

$P2_1/c$

C_{2h}^5

$2/m$

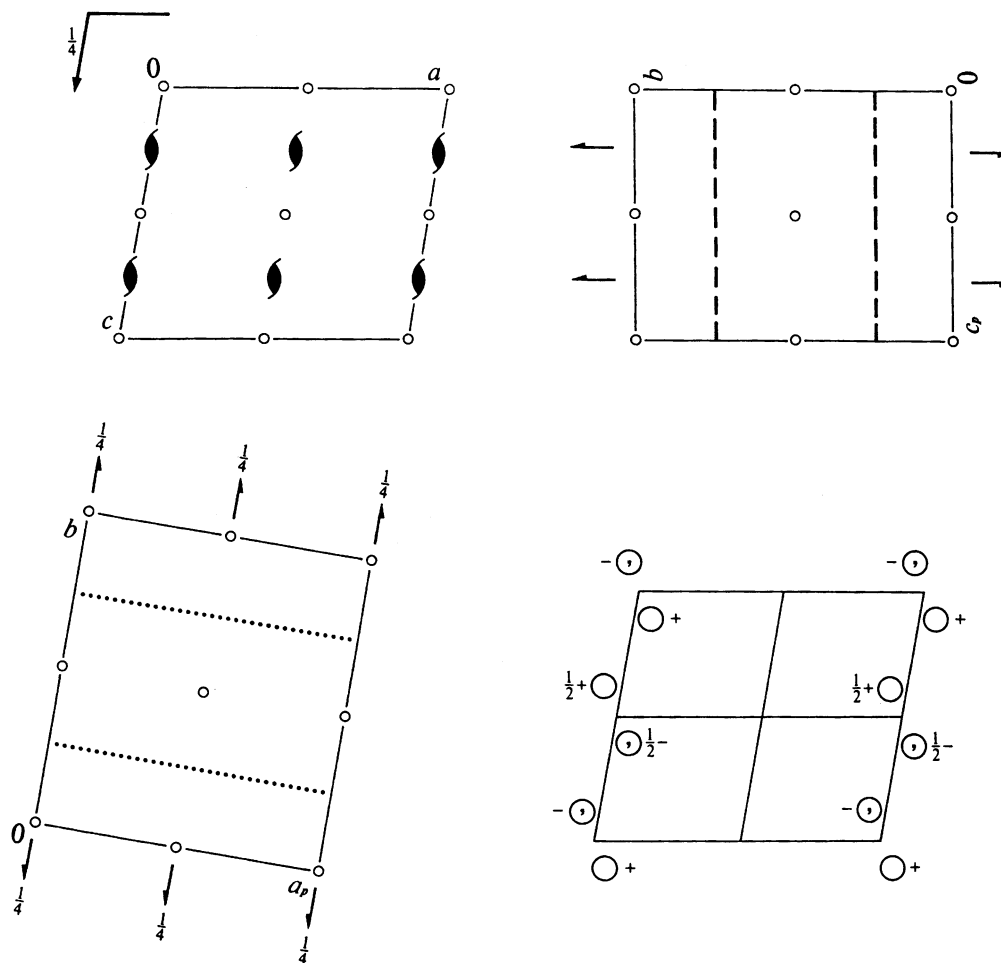
Monoclinic

No. 14

$P12_1/c1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ (3) $\bar{1}$ $0, 0, 0$ (4) c $x, \frac{1}{4}, z$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) x, y, z	(2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	General: $h0l: l = 2n$ $0k0: k = 2n$ $00l: l = 2n$ Special: as above, plus $hkl: k + l = 2n$ $hkl: k + l = 2n$ $hkl: k + l = 2n$ $hkl: k + l = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
2 <i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$			
2 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

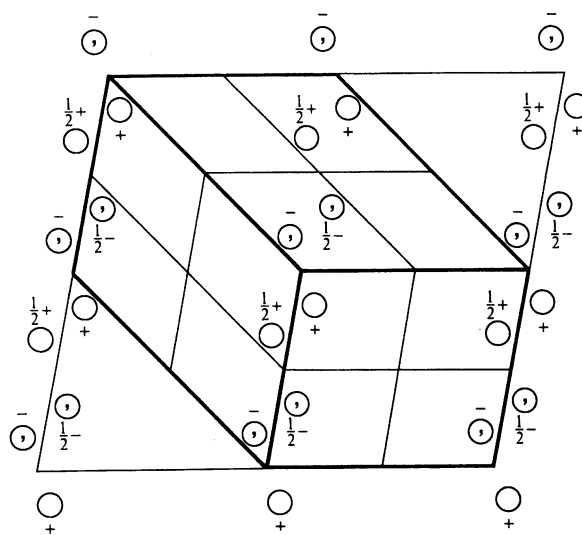
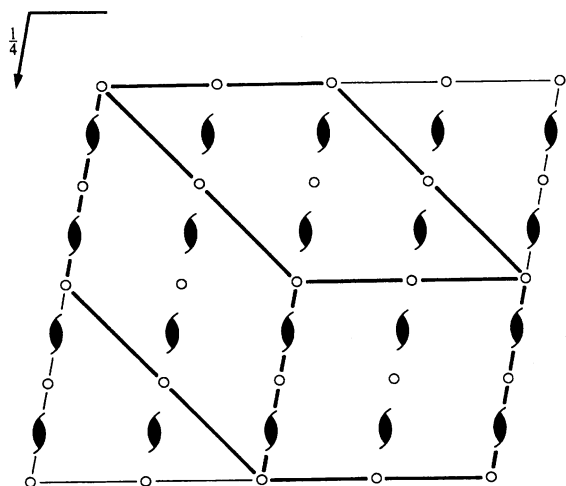
Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x, 0, 0$

Along [010] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

$P2_1/c$ C_{2h}^5 $2/m$

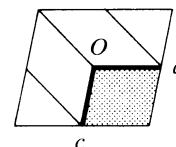
Monoclinic

No. 14

UNIQUE AXIS b , DIFFERENT CELL CHOICES $P12_1/c1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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



Reflection conditions

General:

 $h0l: l = 2n$ $0k0: k = 2n$ $00l: l = 2n$

Special: as above, plus

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

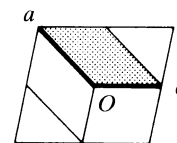
$P12_1/n1$ UNIQUE AXIS b , CELL CHOICE 2Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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



Reflection conditions

General:

$$\begin{aligned} h0l: h+l &= 2n \\ 0k0: k &= 2n \\ h00: h &= 2n \\ 00l: l &= 2n \end{aligned}$$

Special: as above, plus

$$\begin{aligned} hkl: h+k+l &= 2n \\ hkl: h+k+l &= 2n \\ hkl: h+k+l &= 2n \\ hkl: h+k+l &= 2n \end{aligned}$$

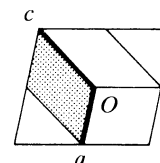
 $P12_1/a1$ UNIQUE AXIS b , CELL CHOICE 3Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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



Reflection conditions

General:

$$\begin{aligned} h0l: h &= 2n \\ 0k0: k &= 2n \\ h00: h &= 2n \end{aligned}$$

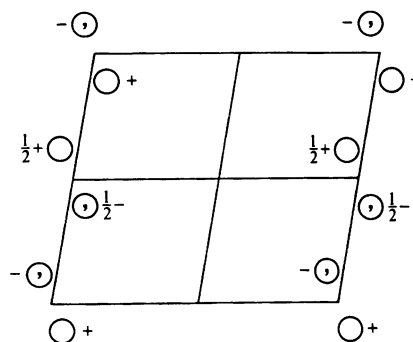
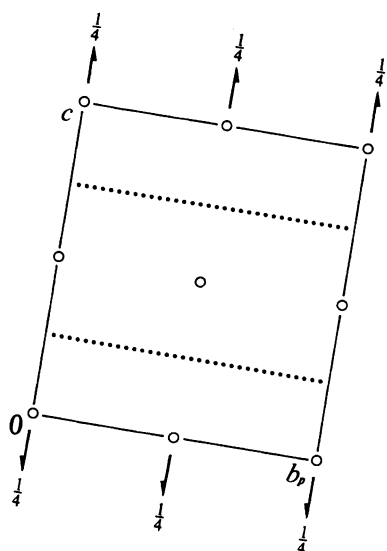
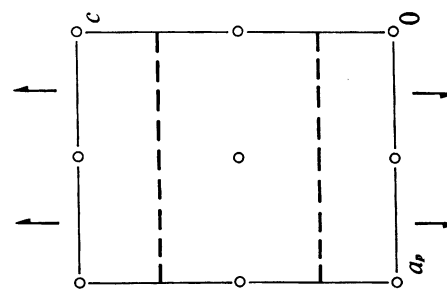
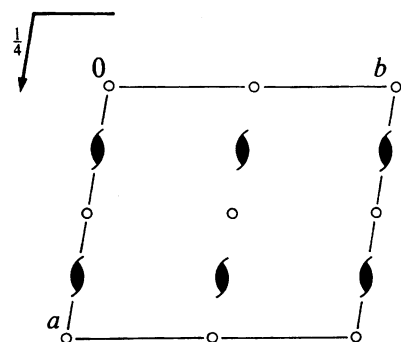
Special: as above, plus

$$\begin{aligned} hkl: h+k &= 2n \\ hkl: h+k &= 2n \\ hkl: h+k &= 2n \\ hkl: h+k &= 2n \end{aligned}$$

$P2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

 $P112_1/a$ Patterson symmetry $P112/m$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

(1) 1 (2) $2(0, 0, \frac{1}{2}) \frac{1}{4}, 0, z$ (3) $\bar{1} 0, 0, 0$ (4) $a \ x, y, \frac{1}{4}$

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

4 e 1 (1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$

General:

$hk0: h = 2n$

$00l: l = 2n$

$h00: h = 2n$

Special: as above, plus

2 d $\bar{1}$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$

$hkl: h + l = 2n$

2 c $\bar{1}$ $\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$

$hkl: h + l = 2n$

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

$hkl: h + l = 2n$

2 a $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$

$hkl: h + l = 2n$

Symmetry of special projectionsAlong $[001]$ $p2$

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

Origin at $0, 0, z$ Along $[100]$ $p2gm$

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

Origin at $x, 0, 0$ Along $[010]$ $p2gg$

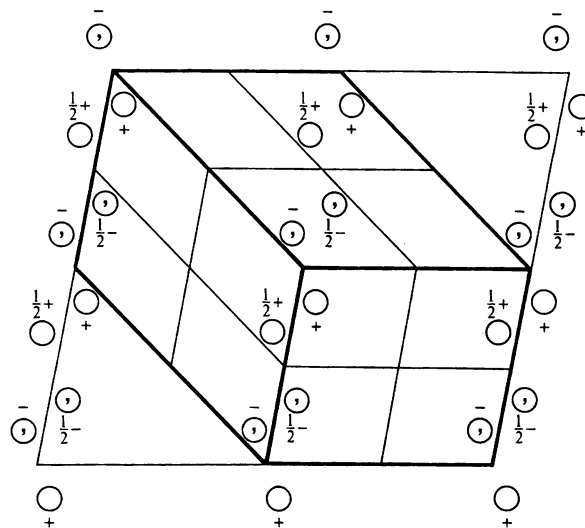
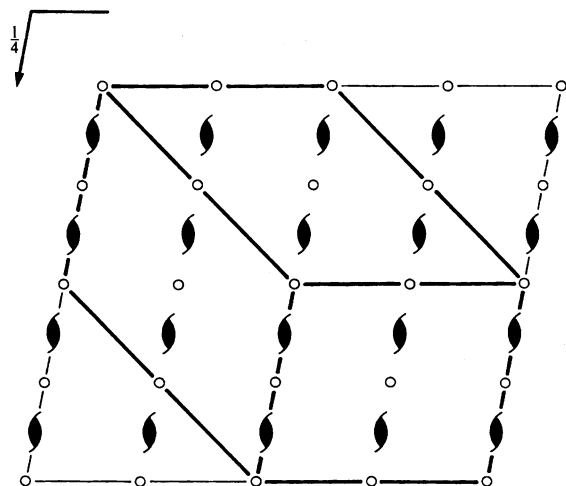
$\mathbf{a}' = \mathbf{c} \quad \mathbf{b}' = \mathbf{a}_p$

Origin at $0, y, 0$

$P2_1/c$ C_{2h}^5 $2/m$

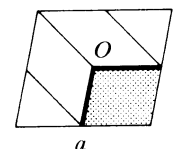
Monoclinic

No. 14

UNIQUE AXIS c , DIFFERENT CELL CHOICES $P112_1/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (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) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$
2 d $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$		
2 c $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$		
2 b $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		
2 a $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$		



Reflection conditions

General:

 $hk0: h = 2n$ $00l: l = 2n$ $h00: h = 2n$

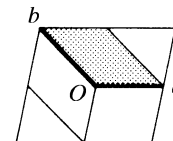
Special: as above, plus

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

$P112_1/n$ UNIQUE AXIS c , CELL CHOICE 2Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

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



Reflection conditions

General:

$hk0: h + k = 2n$

$00l: l = 2n$

$h00: h = 2n$

$0k0: k = 2n$

Special: as above, plus

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

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

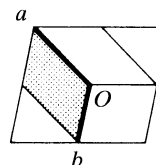
$hkl: h + k + l = 2n$

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

 $P112_1/b$ UNIQUE AXIS c , CELL CHOICE 3Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

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



Reflection conditions

General:

$hk0: k = 2n$

$00l: l = 2n$

$0k0: k = 2n$

Special: as above, plus

$hkl: k + l = 2n$

$hkl: k + l = 2n$

$hkl: k + l = 2n$

$hkl: k + l = 2n$