c}, \mathbf{b}, 3\mathbf{c} x, y, \frac{1}{3}(-x+z); \pm(0, 0, \frac{1}{3})$ [3]  $C121$   $3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$   $\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3}, 0, 0)$  $|2a; 4c| 2b; 4c |3 \times 4c| A121 \mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c} x, y, \frac{1}{3}(x+z); \pm(0, 0, \frac{1}{3})$ [3]  $C121$   $3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$   $\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3}, 0, 0)$  $|2a; 4c| 2b; 4c |3 \times 4c| A121 \mathbf{a}, \mathbf{b}, 3\mathbf{c} x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$ [3]  $C121$   $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$   $x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$  $|2a; 4c| 2b; 4c |3 \times 4c| A121 3\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$ [p]  $C121$   $\mathbf{a}, \mathbf{b}, p\mathbf{c}$   $x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$  $|2a; \frac{p-1}{2} \times 4c| 2b; \frac{p-1}{2} \times 4c |p \times 4c| A121 p\mathbf{a}, \mathbf{b}, \mathbf{c} \frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$  $p = \text{prime} > 2; u = 1, \dots, p-1$  $p = \text{prime} > 2; u = 1, \dots, p-1$ [p]  $C121$   $p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$   $\frac{1}{p}(x-qz), y, z; +(\frac{u}{p}, 0, 0)$  $|2a; \frac{p-1}{2} \times 4c| 2b; \frac{p-1}{2} \times 4c |p \times 4c| A121 \mathbf{a}+q\mathbf{c}, \mathbf{b}, p\mathbf{c} x, y, \frac{1}{p}(-qx+z); +(0, 0, \frac{u}{p})$  $p = \text{prime} > 2; u = 1, \dots, p-1$  $p = \text{prime} > 2; u = 1, \dots, p-1$  $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$  $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$ 

For cell choice 3 see next page

C2

I121

UNIQUE AXIS **b**  
CELL CHOICE 3

No. 5

A112

CONTINUED

UNIQUE AXIS **c**  
CELL CHOICE 1

Axes	Coordinates	Wyckoff positions	Axes	Coordinates	
		2a   2b   4c			
<b>I Maximal translationengleiche subgroups</b>					
[2] P1 (1) <b>a</b> , $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ , <b>c</b>	$x+y, 2y, y+z$	1a   1a   $2 \times 1a$	P1 (1) <b>a</b> , $\frac{1}{2}(\mathbf{b}-\mathbf{c})$ , <b>c</b>	$x, 2y, y+z$	
<b>II Maximal klassengleiche subgroups</b>					
Loss of centring translations					
[2] P12 <sub>1</sub> (4)	$x-\frac{1}{4}, y, z-\frac{1}{4}$	2a   2a   $2 \times 2a$	P112 <sub>1</sub> (4)	$x, y+\frac{1}{4}, z$	
[2] P121 (3)		1a; 1d   1b; 1c   $2 \times 2e$			
		1a; 1c   1b; 1d   $2 \times 2e$	$\Rightarrow P112 (3)$		
		1a; 1b   1c; 1d   $2 \times 2e$	$\Rightarrow$		
Enlarged unit cell, isomorphic					
[3] I121 <b>a</b> , 3 <b>b</b> , <b>c</b>	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$3 \times 2a$	3×2b   3×4c	A112 <b>a</b> , <b>b</b> , 3 <b>c</b>	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$
[p] I121 <b>a</b> , p <b>b</b> , <b>c</b>	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1$	$p \times 2a$	$p \times 2b$	A112 <b>a</b> , <b>b</b> , p <b>c</b>	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ $p = \text{prime} > 2; u = 1, \dots, p-1$
[2] I121    2 <b>a</b> , <b>b</b> , - <b>a</b> + <b>c</b>	$\frac{1}{2}(x+z), y, z; +(\frac{1}{2}, 0, 0)$	2a; 2b	4c   $2 \times 4c$	A112    2 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] I121    2 <b>a</b> , <b>b</b> , - <b>a</b> + <b>c</b>	$\frac{1}{2}(x+z) + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	4c	2a; 2b   $2 \times 4c$	A112    2 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{2}x + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[2] I121    2 <b>a</b> , <b>b</b> , <b>a</b> + <b>c</b>	$\frac{1}{2}(x-z), y, z; +(\frac{1}{2}, 0, 0)$	2a; 2b	4c   $2 \times 4c$	I112    2 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] I121    2 <b>a</b> , <b>b</b> , <b>a</b> + <b>c</b>	$\frac{1}{2}(x-z) + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	4c	2a; 2b   $2 \times 4c$	I112    2 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{2}x + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[3] I121 <b>a</b> , <b>b</b> , 3 <b>c</b>	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	2a; 4c	2b; 4c   $3 \times 4c$	A112 <b>a</b> , 3 <b>b</b> , <b>c</b>	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$
[3] A121    3 <b>a</b> , <b>b</b> , - <b>a</b> + <b>c</b>	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3}, 0, 0)$	2a; 4c	2b; 4c   $3 \times 4c$	A112 <b>a</b> - <b>b</b> , 3 <b>b</b> , <b>c</b>	$x, \frac{1}{3}(x+y), z; \pm(0, \frac{1}{3}, 0)$
[3] I121    3 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	2a; 4c	2b; 4c   $3 \times 4c$	A112 <b>a</b> + <b>b</b> , 3 <b>b</b> , <b>c</b>	$x, \frac{1}{3}(-x+y), z; \pm(0, \frac{1}{3}, 0)$
[3] A121    3 <b>a</b> , <b>b</b> , <b>a</b> + <b>c</b>	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3}, 0, 0)$	2a; 4c	2b; 4c   $3 \times 4c$	A112    3 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$
[p] I121    p <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{p}x, y, z; \pm(\frac{u}{p}, 0, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1$	$2a; \frac{p-1}{2} \times 4c$	$2b; \frac{p-1}{2} \times 4c$	A112    p <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1$
[p] I121 <b>a</b> +2q <b>c</b> , <b>b</b> , p <b>c</b>	$x, y, \frac{1}{p}(-2qx+z); +(0, 0, \frac{u}{p})$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$2a; \frac{p-1}{2} \times 4c$	$2b; \frac{p-1}{2} \times 4c$	A112 <b>a</b> +q <b>b</b> , p <b>b</b> , <b>c</b>	$x, \frac{1}{p}(-qx+y), z; +(0, \frac{u}{p}, 0)$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$

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

For unique axis **b**, cell choices 1 and 2, see preceding page

Axes

Coordinates

Axes

Coordinates

**I Maximal translationengleiche subgroups**

$$[2] P1 \quad \frac{1}{2}(\mathbf{a}-\mathbf{c}), \mathbf{b}, \mathbf{c} \quad 2x, y, y+z$$

$$P1 \quad \mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c}) \quad x+z, y+z, 2z$$

**II Maximal klassengleiche subgroups****Loss of centring translations**

$$[2] P112_1 \quad x+\frac{1}{4}, y, z$$

[2]

$$P112_1 \quad x-\frac{1}{4}, y-\frac{1}{4}, z$$

P112

[2] P112

**Enlarged unit cell, isomorphic**

$$[3] B112 \quad \mathbf{a}, \mathbf{b}, 3\mathbf{c} \quad x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$$

$$[p] B112 \quad \mathbf{a}, \mathbf{b}, p\mathbf{c} \quad x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p}) \\ p = \text{prime} > 2; u = 1, \dots, p-1$$

$$[2] B112 \quad \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$$

$$[2] B112 \quad \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y-\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$$

$$[2] I112 \quad \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$$

$$[2] I112 \quad \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y-\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$$

$$[3] B112 \quad 3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{3}(x-y), y, z; \pm(\frac{1}{3}, 0, 0)$$

$$[3] B112 \quad 3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{3}(x+y), y, z; \pm(\frac{1}{3}, 0, 0)$$

$$[3] B112 \quad 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$$

$$[3] B112 \quad \mathbf{a}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$$

$$[p] B112 \quad \mathbf{a}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0) \\ p = \text{prime} > 2; u = 1, \dots, p-1$$

$$[p] B112 \quad p\mathbf{a}, q\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{p}(x-qy), y, z; +(0, \frac{u}{p}, 0) \\ p = \text{prime} > 2; u = 1, \dots, p-1; \\ -\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$$

$$I112 \quad \mathbf{a}, \mathbf{b}, 3\mathbf{c} \quad x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$$

$$I112 \quad \mathbf{a}, \mathbf{b}, p\mathbf{c} \quad x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p}) \\ p = \text{prime} > 2; u = 1, \dots, p-1$$

$$I112 \quad \mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}(x+y), z; +(0, \frac{1}{2}, 0)$$

$$I112 \quad \mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}(x+y)+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$$

$$I112 \quad \mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}(-x+y), z; +(0, \frac{1}{2}, 0)$$

$$I112 \quad \mathbf{a}, 2\mathbf{b}, \mathbf{c} \quad x, \frac{1}{2}y-\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$$

$$I112 \quad 3\mathbf{a}, \mathbf{b}, \mathbf{c} \quad \frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$$

$$B112 \quad \mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}(x+y), z; \pm(0, \frac{1}{3}, 0)$$

$$I112 \quad \mathbf{a}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$$

$$B112 \quad \mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c} \quad x, \frac{1}{3}(-x+y), z; \pm(0, \frac{1}{3}, 0)$$

$$I112 \quad \mathbf{a}, p\mathbf{b}, \mathbf{c} \quad x, \frac{1}{p}y, z; \pm(0, \frac{u}{p}, 0) \\ p = \text{prime} > 2; u = 1, \dots, p-1$$

$$I112 \quad p\mathbf{a}, 2q\mathbf{a}+\mathbf{b}, \mathbf{c} \quad \frac{1}{p}(x-2qy), y, z; +(\frac{u}{p}, 0, 0)$$

$$p = \text{prime} > 2; u = 1, \dots, p-1;$$

$$-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$$