

$p112/a$

$2/m$

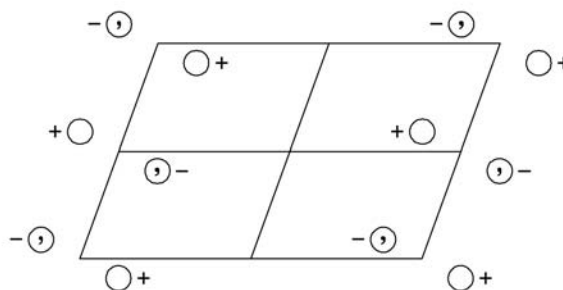
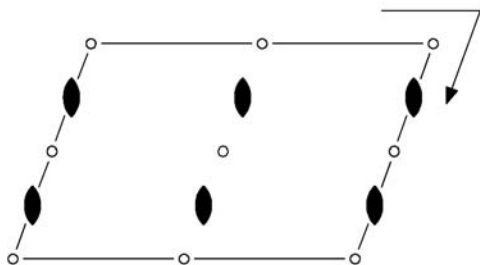
Monoclinic/Oblique

No. 7

$p112/a$

Patterson symmetry  $p112/m$

CELL CHOICE 1



Origin at  $\bar{1}$  on glide plane  $a$

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

Symmetry operations

- |             |                                     |                       |                             |
|-------------|-------------------------------------|-----------------------|-----------------------------|
| (1) 1       | (2) $2 \frac{1}{2}, 0, z$           | (3) $\bar{1} 0, 0, 0$ | (4) $a \ x, y, 0$           |
| (1 0, 0, 0) | (2 <sub>z</sub>  \frac{1}{2}, 0, 0) | ( $\bar{1}$  0, 0, 0) | ( $m_z$  \frac{1}{2}, 0, 0) |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3)

**Positions**

		Coordinates				Reflection conditions
Multiplicity,						General:
Wyckoff letter,						$hk$ : $h = 2n$
Site symmetry						$h0$ : $h = 2n$
4	$e$ 1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z}$	Special: no extra conditions
2	$d$ 2	$\frac{1}{4}, \frac{1}{2}, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$			
2	$c$ 2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$			
2	$b$ $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	$a$ $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$			

**Symmetry of special projections**

Along [001]  $p2$

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

Origin at  $0, 0, z$

Along [100]  $\neq 2mm$

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

Origin at  $x, 0, 0$

Along [010]  $\neq 2mg$

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

Origin at  $0, y, 0$

**Maximal non-isotypic subgroups**

**I** [2]  $p11a$  (5) 1; 4

[2]  $p112$  (3) 1; 2

[2]  $p\bar{1}$  (2) 1; 3

**IIa** none

**IIb** none

**Maximal isotypic subgroups of lowest index**

**IIc** [2]  $p112/a$  ( $\mathbf{b}' = 2\mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}$ ) (7)

**Minimal non-isotypic supergroups**

**I** [2]  $pmaa$  (38); [2]  $pban$  (39); [2]  $pmma$  (41); [2]  $pman$  (42); [2]  $pbaa$  (43); [2]  $pbma$  (45); [2]  $pmmn$  (46); [2]  $cmme$  (48); [2]  $p4/n$  (52)

**II** [2]  $p112/m$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) (6)

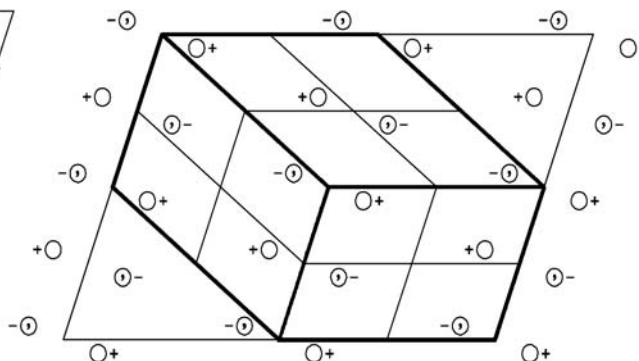
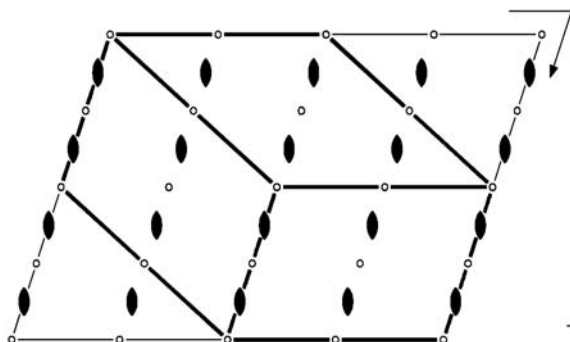
$p112/a$

$2/m$

Monoclinic/Oblique

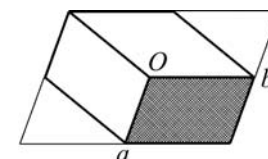
No. 7

DIFFERENT CELL CHOICES



$p112/a$

CELL CHOICE 1



Origin at  $\bar{1}$  on glide plane  $a$

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

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3)

Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

General:

$hk: h = 2n$

$h0: h = 2n$

Special: no extra conditions

4	<i>e</i>	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z}$
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2	<i>d</i>	2	$\frac{1}{4}, \frac{1}{2}, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$
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2	<i>c</i>	2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$
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2	<i>b</i>	$\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$
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2	<i>a</i>	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$
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$p112/n$ 

## CELL CHOICE 2

Origin at  $\bar{1}$  on glide plane  $n$ Asymmetric unit  $0 \leq x \leq \frac{1}{4}$ ;  $0 \leq y \leq 1$ ;  $0 \leq z$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Coordinates	Coordinates	Coordinates
4 $e$ 1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$
2 $d$ 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$		
2 $c$ 2	$\frac{3}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$		
2 $b$ $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$		
2 $a$ $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$		

 $p112/b$ 

## CELL CHOICE 3

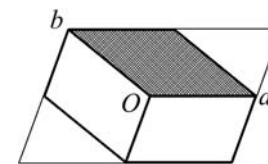
Origin at  $\bar{1}$  on glide plane  $b$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Coordinates	Coordinates	Coordinates
4 $e$ 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, y + \frac{1}{2}, \bar{z}$
2 $d$ 2	$\frac{1}{2}, \frac{3}{4}, z$	$\frac{1}{2}, \frac{1}{4}, \bar{z}$		
2 $c$ 2	$0, \frac{1}{4}, z$	$0, \frac{3}{4}, \bar{z}$		
2 $b$ $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$		
2 $a$ $\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, 0$		



Reflection conditions

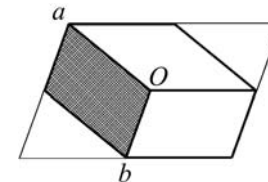
General:

$hk: h + k = 2n$

$h0: h = 2n$

$0k: k = 2n$

Special: no extra conditions



Reflection conditions

General:

$hk: k = 2n$

$0k: k = 2n$

Special: no extra conditions