# Week 9

EBS 209

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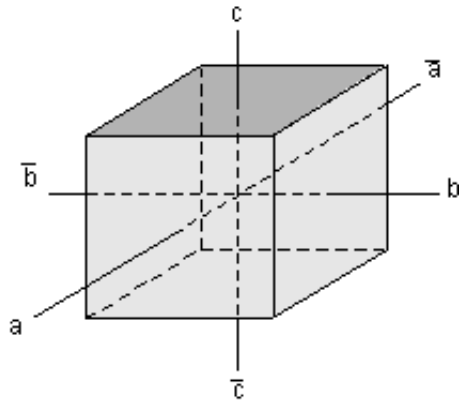
# Intercepts of Crystal Faces (Weiss Parameters)

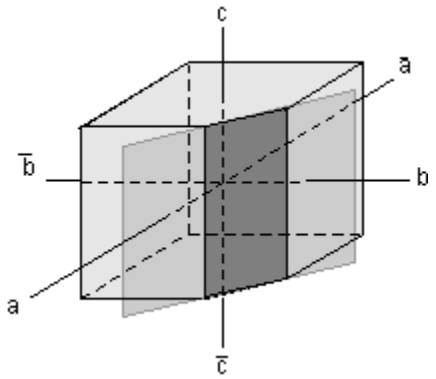
# Intercepts of Crystal Faces (Weiss Parameters)

A crystal face intersects only one of the crystallographic axes.

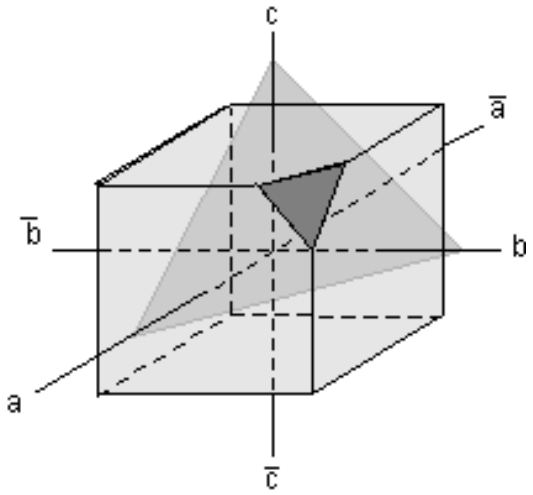
If we assume that the face intercepts the c axis at a distance of 1 unit length, then the intercepts, sometimes called Weiss Parameters, are:

**∞a, ∞b, 1c**




A crystal face intersects two of the crystallographic axes. the parameters for this face are: **1 a, 1 b, ∞c**




A crystal face that intersects all 3 axes.

Thus, the parameters in this example would be:

**1a, 1b, 1c**

Two very important points about intercepts of faces:

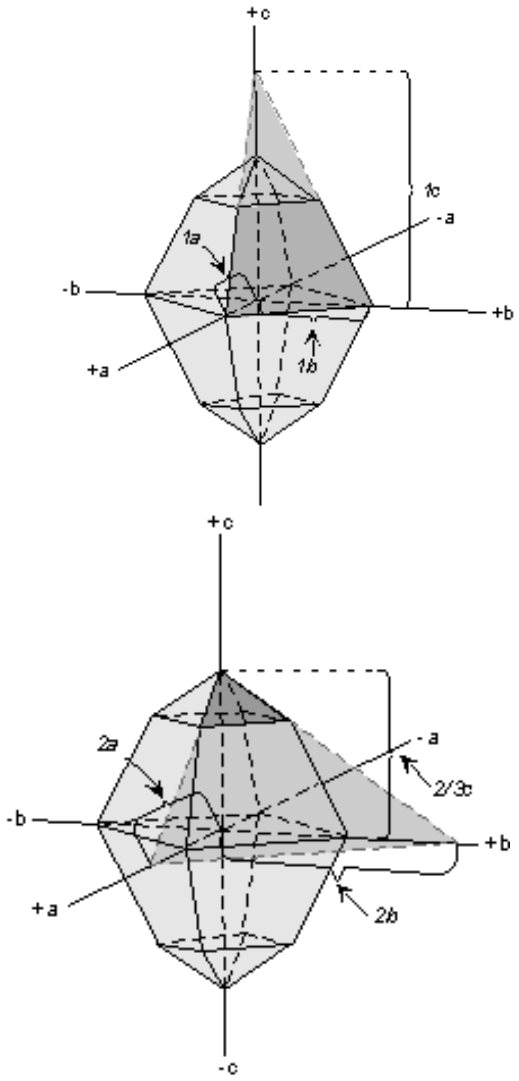
- **The intercepts or parameters are relative values, and do not indicate any actual cutting lengths.**
- **Since they are relative, a face can be moved parallel to itself without changing its relative intercepts or parameters**.

Because one does usually not know the dimensions of the unit cell, it is difficult to know what number to give the intercept of a face, unless one face is chosen arbitrarily to have intercepts of 1.

Thus, the convention is to assign the **largest face that intersects all 3 crystallographic axes the parameters - 1a, 1b, 1c. This face is called the *unit face.***

The orthorhombic crystal shown here, the large dark shaded face is the largest face that cuts all three axes. It is the unit face, and is therefore assigned the parameters 1a, 1b, 1c.

- Once the unit face is defined, the intercepts of the smaller face can be determined.
- These are 2a, 2b, 2/3c. Note that we can divide these parameters by the common factor 2, resulting in 1a,1b,1/3c.
- Again, this illustrates the point that moving a face parallel to itself does not change the relative intercepts.
- Since intercepts or parameters are relative, they do not represent the actual cutting lengths on the axes.
- By specifying the intercepts or parameters of a crystal face, we now have a way to uniquely identify each face of a crystal. But, the notation is cumbersome, so crystallographers have developed another way of identifying or indexing faces.

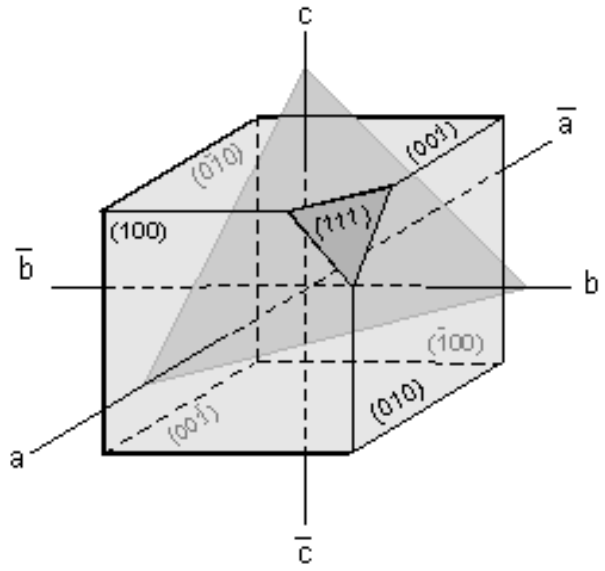


# Miller Indices

# Miller Indices

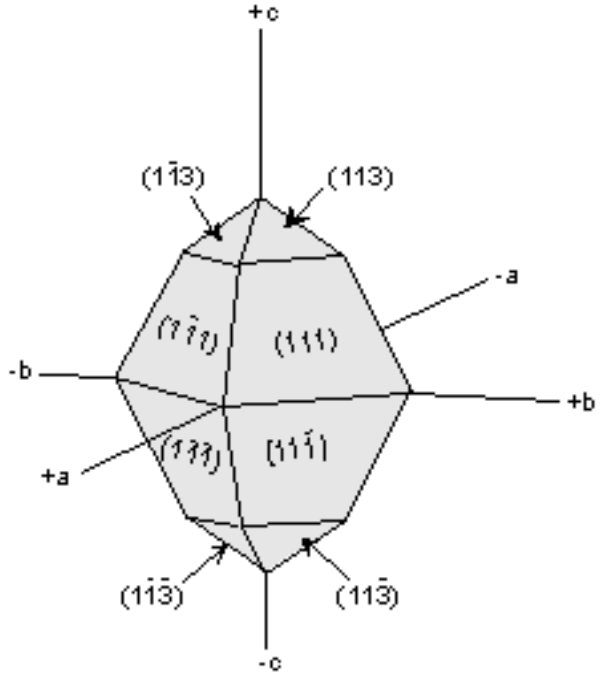
- The Miller Index for a crystal face is found by
  - first determining the parameters
  - second inverting the parameters, and
  - third clearing the fractions.
- For example, if the face has the parameters 1 a, 1 b, ∞ c
- inverting the parameters would be 1/1, 1/1, 1/ ∞
- this would become 1, 1, 0

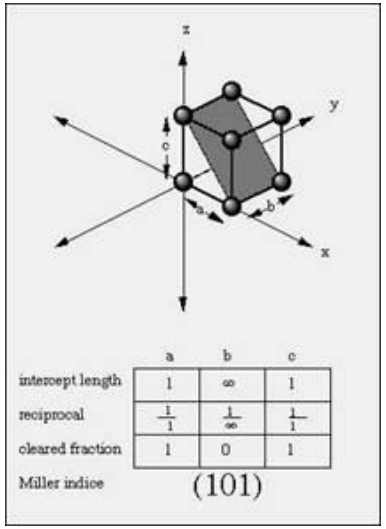
  the Miller Index is written inside parentheses with no commas - thus (110)



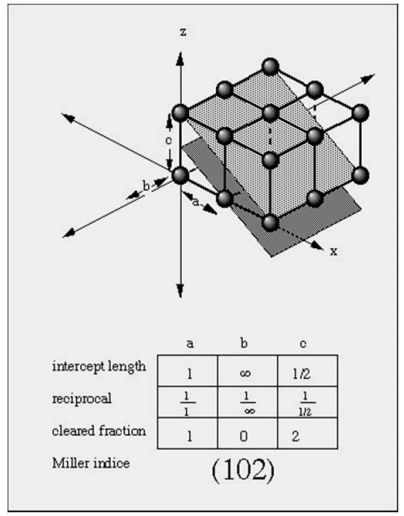

The face [labeled (111)] that cuts all three axes at 1 unit length has the parameters 1a, 1b,
1c. Inverting these, results in 1/1, 1/1, 1/1 to give the Miller Index (111).

Recall that the small triangular face near the top that cuts all three axes had the parameters 1a, 1b, 1/3c. Inverting these becomes 1/1, 1/1, 3/1 to give the Miller Index for this face as (113).

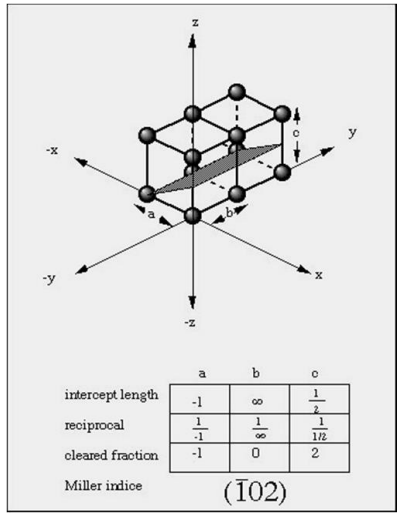




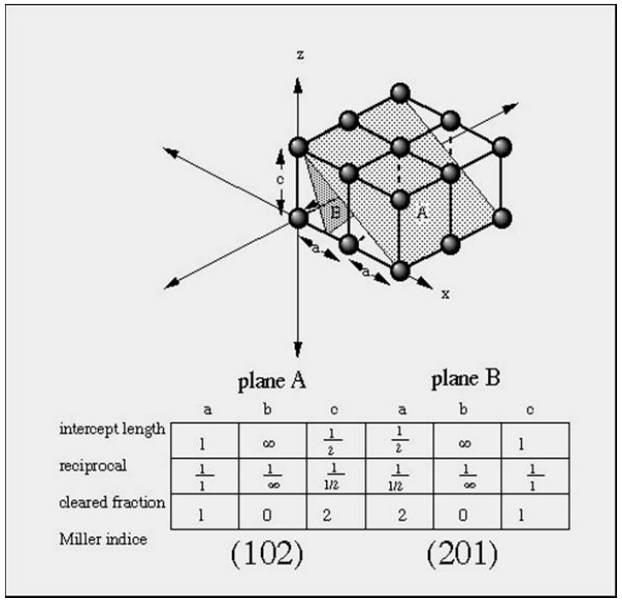

| | a | b | c |
|---|---|---|---|
| intercept length | 1 | ∞ | 1 |
| reciprocal | 1/1 | 1/∞ | 1/1 |
| cleared fraction | 1 | 0 | 1 |
| Miller indice | (101) | | |




| | a | b | c |
|---|---|---|---|
| intercept length | 1 | ∞ | 1/2 |
| reciprocal | 1/1 | 1/∞ | 1/1/2 |
| cleared fraction | 1 | 0 | 2 |
| Miller indice | (102) | | |




| | a | b | c |
|---|---|---|---|
| intercept length | -1 | ∞ | 1/2 |
| reciprocal | 1/-1 | 1/∞ | 1/1/2 |
| cleared fraction | -1 | 0 | 2 |
| Miller indice | (1̄02) | | |




| | plane A | | | plane B | | |
|---|---|---|---|---|---|---|
| | a | b | c | a | b | c |
| intercept length | 1 | ∞ | 1/2 | 1/2 | ∞ | 1 |
| reciprocal | 1/1 | 1/∞ | 1/1/2 | 1/1/2 | 1/∞ | 1/1 |
| cleared fraction | 1 | 0 | 2 | 2 | 0 | 1 |
| Miller indice | (102) | | | (201) | | |

To refer to a general face that intersects all three crystallographic axes where the parameters are not known, we use the notation (hkl). For a face that intersects the b and c axes with general or unknown intercepts the notation would be (0kl), for a face intersecting the a and c axis, but parallel to b the notation would be (h0l), and similarly for a face intersecting the a and b axes, but parallel to c we would use the notation (hk0).

# Miller Bravais Indices

- Since the hexagonal system has three "a" axes perpendicular to the "c" axis, both the parameters of a face and the Miller Index notation must be modified.
- The modified parameters and Miller Indices must reflect the presence of an additional axis.
- This modified notation is referred to as Miller-Bravais Indices, with the general notation (hkil)

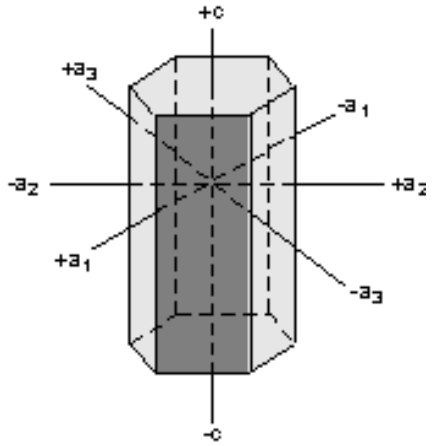
# Miller-Bravais Index

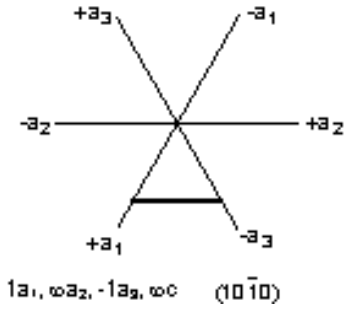
- This face intersects the positive a1 axis at 1 unit length, the negative a3 axis at 1 unit length, and does not intersect the $a_2$ or c axes. This face
- thus has the parameters:
- 1 a1, ∞ $a_2$, -1 $a_3$, ∞ c

  Inverting and clearing fractions gives the Miller-Bravais Index:
- – (10-10)

  An important rule to remember in applying this notation in the hexagonal system, is that whatever indices are determined for h, k, and i,

  $h + k + i = 0$



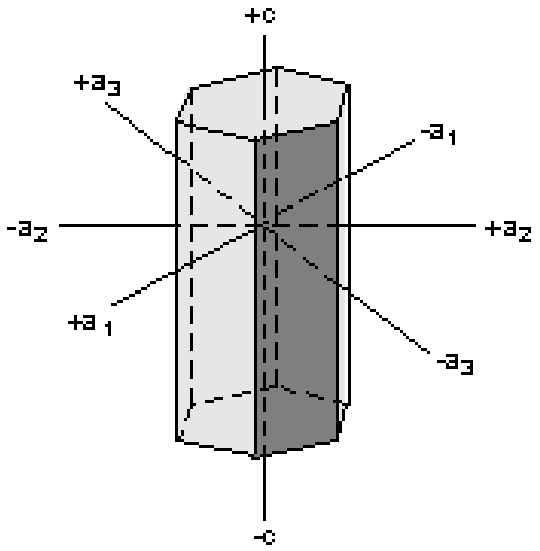
For a similar hexagonal crystal, this time with the shaded face cutting all three axes, we would find for the shaded face in the diagram that the parameters are **1 $a_1$, 1 $a_2$, -1/2 $a_3$, ∞ c.**

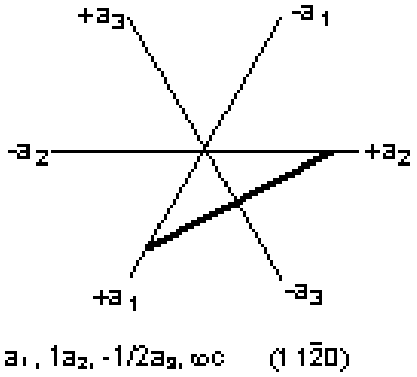
Inverting these intercepts gives:

- **1/1, 1/1, -2/1, 1/∞**

- resulting in a Miller-Bravais Index of
  - **(110)**

Note how the "**h + k + i = 0**" rule applies here!



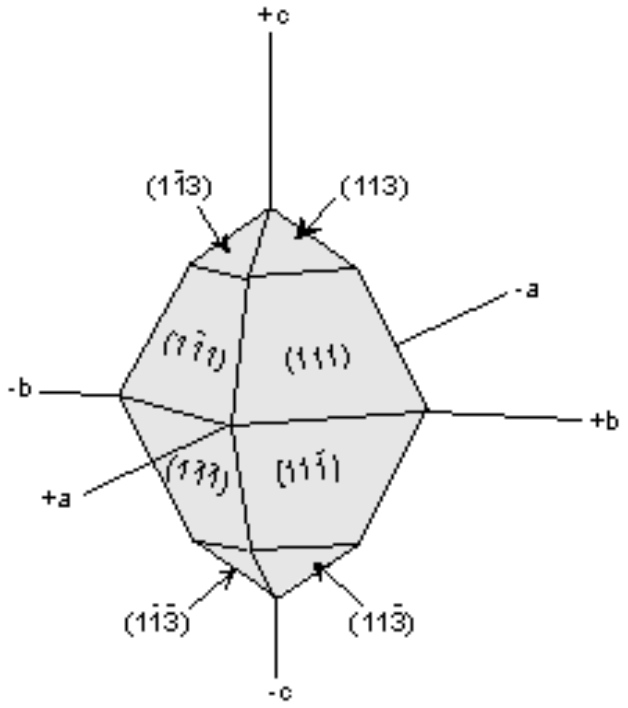
# Crystal Forms

- Although we will not cover this in detail in this lecture, the next step is to use the Miller Index notation to designate crystal forms.
- A ***crystal form*** is **a set of crystal faces that are related to each other by symmetry.**
- To designate a crystal form (which could imply many faces) we use the Miller Index, or Miller-Bravais Index notation enclosing the indices in curly braces, i.e.
  - **{hkl} or {hkil}**
- Such notation is called a ***form symbol***.

As an example, look at the crystal drawing shown here. This crystal is the same orthorhombic crystal discussed above. It has two forms.
The form {111} consists of the following symmetrically 8 related faces:
(111), (11), (11), (1), (11), (1), (1), and ().
This form is called a rhombic-dipyramid.

The other form is also a rhombic-dipyramid, but consists of the triangular shaped faces similar to the face (113).

The form symbol for this form is {113} and consists of the following 8 faces:
(113), (13), (11), (1), (13), (1), (3), and ().



# Forms, Open and Closed

**Any group of crystal faces related by the same symmetry is called a *form*. There are 47 or 48 crystal forms depending on the classification used.**

**Closed forms are those groups of faces all related by symmetry that completely enclose a volume of space. It is possible for a crystal to have entirely faces of one closed form.**

**Open forms are those groups of faces all related by symmetry that do not completely enclose a volume of space.**

**A crystal with open form faces requires additional faces as well. There are 17 or 18 open forms and 30 closed forms.**

# Crystal Form, Zones, Crystal Habit

- As stated at the end of the last lecture, the next step is to use the Miller Index notation to designate crystal forms. A ***crystal form*** is **a set of crystal faces that are related to each other by symmetry.**
- To designate a crystal form (which could imply many faces) we use the Miller Index, or Miller-Bravais Index notation enclosing the indices in curly braces, i.e.
  - {101} or {111}

# General Forms and Special Forms

- A ***general form*** is a form in a particular crystal class that contains faces that intersect all crystallographic axes at different lengths. It has the form symbol **{hkl}** All other forms that may be present are called ***special forms***.

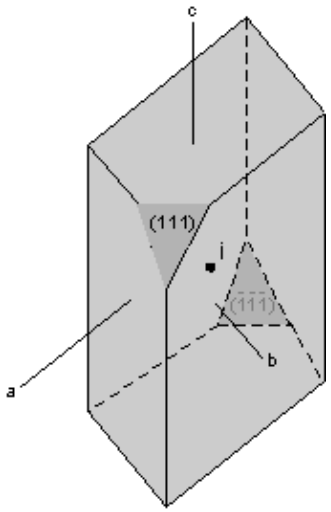
  In the monoclinic, triclinic, and orthorhombic crystal systems, the form {111} is a general form because in these systems faces of this form will intersect the a, b, and c axes at different lengths because the unit lengths are different on each axis.
- In crystals of higher symmetry, where two or more of the axes have equal length, a general form must intersect the equal length axes at different multiples of the unit length.
- Thus in the tetragonal system the form {121} is a general form. In the isometric system a general form would have to be something like {123}.

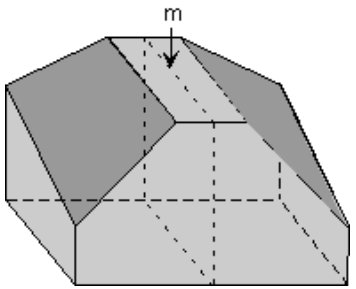
# Open Forms and Closed Forms

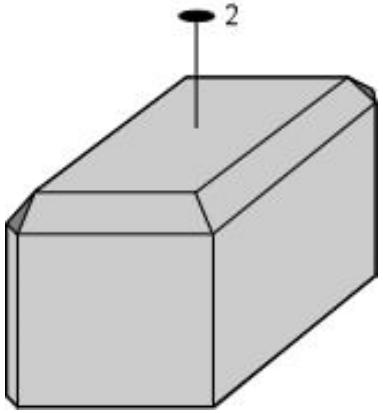
- A ***closed form*** is a set of crystal faces that completely enclose space. Thus, in crystal classes that contain closed forms, a crystal can be made up of a single form.

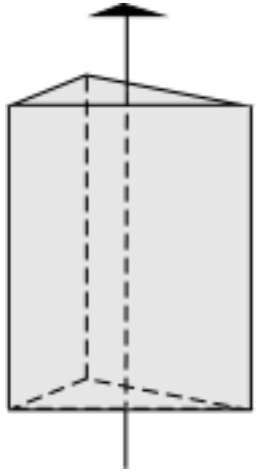
- An ***open form*** is one or more crystal faces that do not completely enclose space.

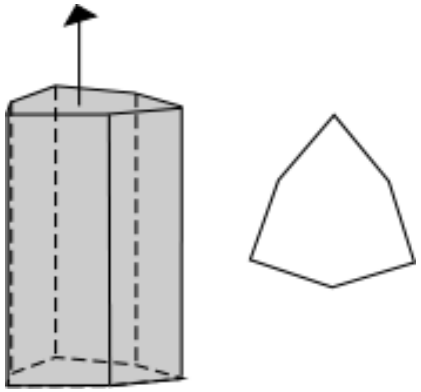
- Eg. 1. Pedions are single faced forms. Since there is only one face in the form a pedion cannot completely enclose space. Thus, a crystal that has only pedions, must have at least 3 different pedions to completely enclose space.
- Eg. 2. A prism is a 3 or more faced form wherein the crystal faces are all parallel to the same line. If the faces are all parallel then they cannot completely enclose space. Thus crystals that have prisms must also have at least one additional form in order to completely enclose space.
- Eg. 3. A dipyramid has at least 6 faces that meet in points at opposite ends of the crystal. These faces can completely enclose space, so a dipyramid is closed form. Although a crystal may be made up of a single dipyramid form, it may also have other forms present.

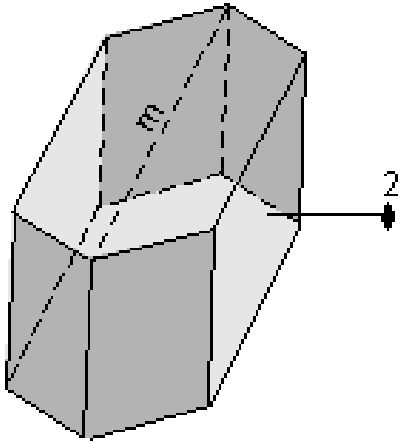

c
(111)
(111)
a
b


m


2



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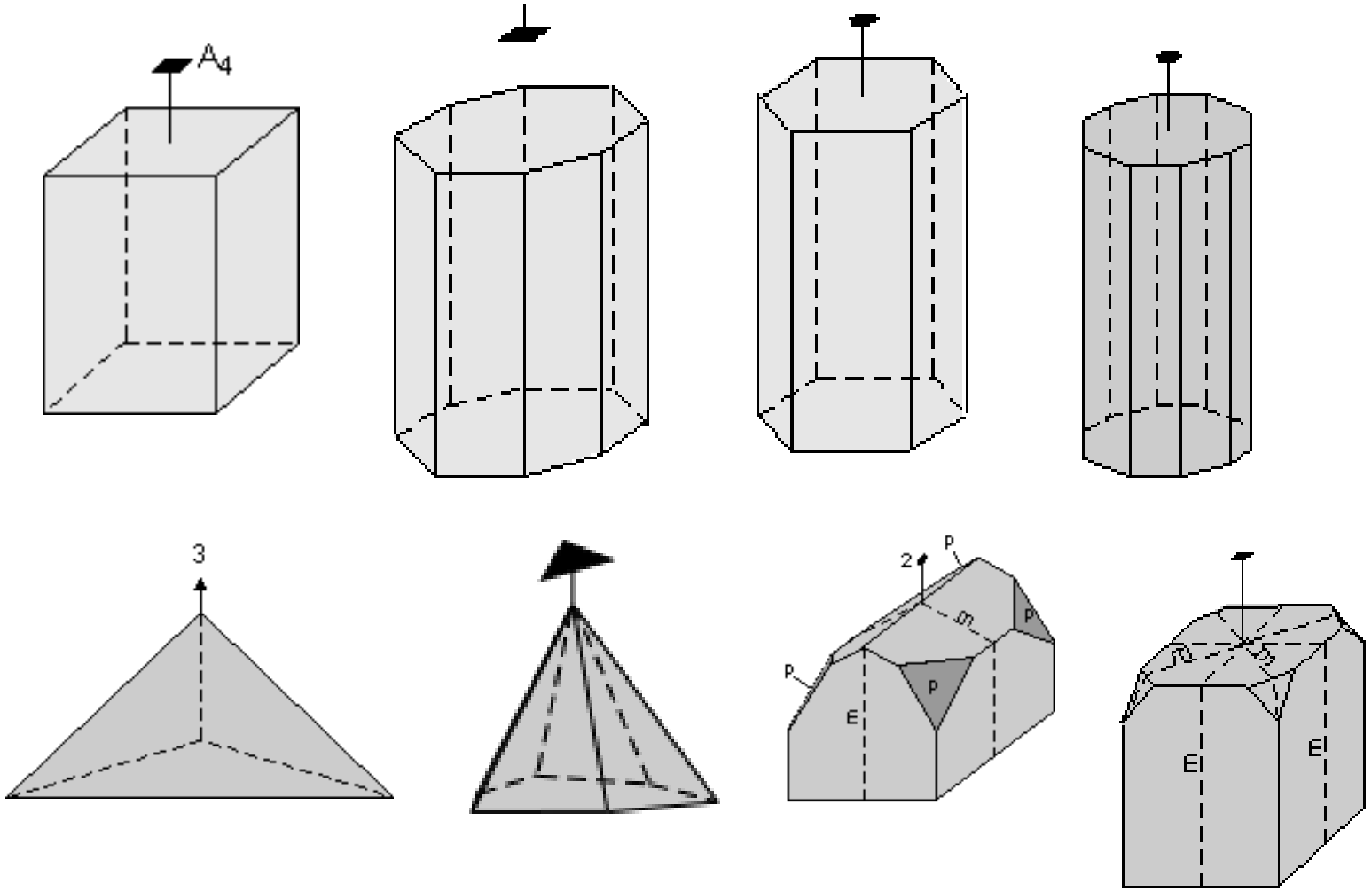
A4
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P
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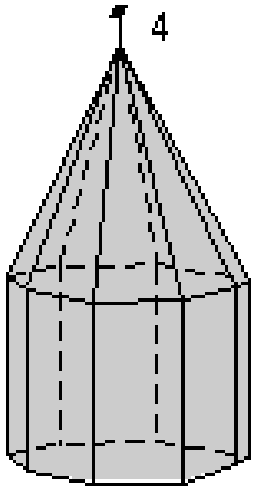
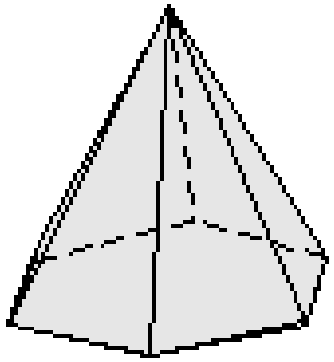
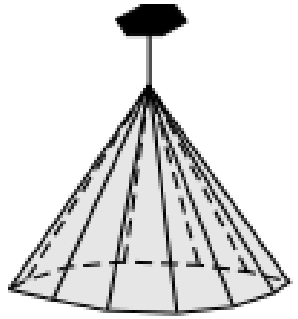
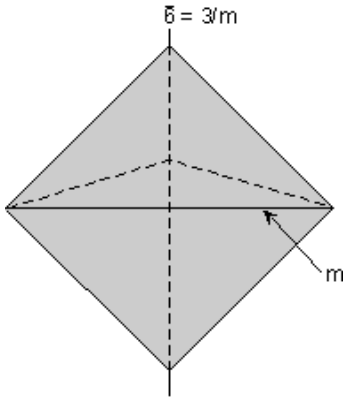
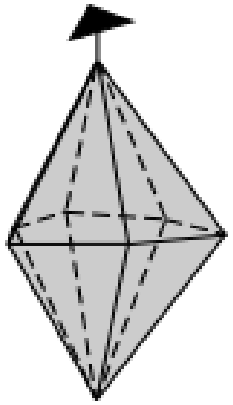
E

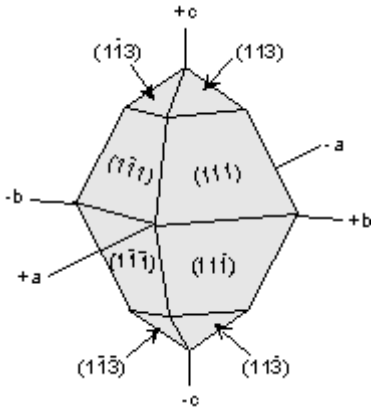

4

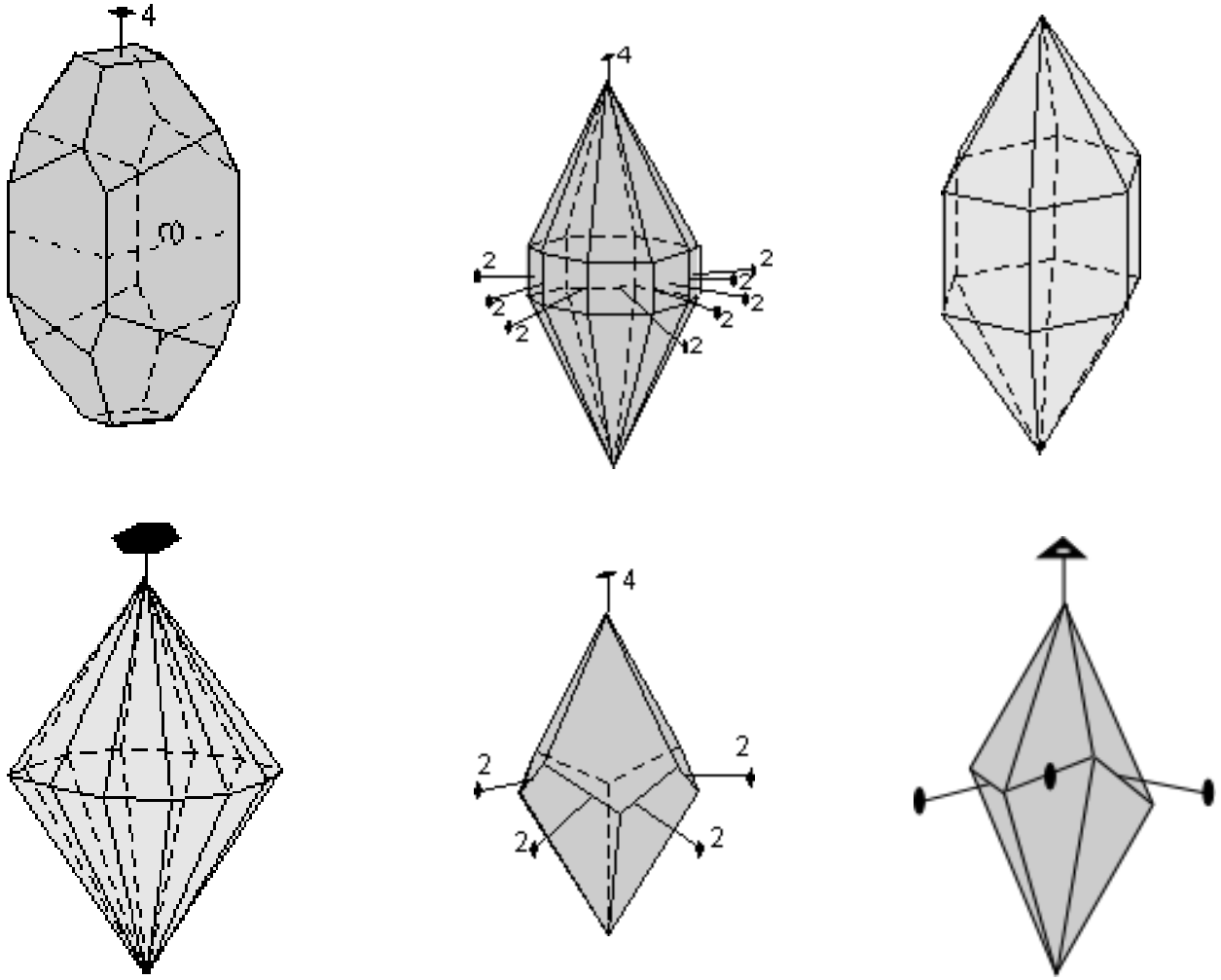





6̄ = 3/m
m




+c
(1$\bar{1}$3)
(113)
-a
(1$\bar{1}\bar{1}$)
(111)
-b
+b
+a
(1$\bar{1}$1)
(11$\bar{1}$)
(1$\bar{1}\bar{3}$)
(11$\bar{3}$)
-c


4
∞
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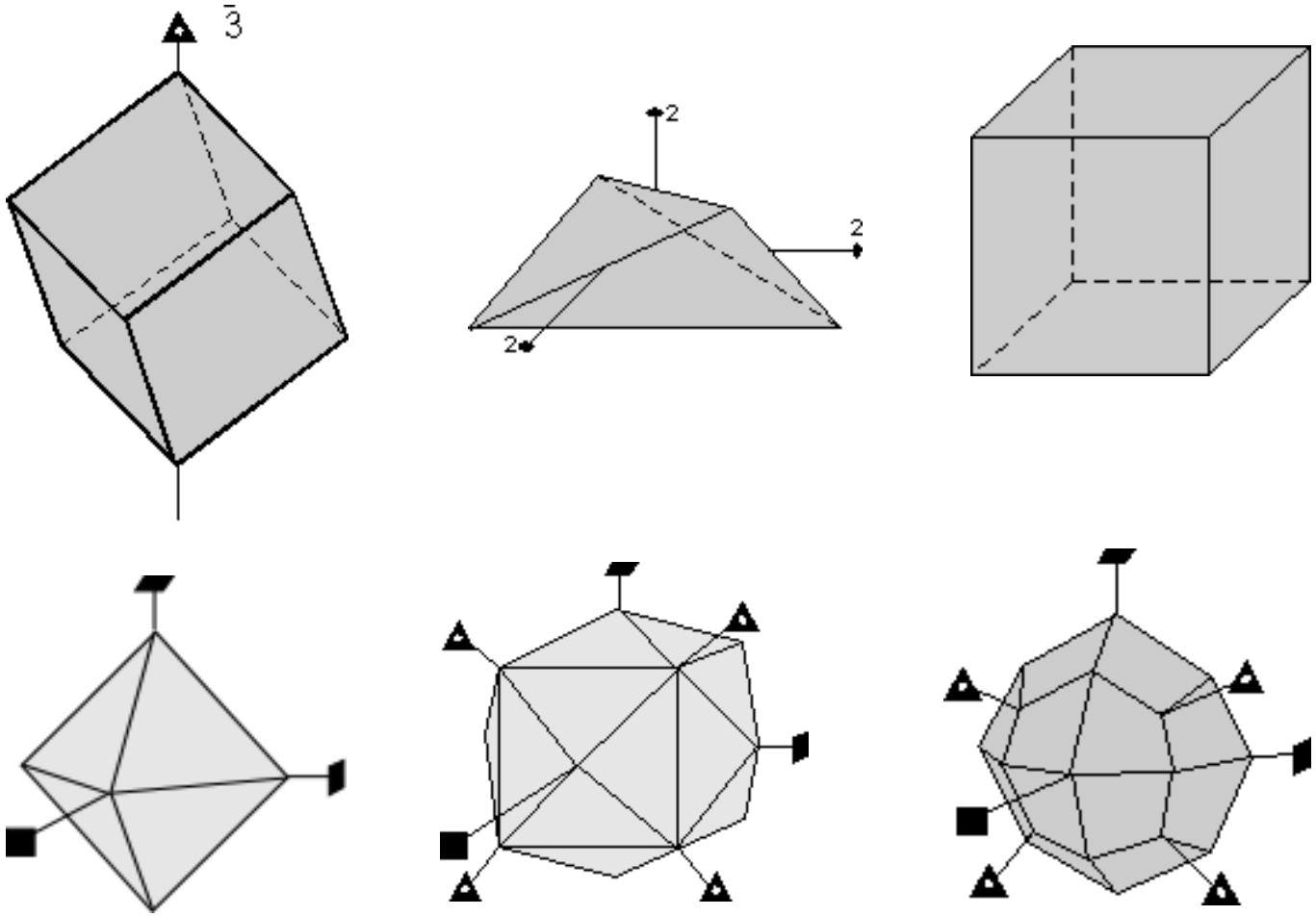
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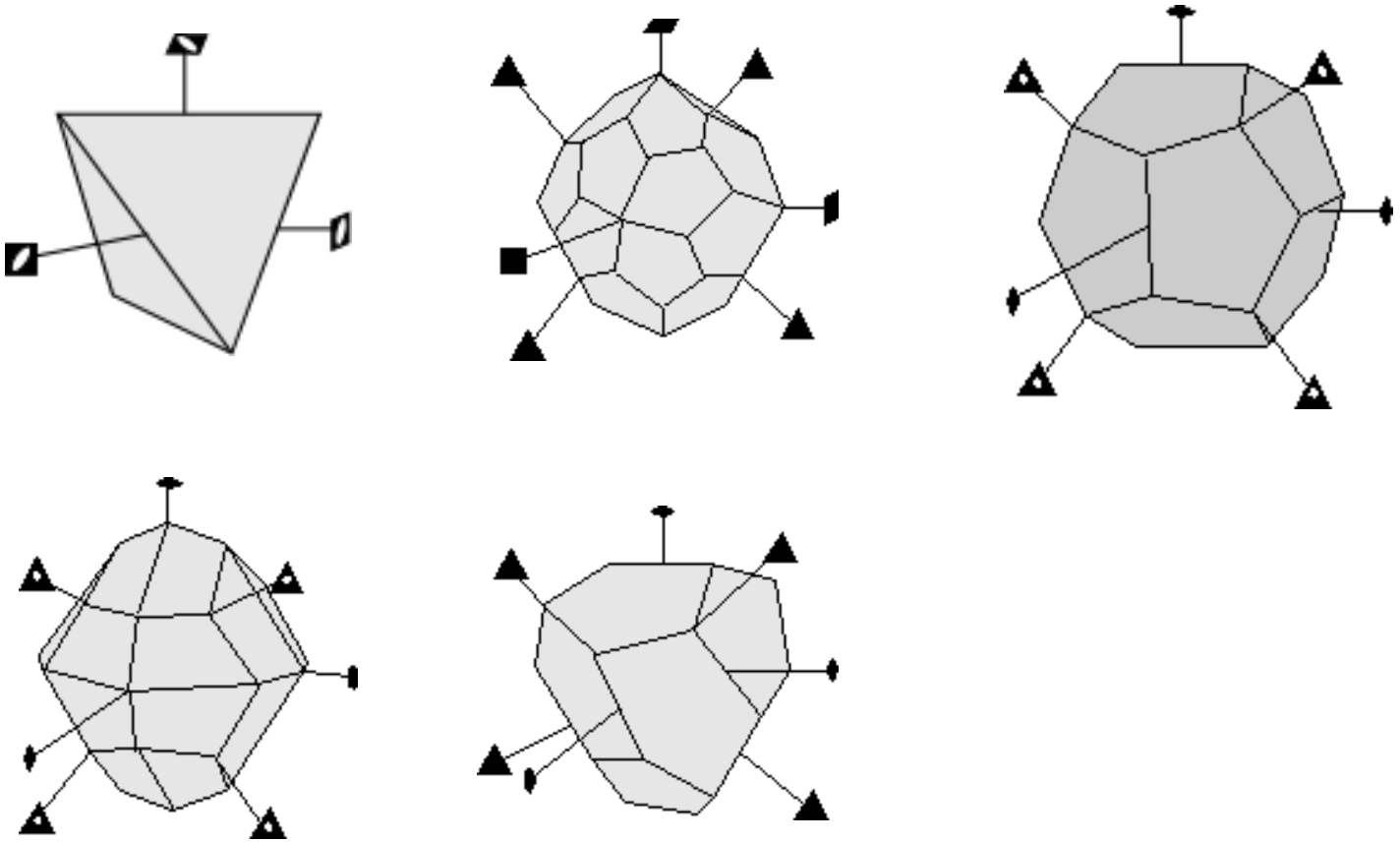


# Understanding Miller Indices, Form Symbols, and Forms

- **Triclinic -** Since this class has such low symmetry there are no constraints on the axes, but the most pronounced face should be taken as parallel to the c axis.
- **Monoclinic -** The 2 fold axis is the b axis, or if only a mirror plane is present, the b axis is perpendicular to the mirror plane.
- **Orthorhombic -** The current convention is to take the longest axis as b, the intermediate axis is a, and the shortest axis is c  An older convention was to take the c axis as the longest, the b axis intermediate, and the a axis as the shortest.
- **Tetragonal** - The c axis is either the 4 fold rotation axis or the rotoinversion axis.
- **Hexagonal** - The c axis is the 6-fold, 3-fold, axis, or .
- **Isometric** - The equal length a axes are either the 3  4-fold rotation axes, rotoinversion axes, or, in cases where no 4 or axes are present, the 3 2-fold axes.

# Vectorial Properties of Crystals

- Although a crystal structure is an ordered arrangement of atoms on a lattice, as we have seen, the order may be different along different directions in the crystal.
- Thus, some properties of crystals depend on direction. These are called vectorial properties, and can be divided into two categories: continuous and discontinuous.

# Continuous Vectorial Properties

- Continuous vectorial properties depend on direction, but along any given the direction the property is the same. Some of the continuous vectorial properties are:
- **Hardness** - In some minerals there is a difference in hardness in different directions in the crystal. Examples: Kyanite, Biotite, Muscovite. This can become an important identifying property and/or may lead to confusion about the hardness if one is not aware of the directional dependence.
- **Velocity of Light (Refractive Index)** - For all minerals except those in the isometric system, the velocity of light is different as the light travels along different directions in the crystal. We will use this directional dependence of light velocity as an important tool in the second half of the course. Refractive Index is defined as the velocity of light in a material divided by the velocity of light in a vacuum. Because the velocity of light depends on direction, the refractive index will also depend on direction.
- **Thermal Conductivity** - The ability of a material to conduct heat is called thermal conductivity. Like light, heat can be conducted at different rates along different directions in crystals.
- **Electrical Conductivity**- The ability of a material to allow the passage of electrons is called electrical conductivity, which is also directionally dependent except in isometric crystals.
- **Thermal Expansion** - How much the crystal lattice expands as it is heated is referred to as thermal expansion. Some crystals expand more in one direction than in others, thus thermal expansion is a vectorial property.
- **Compressibility** - Compressibility is a measure of how the lattice is reduced as atoms are pushed closer together under pressure. Some directions in crystals may be more compressible than others.

# Discontinuous Vectorial Properties

- Discontinuous vectorial properties pertain only to certain directions or planes within a crystal. For these kinds of properties, intermediate directions may have no value of the property. Among the discontinuous vectorial properties are:
- **Cleavage** - Cleavage is defined as a plane within the lattice along which breakage occurs more easily than along other directions. A cleavage direction develops along zones of weakness in the crystal lattice. Cleavage is discontinuous because it only occurs along certain planes.
- **Growth Rate** - Growth rate is defined as the rate at which atoms can be added to the crystal. In some directions fewer atoms must be added to the crystal than in other directions, and thus some directions may allow for faster growth than others.
- **Solution Rate** - Solution rate is the rate at which a solid can be dissolved in a solvent. In this case it depends on how tightly bonded the atoms are in the crystal structure, and this usually depends on direction.

# Crystal Habit

- In nature perfect crystals are rare. The faces that develop on a crystal depend on the space available for the crystals to grow. If crystals grow into one another or in a restricted environment, it is possible that no well-formed crystal faces will be developed.
- However, crystals sometimes develop certain forms more commonly than others, although the symmetry may not be readily apparent from these common forms. The term used to describe general shape of a crystal is ***habit.***

Some common crystal habits are as follows.

- ***Cubic*** **- cube shapes**

  ***Octahedral*** **- shaped like octahedrons, as described above.**
- ***Tabular*** **- rectangular shapes.**

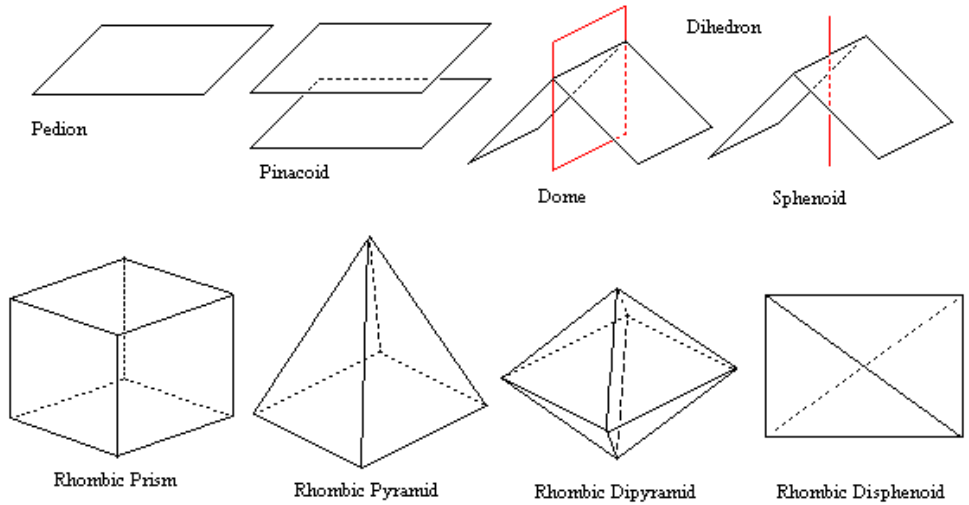
  ***Equant*** **- a term used to describe minerals that have all of their boundaries of approximately equal length.**
- ***Fibrous*** **- elongated clusters of fibers.**
- ***Acicular*** **- long, slender crystals.**
- ***Prismatic*** **- abundance of prism faces.**
- ***Bladed*** **- like a wedge or knife blade**
- ***Dendritic*** **- tree-like growths**
- ***Botryoidal*** **- smooth bulbous shapes**

| Symmetry | {010} | | | {001} | | |
|---|---|---|---|---|---|---|
| | #Faces | Form | #Cleavage Directions | #Faces | Form | #Cleavage Directions |
| 1 | | | | | | |
| 2 | | | | | | |
| 2/m | | | | | | |
| 2/m2/m2/m | | | | | | |
| 4/m2/m2/m | | | | | | |
| 4/m $\bar{3}$ 2/m | | | | | | |

| Symmetry | {110} | | | {111} | | |
|---|---|---|---|---|---|---|
| | #Faces | Form | #Cleavage Directions | #Faces | Form | #Cleavage Directions |
| 1 | | | | | | |
| 2 | | | | | | |
| 2/m | | | | | | |
| 2/m2/m2/m | | | | | | |
| 4/m2/m2/m | | | | | | |
| 4/m $\bar{3}$ 2/m | | | | | | |

# Triclinic, Monoclinic and Orthorhombic Forms

- **Pedion**
  - A single face unrelated to any other by symmetry. Open
- **Pinacoid**
  - A pair of parallel faces related by mirror plane or 2-fold symmetry axis. Open
- **Dihedron**
- A pair of intersecting faces related by mirror plane or twofold symmetry axis. Some crystallographers distinguish between **domes** (pairs of intersecting faces related by mirror plane) and
- **Sphenoids** (pairs of intersecting faces related by twofold symmetry axis). All are open forms



| Crystal System | Crystal Class | Symmetry | Name of Class |
|---|---|---|---|
| Triclinic | 1 | none | Pedial |
| | $\bar{1}$ | i | Pinacoidal |
| Monoclinic | 2 | $1A_2$ | Sphenoidal |
| | m | 1m | Domatic |
| | 2/m | i, $1A_2$, 1m | Prismatic |

Hermann Mauguin

# Crystallographic Calculations

- Crystallographic calculations involve the following:
- Miller Indices (hkl)
- Axial ratios - . a: 1: c
- $\rho$ and $\phi$ angles corresponding to a Miller Index (hkl)
- angles between crystallographic axes if in monoclinic, or triclinic systems.

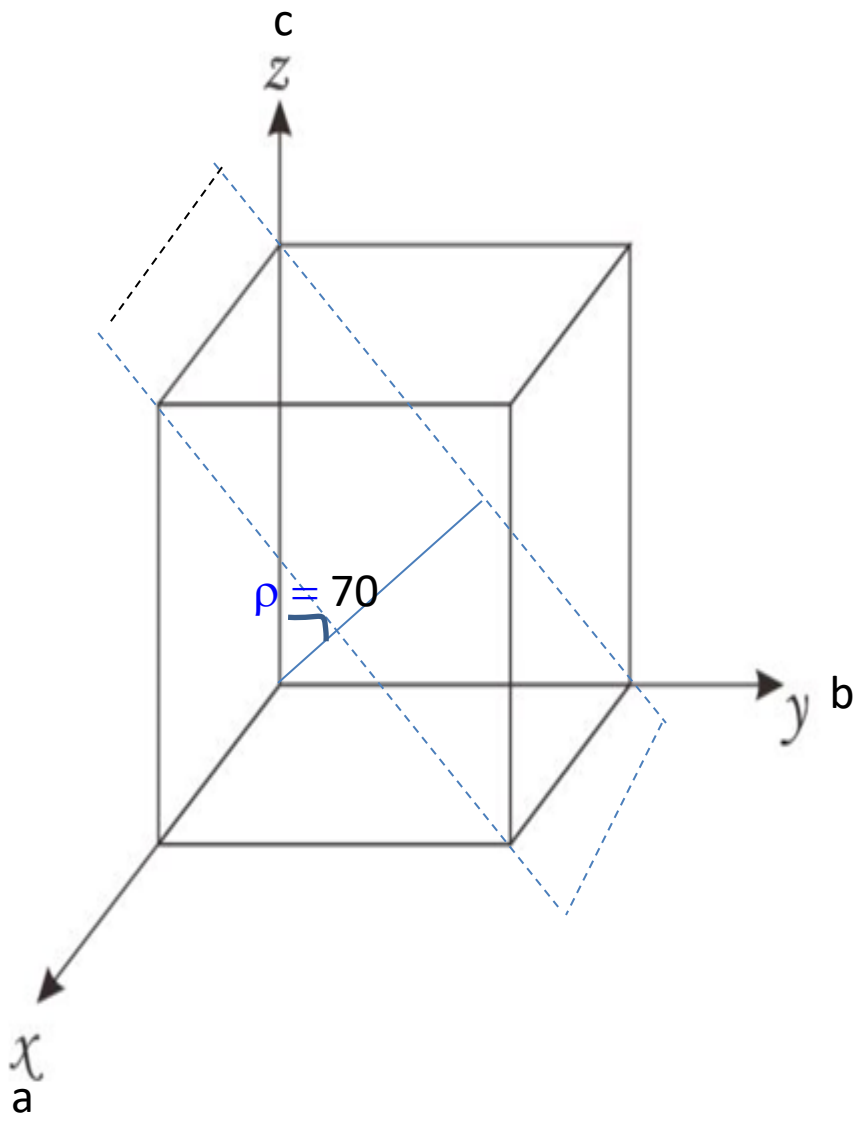
# Miller indices and $\rho$ and $\phi$ angles. In the orthorhombic, tetragonal, or isometric systems.

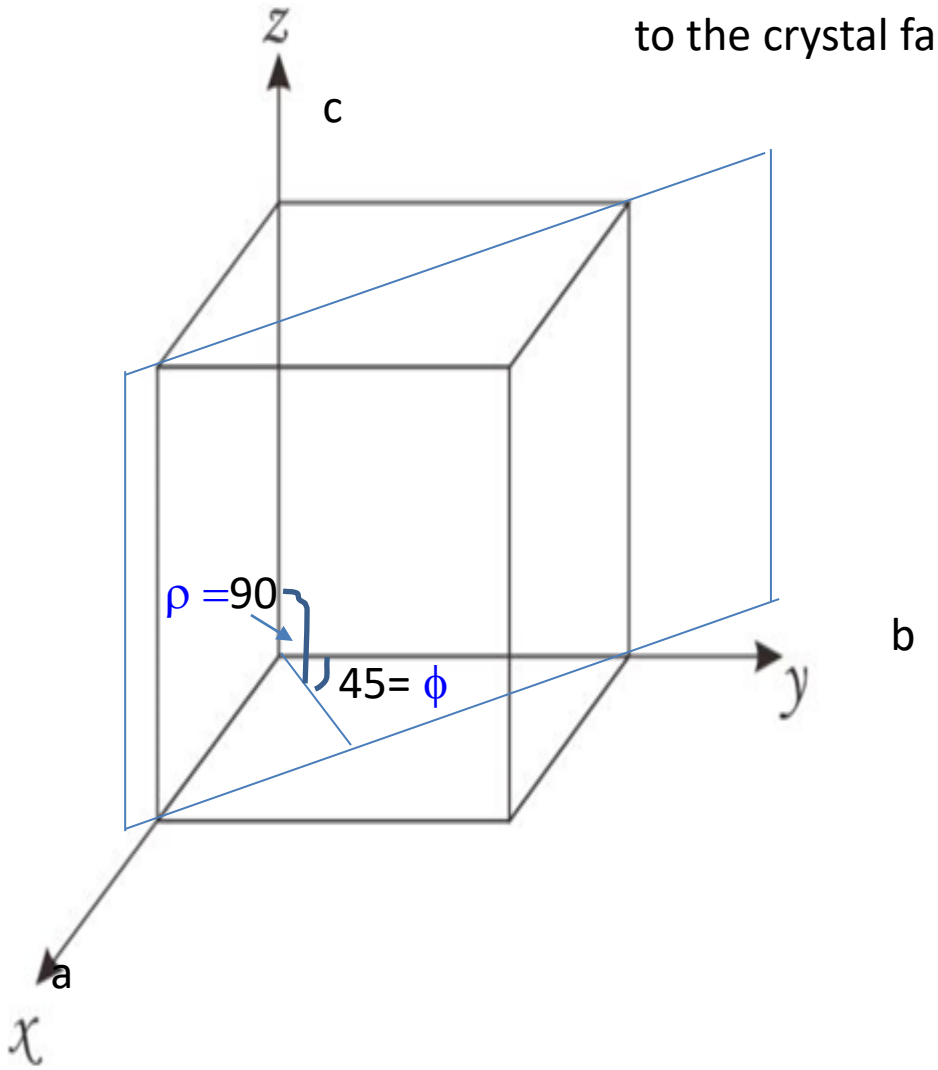
- If h is 0, i.e. (0kl) is the Miller Index, then the face is parallel to the **a** crystallographic axis.
  - So, $\phi = 0^o$ or $\phi = 180^o$
- If k is 0 i.e. (h0l) is the Miller Index, then the face is parallel to the **b** crystallographic axis.
  - So, $\phi = 90^o$ or $\phi = 270^o$
- If l is 0, i.e. (hk0) is the Miller Index, then the face is parallel to the **c** crystallographic axis.
  - So, $\rho = 90^o$
- If h & k are 0, i.e. (00l) is the Miller Index, then the face is perpendicular to the **c** axis.
  - So, r = $0^o$ or $\rho = 180^o$, and f is undefined.
- If h & l are 0, i.e. (0k0) is the Miller Index, then the face is perpendicular to the **b** axis.
  - So, $\rho = 90^o$ and $\phi = 0^o$ or $\phi = 180^o$.
- If l and k are 0, i.e. (h00) is the Miller Index, then the face is perpendicular to the **a** axis.
  - So, $\rho = 90^o$ and $\phi = 90^o$ or $\phi = 270^o$.

We define this face (010) as having a Φ angle of $0^o$. For any other face, the Φ angle will be measured from the b axis in a clockwise sense in the plane of the equator.

We define the ρ angle, as the angle between the c axis and the pole to the crystal face, measured downward from the North pole of the sphere. In the diagram shown here, a crystal face has a ρ angle measured in the vertical plane containing the axis of the sphere and the face pole, and a Φ angle measured in the horizontal equatorial plane. Note that the (010) face has a ρ angle = $90^o$.

We define the ρ angle, as the angle between the c axis and the pole to the crystal face,

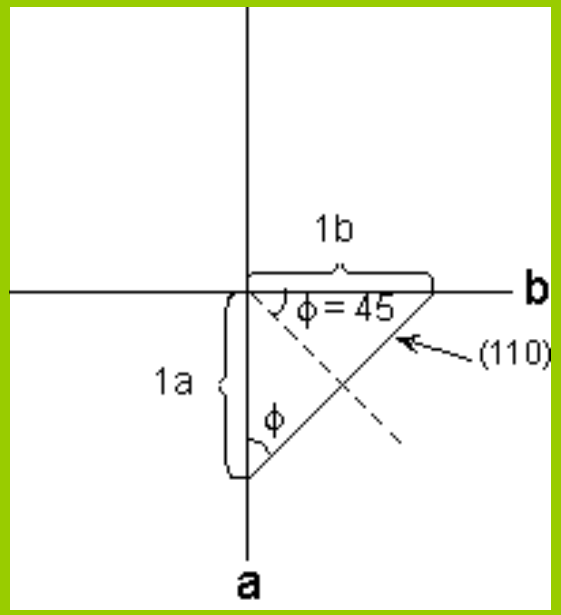


Given Miller indices and ρ and ϕ angles for crystal faces that, in combination, intersect all crystallographic axes, calculate the axial ratios of the mineral.

| Faces | ρ | ϕ |
|---|---|---|
| (1$\bar{1}$0) | 90° | 45° |
| (011) | 70° | 0° |

Since the ϕ angle is the angle between the normal to the face and the b axis, the ϕ angle also occurs between the a axis and the face



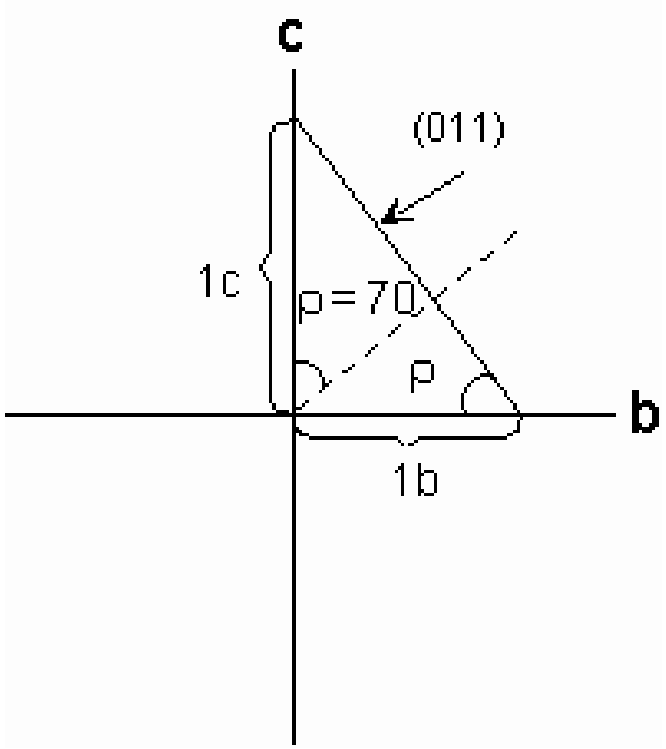

Thus, we can write:

$\tan 45^o = 1b/1a$

Then

$1a/1b = 1/\tan 45^o = 1$

So, a/b: b/b = 1: 1




Thus, we can write:

$\tan 70^o = 1c/1b$

then

$c/b = \arctan 70^o$

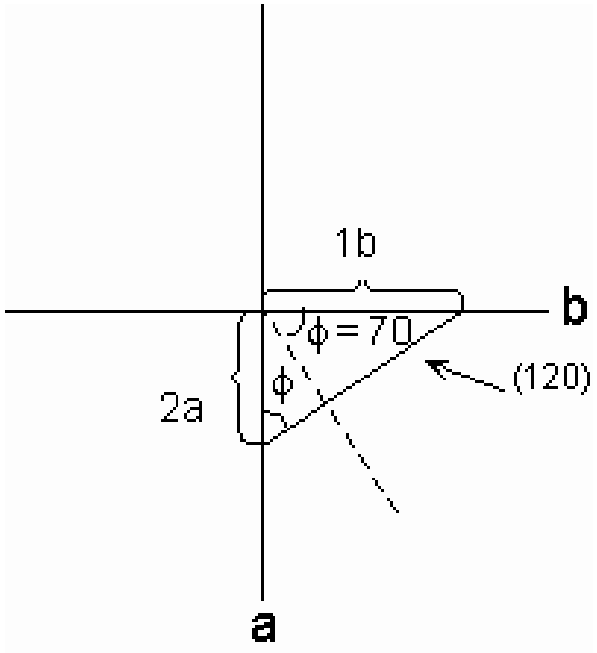
So, c/b = 2.7475

so, a : b : c = 1 : 1 : 2.7475 and the mineral must be tetragonal, since a/b =1.

the $\rho$ angle also occurs between the b axis and the (011) face

# Example 2:

| Faces | ρ | ϕ |
|---|---|---|
| (120) | 90° | 70° |
| (011) | 32° | 0° |

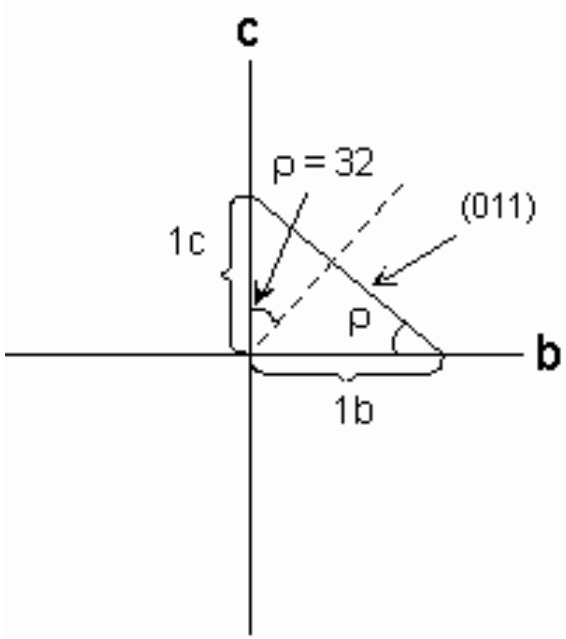



Then we can write:

$\tan 70^o = 1b/2a$

$a/b = ½ \tan 70^o$

$1a/1b = 0.18199$




For this face we can determine that

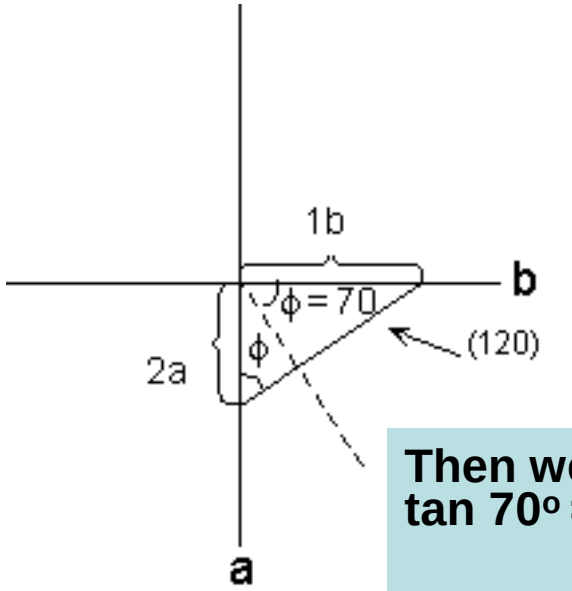
$\tan 32^o = 1c/1b$

$1c/1b = 0.6248$

so, a : b : c = 0.18199 : 1 : 0.6248, and the mineral is orthorhombic

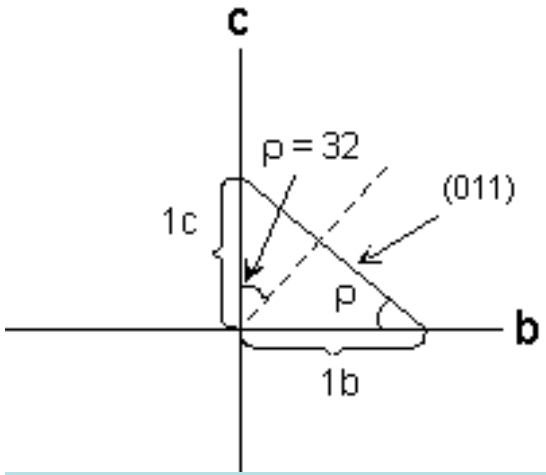
# Example 3:

| Faces | ρ | ϕ |
|---|---|---|
| (120) | 90° | 70° |
| (011) | 32° | 0° |




**Then we can write:**
**tan 70° = 1b/2a**

**a/b = ½ tan70°**
**1a/1b = 0.18199**




**For this face we can determine that**

**tan 32° = 1c/1b**

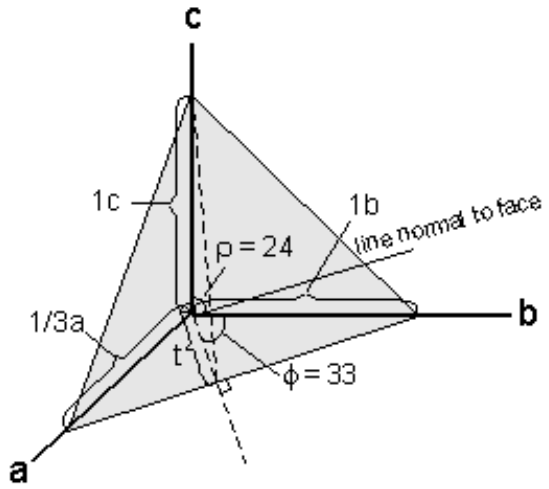
**1c/1b = 0.6248**

**so, a : b : c = 0.18199 : 1 : 0.6248, and the mineral is orthorhombic**

# Example 4:

| Faces | ρ | ϕ |
|---|---|---|
| **(311)** | **24°** | **33°** |

This face is more complicated because it intersects all three axes.

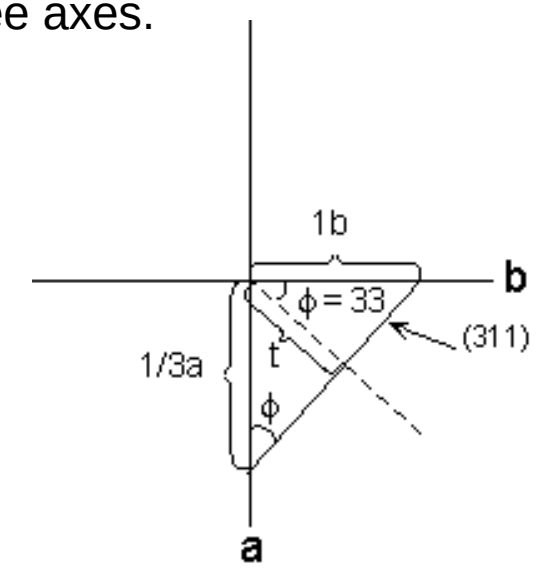



**Face in the a - b plane.**
**1b/(1/3)a = tan 33°**

**1a/3b = 1/tan 33**

**1a/1b = 3/tan 33**

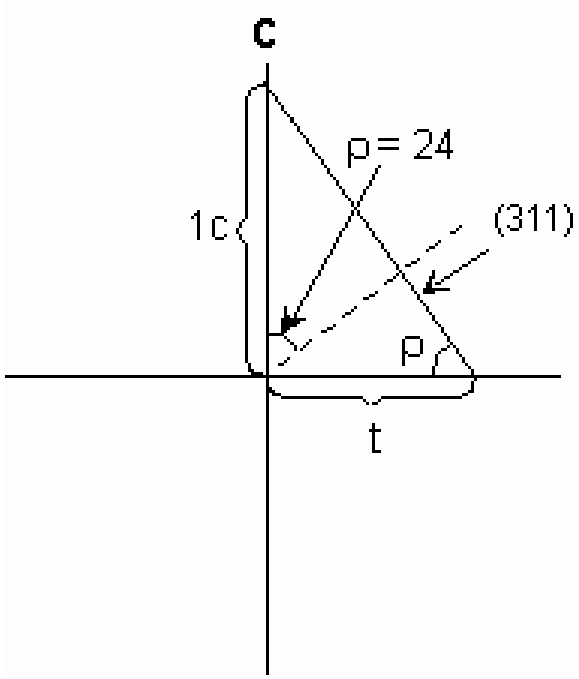
**1a/1b = 4.6196**




**The length of the line t is: t/b = cos 33°**

**t/b = 0.8397**

**t = 0.8397 b**




**We can now use this to determine the c/b axial ratio.**

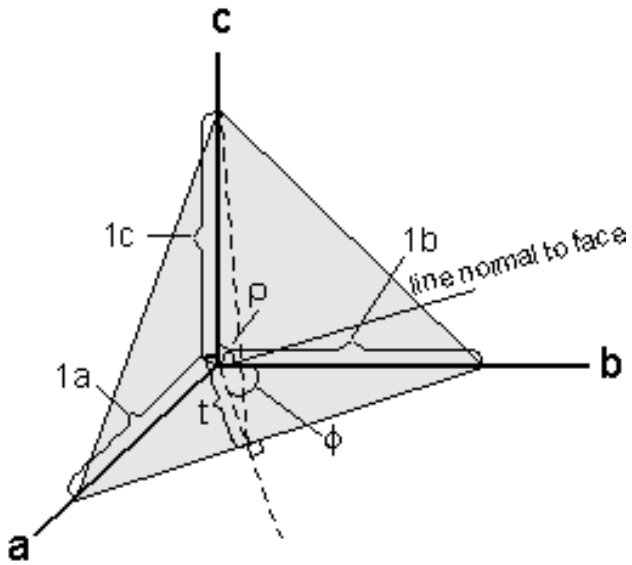
**$1c/t = \tan 24^o$**

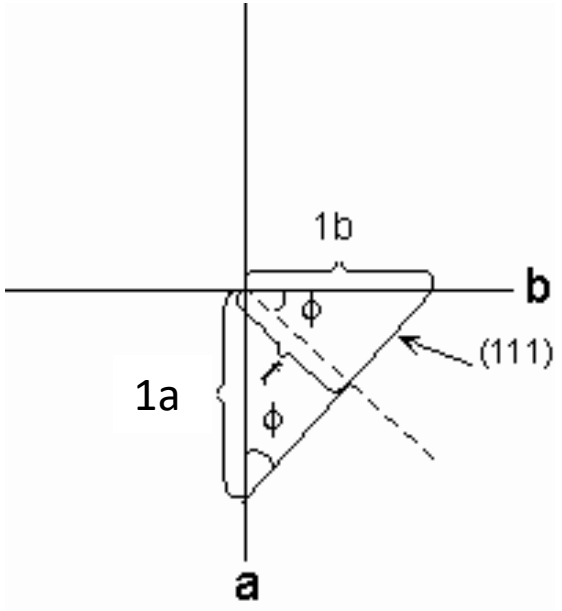
**$1c = 0.8387\ b \tan 24^o$**
**$c/b = 0.3747$**

**Thus, the axial ratio for this mineral is 4.6196 : 1 : 0.3747**

# Example 4:

**Given the axial ratio for a mineral is 1 : 1 : 5.0, what are ρ and ϕ for the face (111).**




**Since the ϕ angle for this face is measured in the horizontal a - b plane, draw the plane containing only the a and b axes to determine the angle. Since the axial ratio tells us that the relative lengths of the a and b axes are equal**

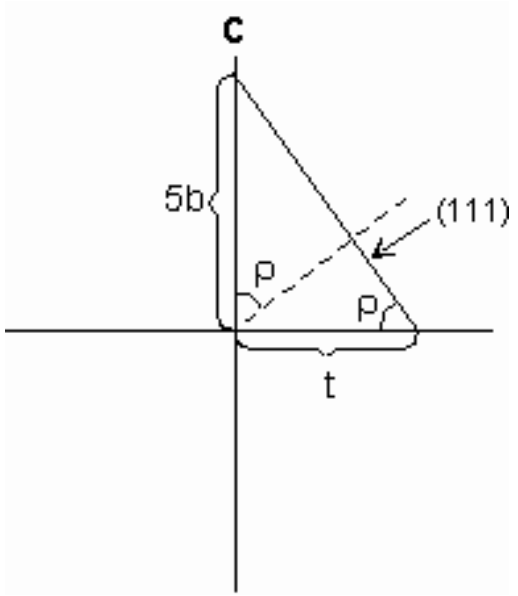
$$\tan \phi = 1a/1b = 1$$

$$\phi = 45^{o}$$

**the ρ angle, we need to know the length of the line labeled t,**

**The length of the line t is:**
**t/b = cos 45°**

**t = 0.7071 b**



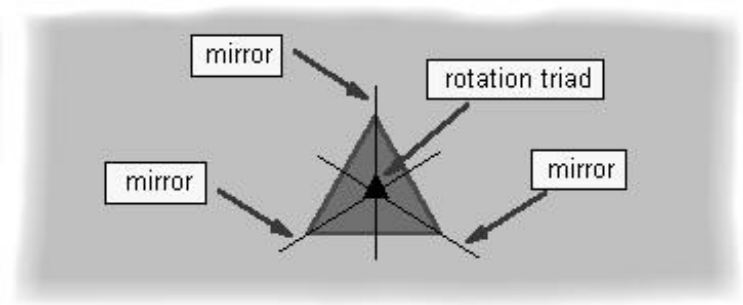

Now we can determine the angle by drawing the plane that includes the c axis and the line t. In this plane we can let the length of the c = 5b, from the axial ratio.

***Then:***

tan ρ = 5b/t
tan ρ = 5b/0.7071b
tan ρ = 5/0.7071
tan ρ = 7.071
ρ = arctan (7.071) = 81.95°

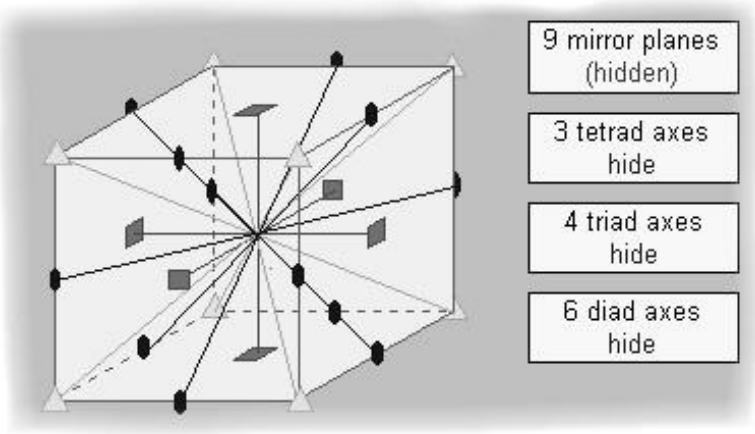
**So for the (111) face in this crystal ρ =81.95° and ϕ = 45°.**

The combination of reflection and rotation symmetry to give the ten plane point symmetry groups follows.

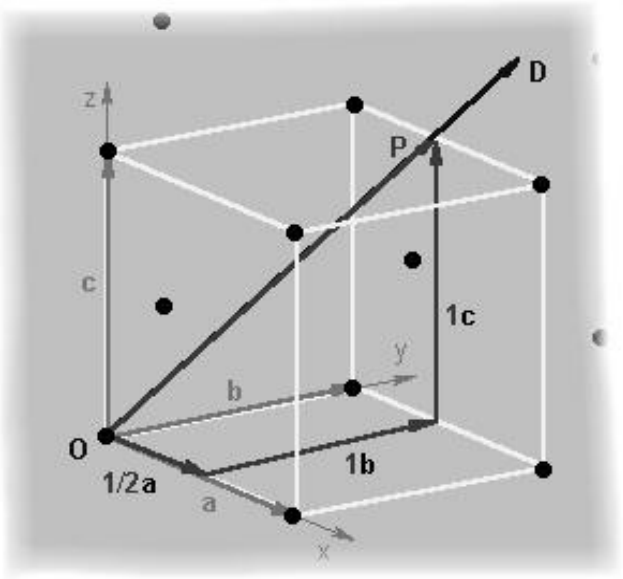



All crystals can be assigned to be in one of seven crystal systems.depending on the shape of their unit cell. Seven distinct unit cells exist, the shape of these unit cells is determined by the symmetry of the crystal system. Within each of the crystal systems, different lattices are possible. There are 14 different lattices, known as the Bravais lattices. By clicking on the crystal system name, the Bravais lattices are illustrated.

This section then addresses symmetry elements in three dimensions. Mirrors lines become mirror planes, and objects can have more than one rotation axis in different directions. These symmetry elements all pass through the centre of the object, through a single point. This combination of symmetry elements is called the point symmetry group for an object.



# Indexing Directions and Planes




It is often necessary to state the direction in a crystal. A method is described which shows how to calculate the Miller index for a direction in a 2-D lattice. It is important to be able to identify the unit vectors in the lattice of the crystal, since the Miller index expresses direction in terms of ratios of these vectors. This method is easily extended to three dimensions.

| Crystal System | Crystal Class | Symmetry | Name of Class |
|---|---|---|---|
| Triclinic | 1 | none | Pedial |
| | $\bar{1}$ | i | Pinacoidal |
| Monoclinic | 2 | $1A_2$ | Sphenoidal |
| | m | 1m | Domatic |
| | 2/m | i, $1A_2$, 1m | Prismatic |

END