

$C2$

$C_2^3$

2

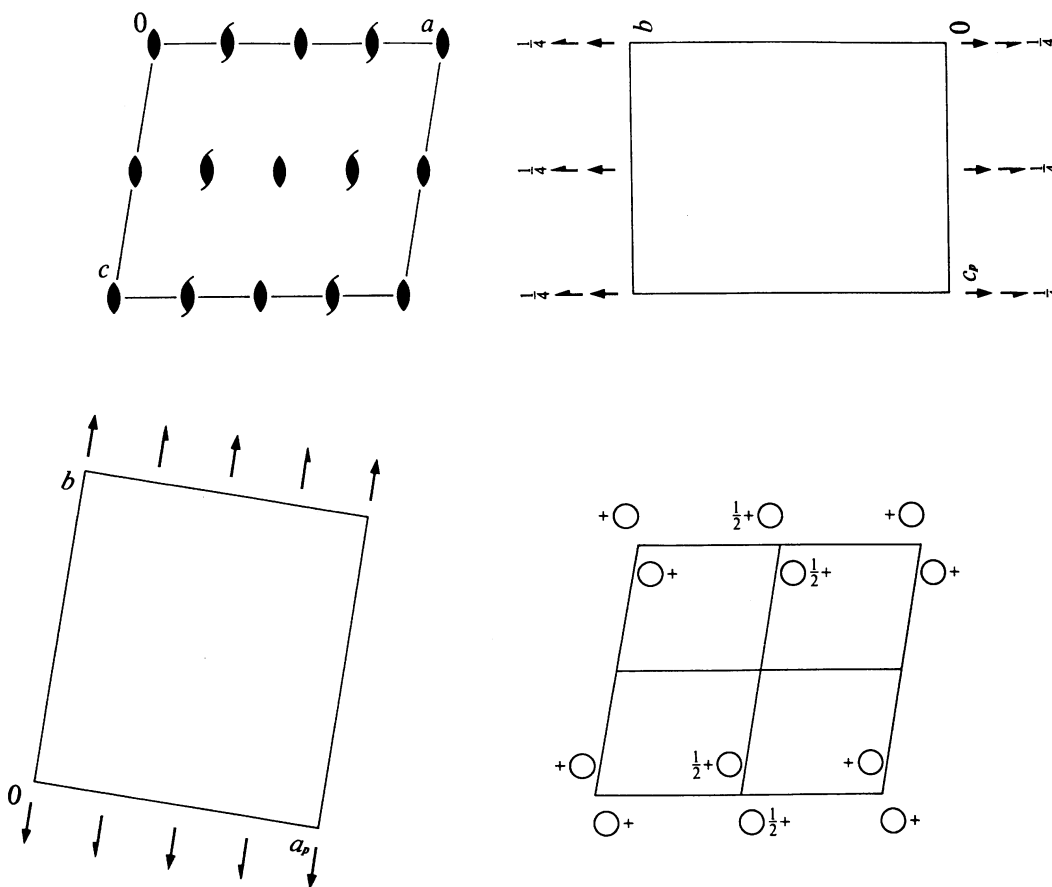
Monoclinic

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	Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$	General:
4	<i>c</i> 1	(1) $x,y,z$ (2) $\bar{x},y,\bar{z}$	$hkl : h+k=2n$ $h0l : h=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$
			Special: no extra conditions
2	<i>b</i> 2	$0,y,\frac{1}{2}$	
2	<i>a</i> 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  $0,y,0$

**Maximal non-isomorphic subgroups**

- I** [2]  $C1(P1, 1)$  1+
- IIa** [2]  $P12_11(P2_1, 4)$  1;  $2 + (\frac{1}{2}, \frac{1}{2}, 0)$   
[2]  $P121(P2, 3)$  1; 2
- IIb** none

**Maximal isomorphic subgroups of lowest index**

- IIc** [2]  $C121(\mathbf{c}' = 2\mathbf{c}$  or  $\mathbf{a}' = \mathbf{a} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$ ; [3]  $C121(\mathbf{b}' = 3\mathbf{b})(C2, 5)$

**Minimal non-isomorphic supergroups**

- I** [2]  $C2/m(12)$ ; [2]  $C2/c(15)$ ; [2]  $C222_1(20)$ ; [2]  $C222(21)$ ; [2]  $F222(22)$ ; [2]  $I222(23)$ ; [2]  $I2_12_1(24)$ ; [2]  $Amm2(38)$ ;  
[2]  $Aem2(39)$ ; [2]  $Ama2(40)$ ; [2]  $Aea2(41)$ ; [2]  $Fmm2(42)$ ; [2]  $Fdd2(43)$ ; [2]  $Imm2(44)$ ; [2]  $Iba2(45)$ ; [2]  $Ima2(46)$ ;  
[2]  $I4(79)$ ; [2]  $I4_1(80)$ ; [2]  $I\bar{4}(82)$ ; [3]  $P312(149)$ ; [3]  $P321(150)$ ; [3]  $P3_112(151)$ ; [3]  $P3_121(152)$ ; [3]  $P3_212(153)$ ;  
[3]  $P3_221(154)$ ; [3]  $R32(155)$
- II** [2]  $P121(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b})(P2, 3)$

$C_2$

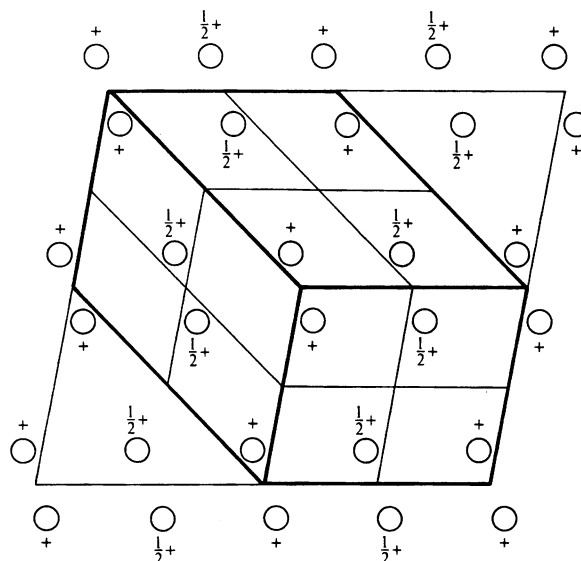
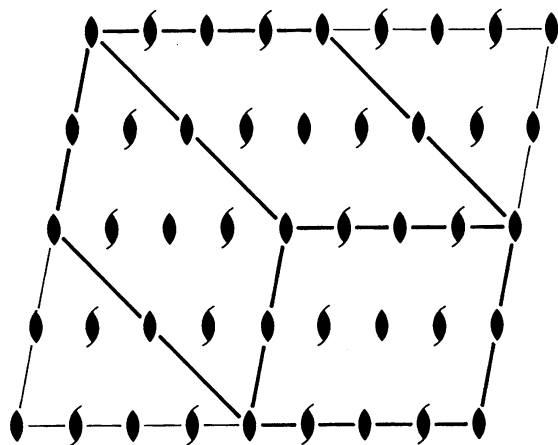
$C_2^3$

2

Monoclinic

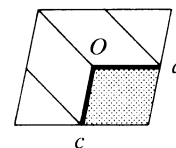
No. 5

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES



$C_{121}$

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

2	$b$	2	$0, y, \frac{1}{2}$
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2	$a$	2	$0, y, 0$
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## 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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## 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)

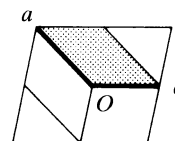
## Positions

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) $\bar{x},y,\bar{z}$
---	-----	---	-------------	-------------------------

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:

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

$$h0l : l = 2n$$

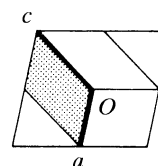
$$0kl : k + l = 2n$$

$$hk0 : k = 2n$$

$$0k0 : k = 2n$$

$$00l : l = 2n$$

Special: no extra conditions



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

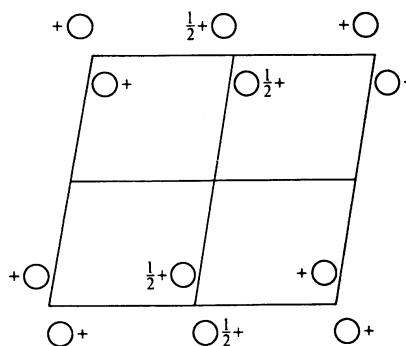
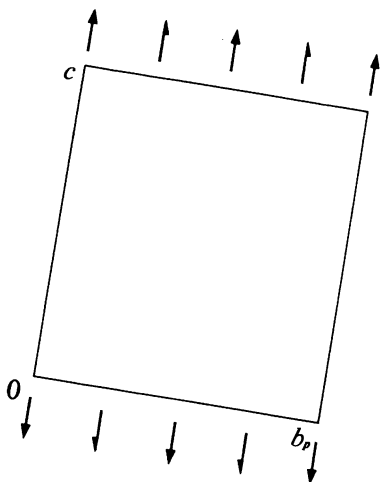
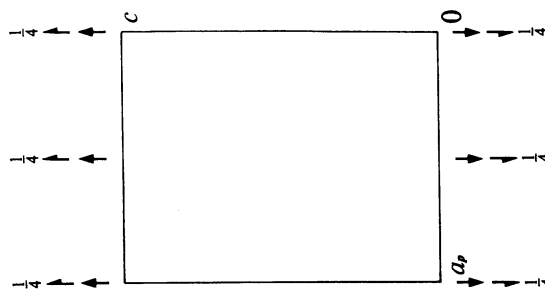
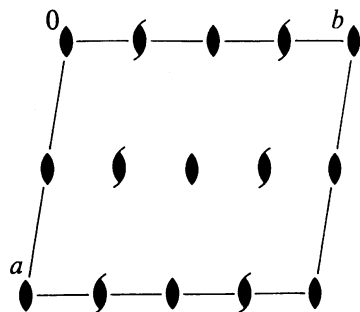
Monoclinic

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

**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

Reflection conditions

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

General:

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

$hkl : k+l=2n$

$hk0 : k=2n$

$0kl : k+l=2n$

$h0l : l=2n$

$00l : l=2n$

$0k0 : k=2n$

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  $0,y,0$

**Maximal non-isomorphic subgroups**

**I** [2]  $A1 (P1, 1)$  1+

**IIa** [2]  $P112_1 (P2_1, 4)$  1;  $2 + (0, \frac{1}{2}, \frac{1}{2})$

[2]  $P112 (P2, 3)$  1; 2

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $A112 (\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}) (C2, 5)$ ; [3]  $A112 (\mathbf{c}' = 3\mathbf{c}) (C2, 5)$

**Minimal non-isomorphic supergroups**

**I** [2]  $C2/m (12)$ ; [2]  $C2/c (15)$ ; [2]  $C222_1 (20)$ ; [2]  $C222 (21)$ ; [2]  $F222 (22)$ ; [2]  $I222 (23)$ ; [2]  $I2_12_1 (24)$ ; [2]  $Amm2 (38)$ ;  
[2]  $Aem2 (39)$ ; [2]  $Ama2 (40)$ ; [2]  $Aea2 (41)$ ; [2]  $Fmm2 (42)$ ; [2]  $Fdd2 (43)$ ; [2]  $Imm2 (44)$ ; [2]  $Iba2 (45)$ ; [2]  $Ima2 (46)$ ;  
[2]  $I4 (79)$ ; [2]  $I4_1 (80)$ ; [2]  $I\bar{4} (82)$ ; [3]  $P312 (149)$ ; [3]  $P321 (150)$ ; [3]  $P3_112 (151)$ ; [3]  $P3_21 (152)$ ; [3]  $P3_212 (153)$ ;  
[3]  $P3_221 (154)$ ; [3]  $R32 (155)$

**II** [2]  $P112 (\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2, 3)$

$C_2$

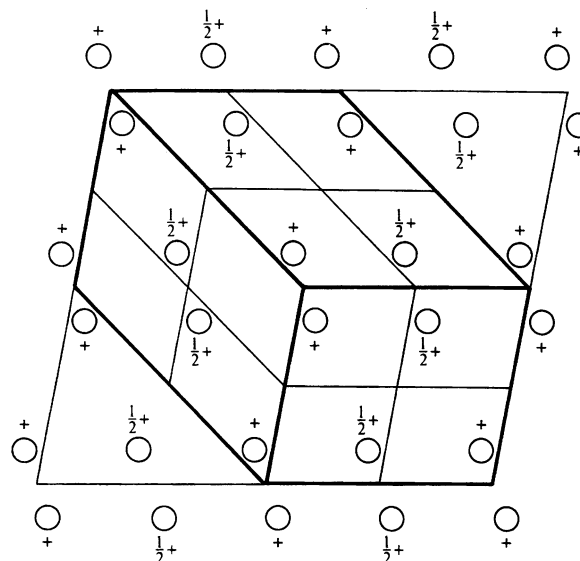
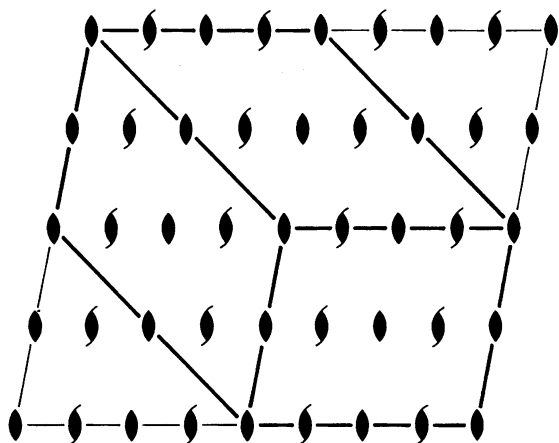
$C_2^3$

2

Monoclinic

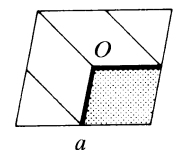
No. 5

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

2	$b$	2	$\frac{1}{2}, 0, z$
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2	$a$	2	$0, 0, z$
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**B112**UNIQUE 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) $\bar{x},\bar{y},z$
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2	$b$	2	$\frac{1}{2},\frac{1}{2},z$
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2	$a$	2	$0,0,z$
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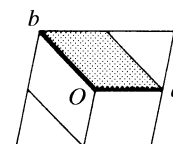
**I112**UNIQUE AXIS  $c$ , CELL CHOICE 3**Origin** on 2**Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ ; (2)**Positions**

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) $\bar{x},\bar{y},z$
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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:

$hkl : h + l = 2n$

$hk0 : h = 2n$

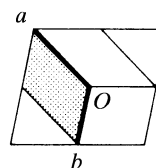
$0kl : l = 2n$

$h0l : h + l = 2n$

$00l : l = 2n$

$h00 : h = 2n$

Special: no extra conditions



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