

$C2$

C_2^3

2

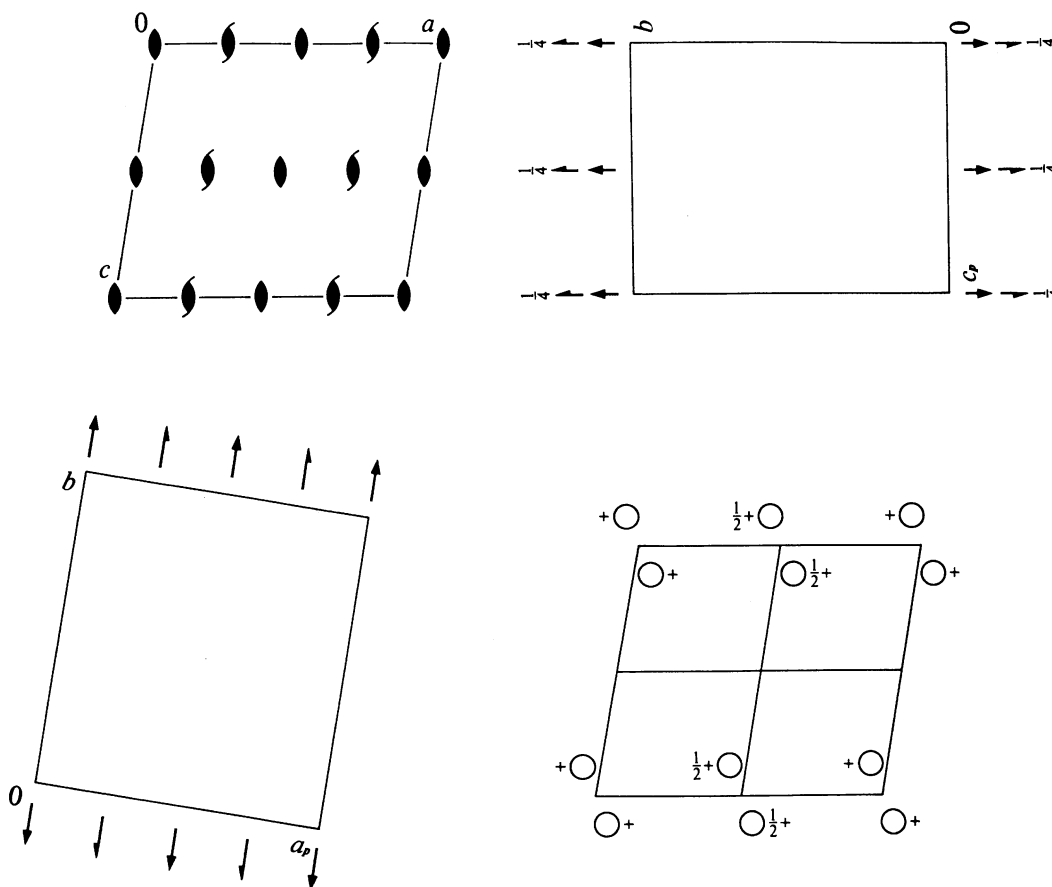
Monoclinic

No. 5

$C121$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2 \ 0,y,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0) \ \frac{1}{4},y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, 0)+$

Reflection conditions

4 *c* 1 (1) x, y, z (2) \bar{x}, y, \bar{z}

General:

$$hkl: h + k = 2n$$

$$h0l: h = 2n$$

$$0kl: k = 2n$$

$$hk0: h + k = 2n$$

$$0k0: k = 2n$$

$$h00: h = 2n$$

Special: no extra conditions

2 *b* 2 $0, y, \frac{1}{2}$

2 *a* 2 $0, y, 0$

Symmetry of special projections

Along $[001]$ $c1m1$

$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along $[100]$ $p11m$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$

Origin at $x, 0, 0$

Along $[010]$ $p2$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at $0, y, 0$

C2

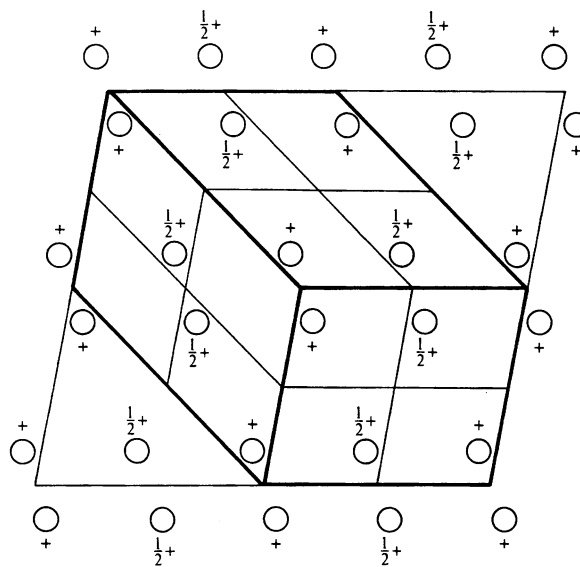
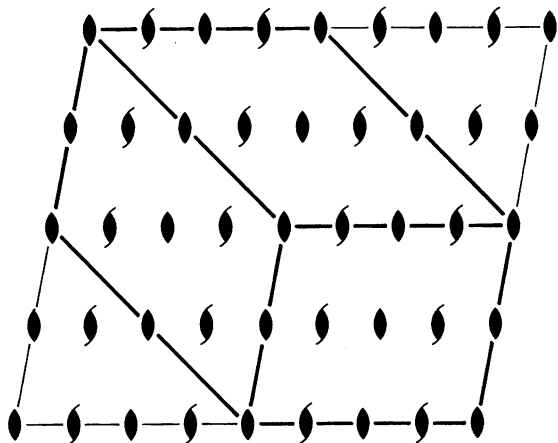
C₂³

2

Monoclinic

No. 5

UNIQUE AXIS *b*, DIFFERENT CELL CHOICES



C121

UNIQUE AXIS *b*, CELL CHOICE 1

Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2)

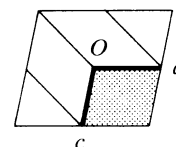
Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, 0)+$

4	<i>c</i>	1	(1) x,y,z	(2) \bar{x},y,\bar{z}
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2	<i>b</i>	2	$0,y,\frac{1}{2}$
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2	<i>a</i>	2	$0,y,0$
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Reflection conditions

General:

$hkl: h+k=2n$
 $h0l: h=2n$
 $0kl: k=2n$
 $hk0: h+k=2n$
 $0k0: k=2n$
 $h00: h=2n$

Special: no extra conditions

A121

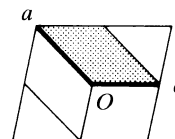
UNIQUE AXIS b , CELL CHOICE 2**Origin** on 2**Asymmetric unit** $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$

4	c	1	(1) x, y, z	(2) \bar{x}, y, \bar{z}
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2	b	2	$\frac{1}{2}, y, \frac{1}{2}$
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2	a	2	$0, y, 0$
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Reflection conditions

General:

 hkl : $k + l = 2n$ $h0l$: $l = 2n$ $0kl$: $k + l = 2n$ $hk0$: $k = 2n$ $0k0$: $k = 2n$ $00l$: $l = 2n$

Special: no extra conditions

I121

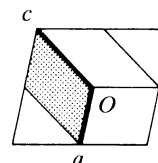
UNIQUE AXIS b , CELL CHOICE 3**Origin** on 2**Asymmetric unit** $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$

4	c	1	(1) x, y, z	(2) \bar{x}, y, \bar{z}
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2	b	2	$\frac{1}{2}, y, 0$
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2	a	2	$0, y, 0$
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Reflection conditions

General:

 hkl : $h + k + l = 2n$ $h0l$: $h + l = 2n$ $0kl$: $k + l = 2n$ $hk0$: $h + k = 2n$ $0k0$: $k = 2n$ $h00$: $h = 2n$ $00l$: $l = 2n$

Special: no extra conditions

C_2

C_2^3

2

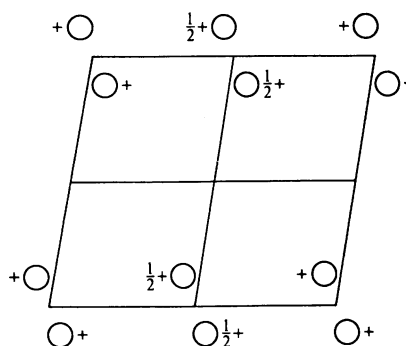
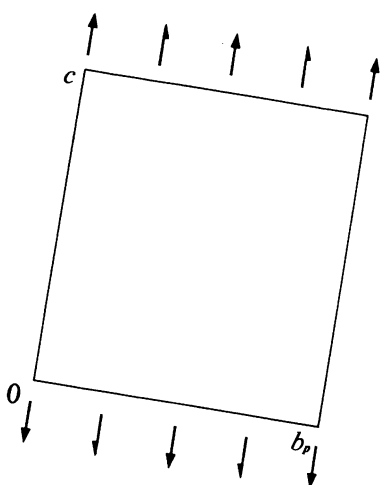
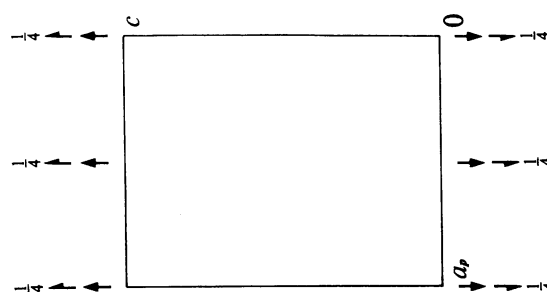
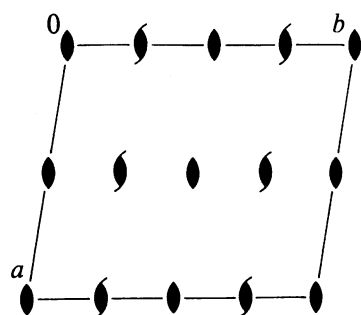
Monoclinic

No. 5

A112

Patterson symmetry A112/m

UNIQUE AXIS c , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1
- (2) 2 $0,0,z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$
- (2) $2(0,0, \frac{1}{2}) 0, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$

Reflection conditions

4 c 1 (1) x, y, z (2) \bar{x}, \bar{y}, z

General:

$$hkl: k + l = 2n$$

$$hk0: k = 2n$$

$$0kl: k + l = 2n$$

$$h0l: l = 2n$$

$$00l: l = 2n$$

$$0k0: k = 2n$$

Special: no extra conditions

2 b 2 $\frac{1}{2}, 0, z$

2 a 2 $0, 0, z$

Symmetry of special projections

Along $[001]$ $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $c1m1$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[010]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0, y, 0$

C2

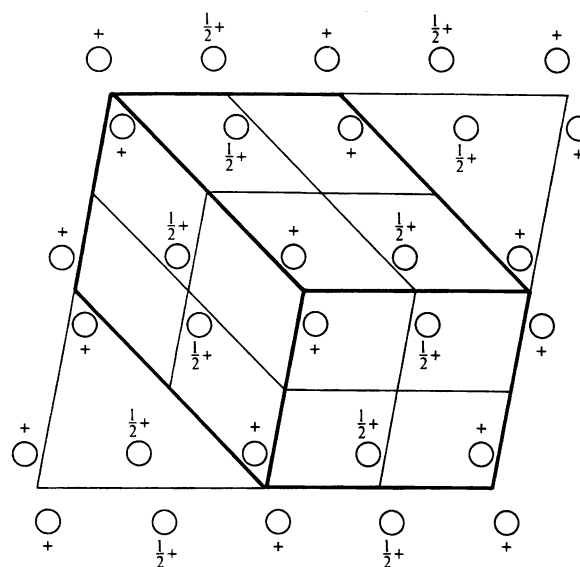
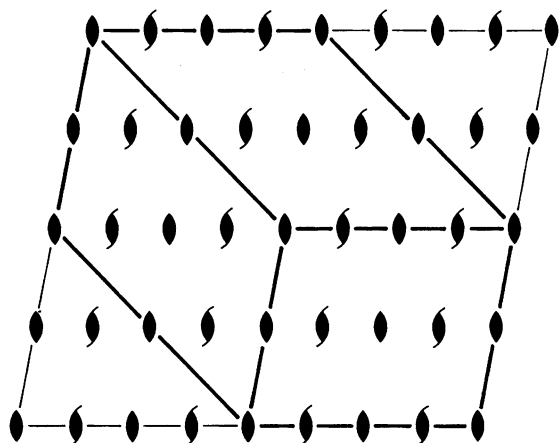
C₂³

2

Monoclinic

No. 5

UNIQUE AXIS *c*, DIFFERENT CELL CHOICES



A112

UNIQUE AXIS *c*, CELL CHOICE 1

Origin on 2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Generators selected $(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0, \frac{1}{2}, \frac{1}{2}); (2)$

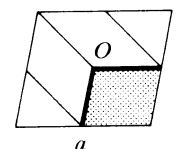
Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

4	<i>c</i>	1	(1) <i>x,y,z</i>	(2) \bar{x}, \bar{y}, z
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2	<i>b</i>	2	$\frac{1}{2}, 0, z$
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2	<i>a</i>	2	$0, 0, z$
---	----------	---	-----------



Reflection conditions

General:

hkl: $k + l = 2n$
hk0: $k = 2n$
0kl: $k + l = 2n$
h0l: $l = 2n$
00l: $l = 2n$
0k0: $k = 2n$

Special: no extra conditions

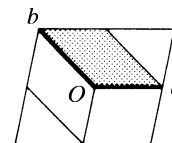
B112UNIQUE AXIS c , CELL CHOICE 2**Origin** on 2**Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},0,\frac{1}{2}) +$

4	c	1	(1) x,y,z	(2) \bar{x},\bar{y},z
---	-----	---	-------------	-------------------------

2	b	2	$\frac{1}{2},\frac{1}{2},z$
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2	a	2	$0,0,z$
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Reflection conditions

General:

$hkl: h+l=2n$

$hk0: h=2n$

$0kl: l=2n$

$h0l: h+l=2n$

$00l: l=2n$

$h00: h=2n$

Special: no extra conditions

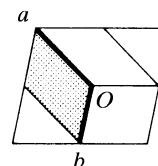
I112UNIQUE AXIS c , CELL CHOICE 3**Origin** on 2**Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$

4	c	1	(1) x,y,z	(2) \bar{x},\bar{y},z
---	-----	---	-------------	-------------------------

2	b	2	$0,\frac{1}{2},z$
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2	a	2	$0,0,z$
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Reflection conditions

General:

$hkl: h+k+l=2n$

$hk0: h+k=2n$

$0kl: k+l=2n$

$h0l: h+l=2n$

$00l: l=2n$

$h00: h=2n$

$0k0: k=2n$

Special: no extra conditions