



# Guide

# Crystallography Miller-Bravais Indices: Hexagonal Planes and Directions

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## Summary

This guide was created to help instructors support students learning Hexagonal Miller-Bravais Indices. The goal is for students to be able to use this alongside homework assignments.

Detailed steps on how to draw and label directions and planes are included with two different example for each.

This method of identifying and drawing planes and directions is also covered in the Lecture from the Crystallography Teaching Package.

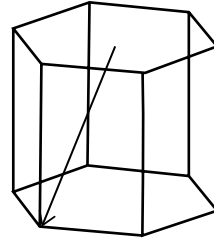
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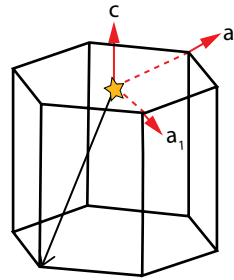
## 1. How to Label Directions

### 1.1 Example 1

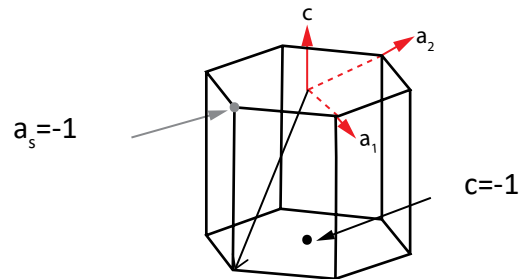
Direction of Interest:



1. Identify the origin of the direction and label origin and axis accordingly



2. Identify intercept coordinates



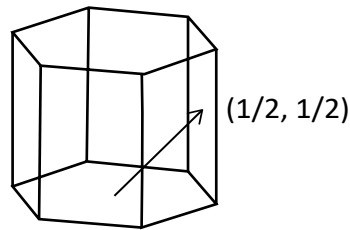
3. Convert  $a_1$ ,  $a_2$ , and  $c$  coordinates to a four coordinate system using the equations below  $[UVW] \rightarrow [u'v't'w']$

4. Label direction with appropriate notation

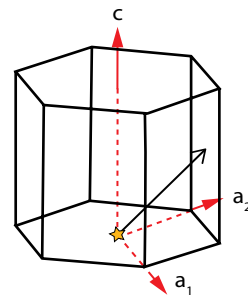
$[11\bar{2}]$

## 1.2 Example 2

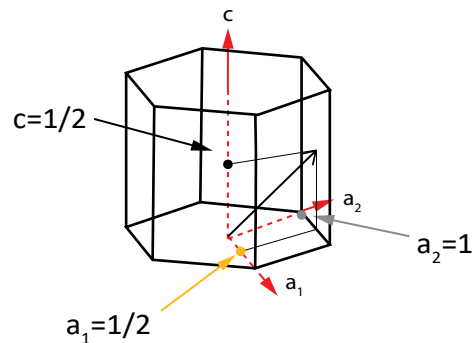
Direction of Interest:



1. Identify the origin of the direction and label origin and axis accordingly



2. Identify intercept coordinates



3. Convert  $a_1$ ,  $a_2$ , and  $c$  coordinates to a four coordinate system using the equations below  
[UVW] → [u'v't'w']

$$\begin{aligned} u' &= (1/3) * (2U - V) \\ v' &= (1/3) * (2V - U) \\ t' &= -(u' + v') \\ w' &= W \end{aligned}$$

$$u' = (1/3) * (2(1/2) - (1)) = 0$$

$$v' = (1/3) * (2(1) - (1/2)) = 1/2$$

$$t' = -(u' + v') = -((0) + (1/2)) = -(1/2) = -1/2$$

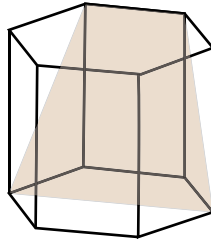
$$w' = 1/2$$

4. Reduce fractions and Label direction with appropriate notation

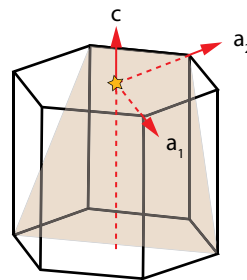
$$2 \times \begin{pmatrix} u' & v' & t' & w' \\ 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \rightarrow \boxed{[01\bar{1}1]}$$

## 2. How to Label Planes (3-axis)

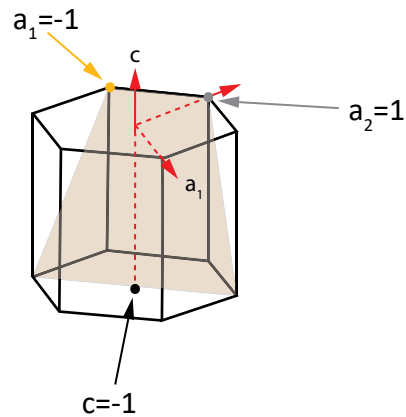
Plane of Interest:



1. Choose origin and label axis. \*Note: plane cannot pass through the origin



2. Identify intercept for each axis



3. Use the following equations to get the indices (hkl). Reduce fractions as necessary

$$h = \frac{1}{a_1} \quad k = \frac{1}{a_2} \quad i = -(h+k) \quad l = \frac{1}{c}$$

$$h = 1/-1 = -1$$

$$k = 1/1 = 1$$

$$i = -(-1+1) = 0$$

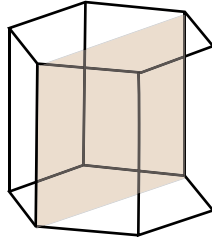
$$l = 1/-1 = -1$$

4. Label plane with appropriate notation

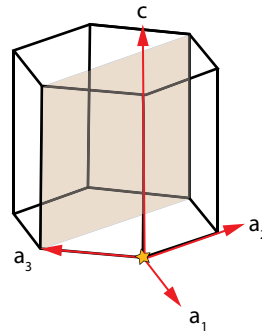
$$(\bar{1}10\bar{1})$$

### 3. How to Label Planes (4-axis)

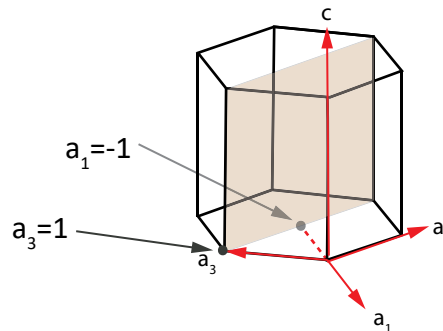
Plane of Interest:



1. Choose origin and label axis. \*Note: plane cannot pass through the origin



2. Identify intercept for each axis



3. Take reciprocals of intercepts to get indices (hkl)

$$h = \frac{1}{a_1} = \frac{1}{-1} = -1$$

$$k = \frac{1}{a_2} = \frac{1}{\infty} = 0$$

$$i = \frac{1}{a_3} = \frac{1}{1} = 1$$

$$l = \frac{1}{c} = \frac{1}{\infty} = 0$$

4. Label plane with appropriate notation

$(\bar{1}010)$

## 4. How to Draw Directions

### 4.1 Example 1

Direction of Interest:  $[011\bar{2}]$

1. Transform 4-axis coordinates to 3-axis.

Reduce as necessary

$[u'v't'w'] \rightarrow [UVW]$

$$U = 2u' + v'$$

$$V = 2v' + u'$$

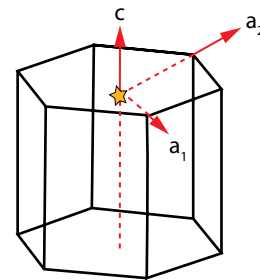
$$W = w'$$

$$U = 2(0) + (1) = 1 \rightarrow \frac{1}{2}$$

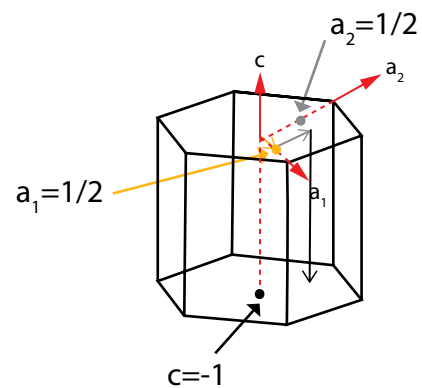
$$[011\bar{2}] \rightarrow V = 2(1) + (0) = 2 \rightarrow 1$$

$$W = -2 \rightarrow -1$$

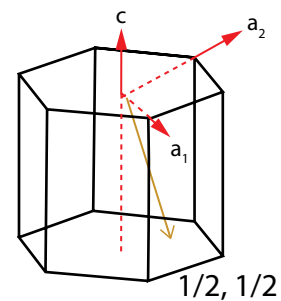
2. Choose origin and label axis on unit cell based on the sign of the U,V,W coordinates (which correspond to  $a_1$ ,  $a_2$ , and c) from Step 1



3. Note coordinates on unit cell and trace to find the end point of the direction



4. Draw direction from origin to end point from Step 3



## 4.2 Example 2

Direction of Interest:  $[1\bar{1}00]$

1. Transform 4-axis coordinates to 3-axis.

Reduce as necessary

$[u'v't'w'] \rightarrow [UVW]$

$$U = 2u' + v'$$

$$V = 2v' + u'$$

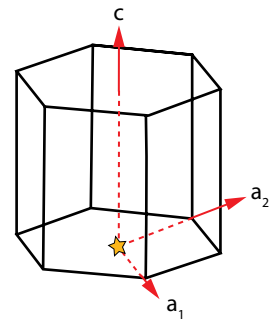
$$W = w'$$

$$U = 2(1) + (-1) = 1$$

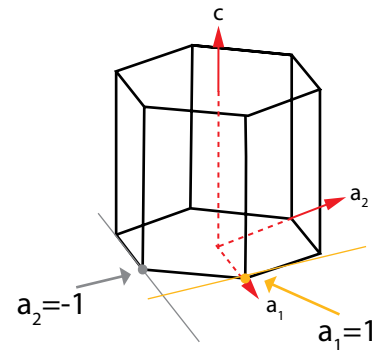
$$[1\bar{1}00] \rightarrow V = 2(-1) + (1) = -1$$

$$W = 0$$

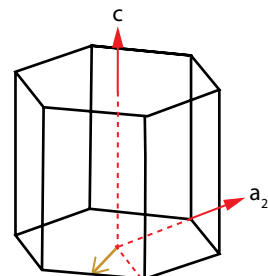
2. Choose origin and label axis on unit cell based on the sign of the U,V,W coordinates (which correspond to  $a_1$ ,  $a_2$ , and c) from Step 1



3. Note coordinates on unit cell and trace to find the end point of the direction



4. Draw direction from origin to end point from Step 3





## 5. How to Draw Planes

### 5.1 Example 1

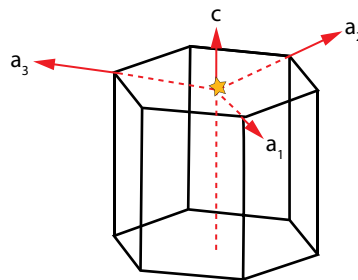
Plane of Interest:  $(11\bar{2}0)$

1. Take the reciprocal of each index to find the intercepts. \*Note that infinity means the plane is parallel to the axis

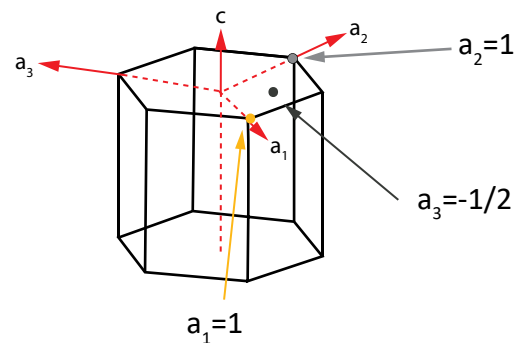
$$\begin{aligned} a_1 &= \frac{1}{1} = 1 \\ a_2 &= \frac{1}{1} = 1 \\ a_3 &= \frac{1}{-2} = -1/2 \\ c &= \frac{1}{0} = \infty \end{aligned}$$

$(11\bar{2}0) \rightarrow$

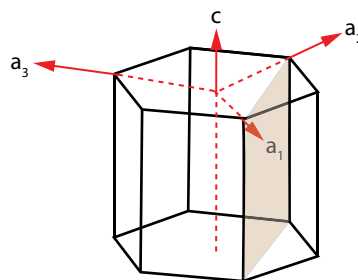
2. Choose origin and label axis based on intercepts and shape. \*Note: plane cannot pass through the origin



3. Mark intercepts for all four points



4. Draw plane



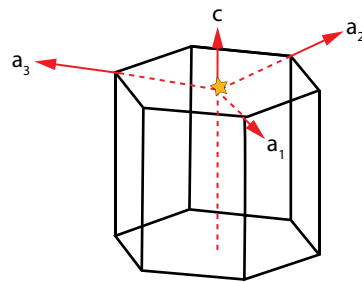
## 5.2 Example 2

*Plane of Interest:  $(11\bar{2}0)$*

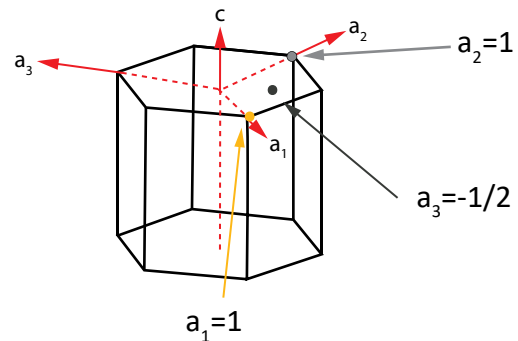
1. Take the reciprocal of each index to find the intercepts. \*Note that infinity means the plane is parallel to the axis

$$\begin{aligned} a_1 &= \frac{1}{1} = 1 \\ a_2 &= \frac{1}{1} = 1 \\ a_3 &= \frac{1}{-2} = -1/2 \\ c &= \frac{1}{0} = \infty \end{aligned} \quad (11\bar{2}0) \rightarrow$$

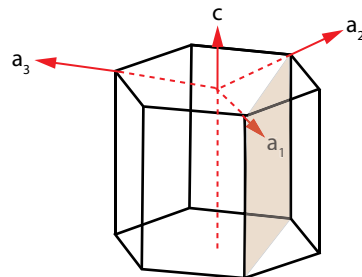
2. Choose origin and label axis based on intercepts and shape. \*Note: plane cannot pass through the origin



3. Mark intercepts for all four points



4. Draw plane



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