Crystal Axes, Systems, Mineral Face Notation (Miller Indices)

Drusy Quartz on Barite

A CRYSTAL is the outward form of the internal structure of the mineral.

The 6 basic crystal systems are:

ISOMETRIC

HEXAGONAL

TETRAGONAL

ORTHORHOMBIC

MONOCLINIC

TRICLINIC

Acknowledgement: the following images from Susan and Stan Celestian, Glendale Community College

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Crystal Systems

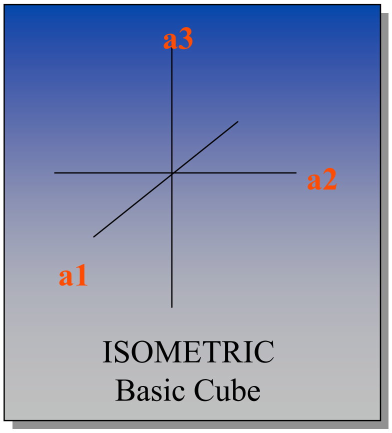
CRYSTAL SYSTEMS are divided into 6 main groups.

ISOMETRIC - Fluorite Crystals

The first group is the ISOMETRIC. This literally means "equal measure" and refers to the equal size of the crystal axes.

Crystal Systems

- **ISOMETRIC** **CRYSTALS**



ISOMETRIC
Basic Cube

ISOMETRIC

In this crystal system there are 3 axes. Each has the same length (as indicated by the same letter “a”).

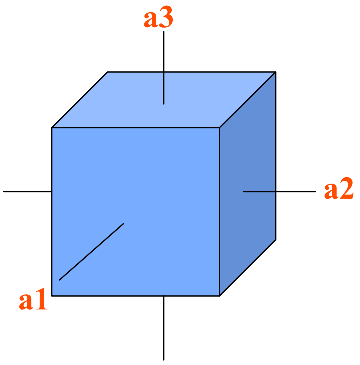
They all meet at mutual 90^{o} angles in the center of the crystal.

Crystals in this system are typically blocky or ball-like.

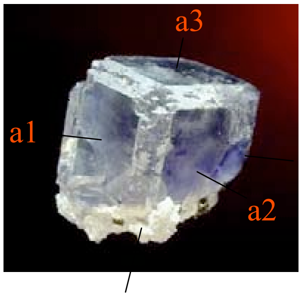
ALL ISOMETRIC CRYSTALS HAVE 4 3-FOLD AXES

Crystal Systems

- **ISOMETRIC** **CRYSTALS**



ISOMETRIC - Basic Cube



Fluorite cube with crystal axes.

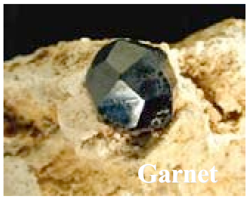
Crystal Systems

- **ISOMETRIC** BASIC CRYSTAL SHAPES

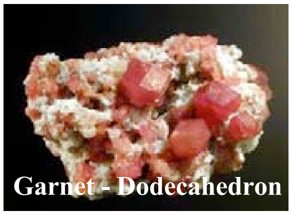
Octahedron

Cube

Cube with
Pyritohedron
Striations

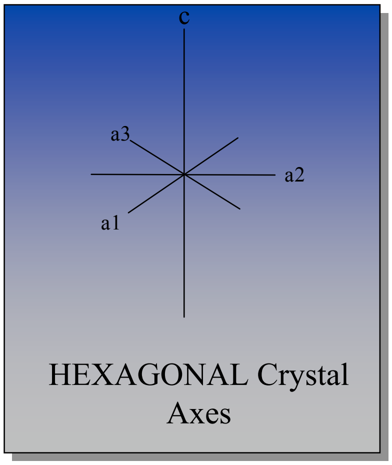


Trapezohedron



Crystal Systems

- **HEXAGONAL** CRYSTALS



HEXAGONAL Crystal Axes

HEXAGONAL - Three horizontal axes meeting at angles of 120^o and one perpendicular axis.

ALL HEXAGONAL CRYSTALS HAVE A SINGLE 3- OR 6-FOLD AXIS = C

Crystal Systems

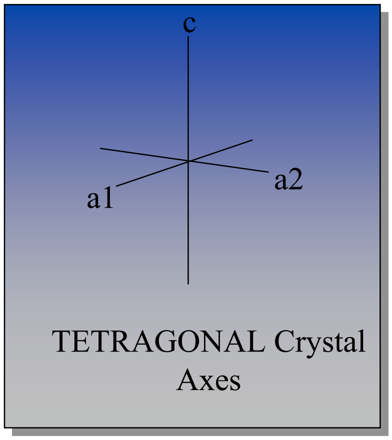
- **HEXAGONAL** CRYSTALS

These hexagonal CALCITE crystals nicely show the six sided prisms as well as the basal pinacoid.

Two subsytems:
1. Hexagonal
2. Trigonal

Crystal Systems

- **TETRAGONAL** CRYSTALS

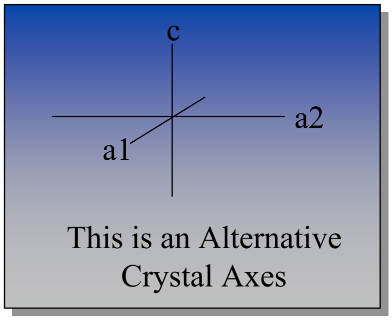


TETRAGONAL Crystal Axes

TETRAGONAL

Two equal, horizontal, mutually perpendicular axes (a1, a2)

Vertical axis (c) is perpendicular to the horizontal axes and is of a different length.

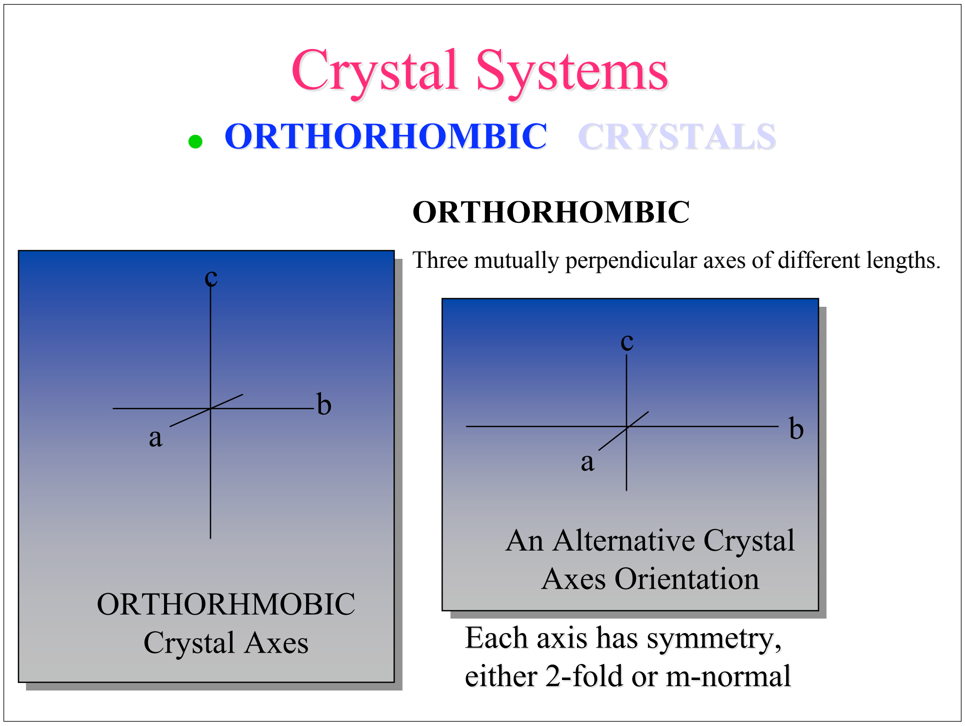


This is an Alternative Crystal Axes

Crystal Systems

- **TETRAGONAL** CRYSTALS

ALL HEXAGONAL CRYSTALS HAVE A SINGLE 3- OR 6-FOLD AXIS = C



Crystal Systems

- **ORTHORHOMBIC** CRYSTALS

ORTHORHOMBIC

Three mutually perpendicular axes of different lengths.

ORTHORHMOBIC
Crystal Axes

An Alternative Crystal
Axes Orientation

Each axis has symmetry,
either 2-fold or m-normal

Crystal Systems

- **ORTHORHOMBIC** CRYSTALS

Topaz from Topaz Mountain, Utah.

Crystal Systems

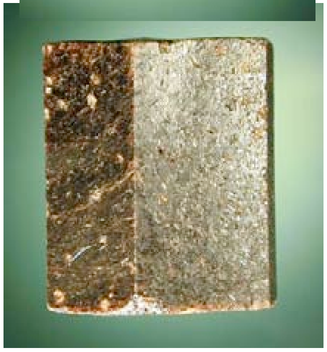
- **ORTHORHOMBIC** CRYSTALS

BARITE is also orthorhombic. The view above is looking down the “c” axis of the crystal.

Crystal Systems

- **ORTHORHOMBIC** CRYSTALS

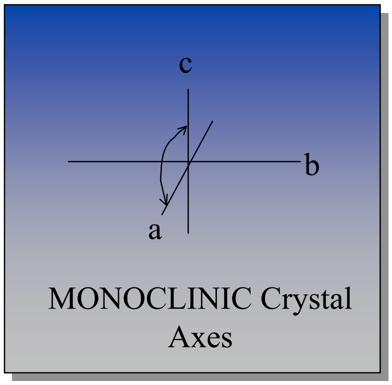
Pinacoid
View



Prism View

Crystal Systems

- **MONOCLINIC** CRYSTALS



MONOCLINIC Crystal
Axes

MONOCLINIC

In this crystal form the axes are of unequal length.

Axes a and b are perpendicular.

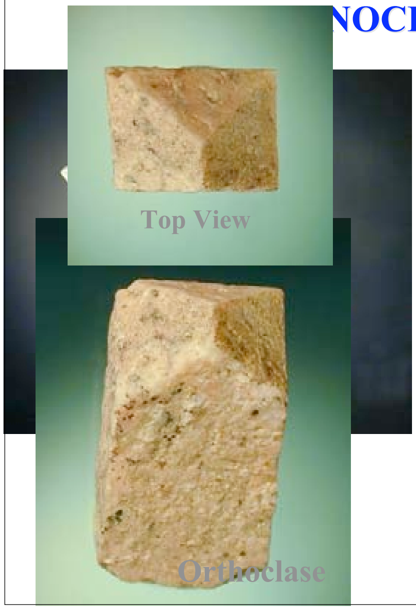
Axes b and c are perpendicular.

But a and c make some oblique angle and with each other.

MONO = ONE AXIS OF
SYMMETRY (2-FOLD OR
MIRROR) = TO “b”

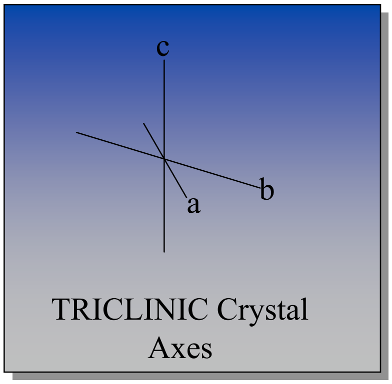
Crystal Systems

NOCLINIC **CRYSTALS**



Crystal Systems

- **TRICLINIC** **CRYSTALS**



TRICLINIC Crystal Axes

TRICLINIC

In this system, all of the axes are of different lengths and none are perpendicular to any of the others.

SYMMETRY: ONLY 1 OR 1-BAR

Crystal Systems

- **TRICLINIC** **CRYSTALS**

Microcline, variety Amazonite

Crystal Faces

Remember:

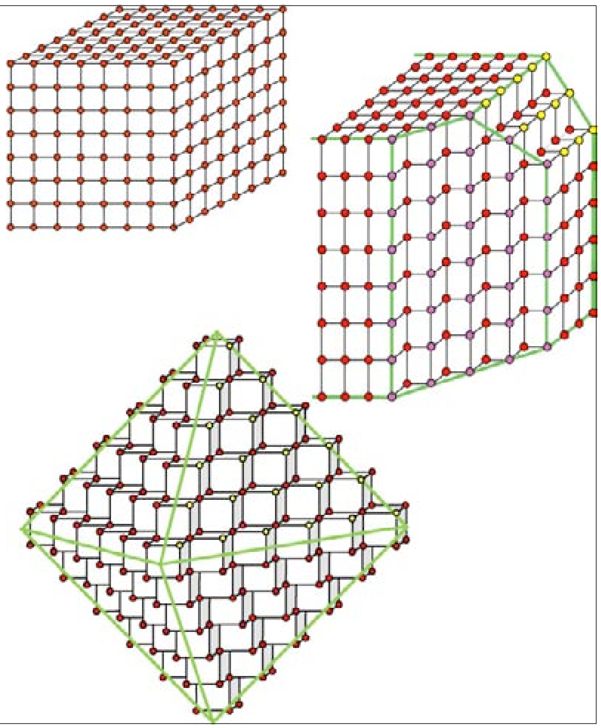
- ✦Space groups for atom symmetry
- ✦Point groups for crystal face symmetry

Crystal Faces = limiting surfaces of growth

Depends in part on shape of building units & physical conditions (T, P, matrix, nature & flow direction of solutions)

Acknowledgement: the following images from John Winter, Whitman College, WA

Crystal Morphology



Observation:

The frequency with which a given face in a crystal is observed is proportional to the density of lattice nodes along that plane

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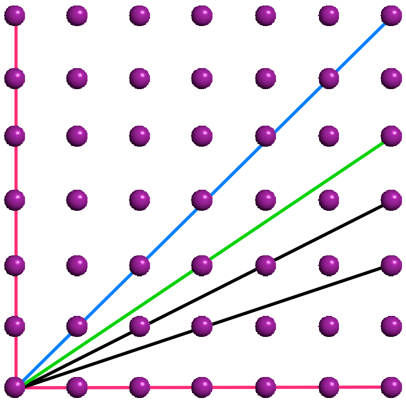
Crystal Morphology

Observation:

The frequency with which a given face in a crystal is observed is proportional to the density of lattice nodes along that plane



Crystal Morphology

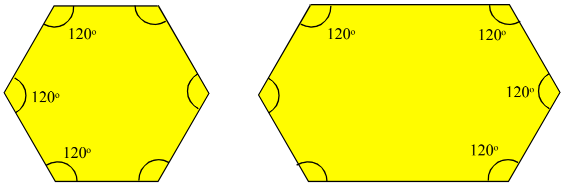
Because faces have direct relationship to the internal structure, they must have a direct and consistent angular relationship to each other

Corundum, var. ruby

Crystal Morphology

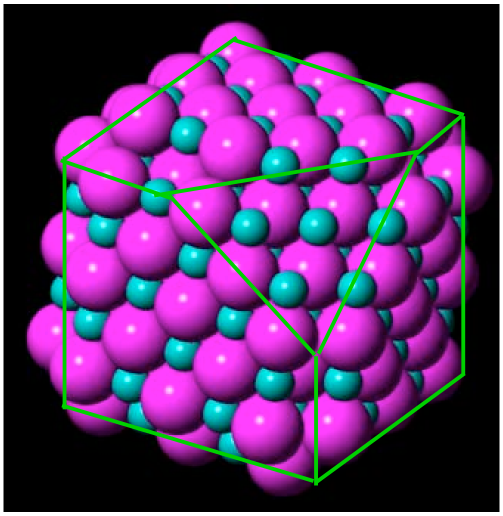
Nicholas Steno (1669): Law of Constancy of Interfacial Angles

Quartz



Crystal Morphology

Diff planes have diff atomic environments



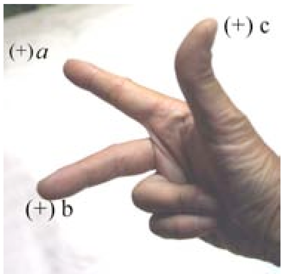
Crystal Morphology

Crystal symmetry conforms to 32 point groups → 32 crystal classes in 6 crystal systems

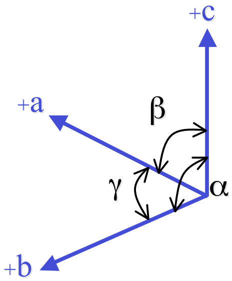
Crystal faces have symmetry about the center of the crystal so the point groups and the crystal classes are the same

Crystal System	No Center	Center
Triclinic	1	$\bar{1}$
Monoclinic	2, $\bar{2}$ (= m)	2/m
Orthorhombic	222, 2mm	2/m 2/m 2/m
Tetragonal	4, $\bar{4}$, 422, 4mm, $\bar{4}$2m	4/m, 4/m 2/m 2/m
Hexagonal	3, 32, 3m 6, $\bar{6}$, 622, 6mm, $\bar{6}$2m	$\bar{3}$, $\bar{3}$ 2/m 6/m, 6/m 2/m 2/m
Isometric	23, 432, $\bar{4}$3m	2/m $\bar{3}$, 4/m $\bar{3}$ 2/m

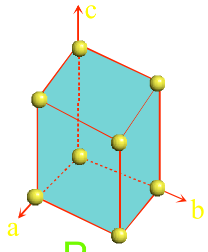
Six Crystal Systems



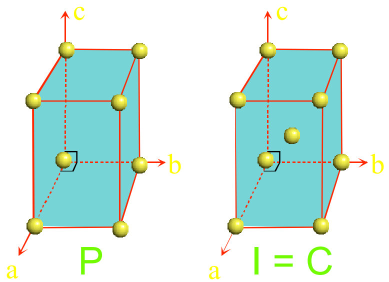
3-D Lattice Types		
Name	**axes**	**angles**
Triclinic	a ≠ b ≠ c	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
Monoclinic	a ≠ b ≠ c	$\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$
Orthorhombic	a ≠ b ≠ c	$\alpha = \beta = \gamma = 90^\circ$
Tetragonal	$a_1 = a_2 \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Hexagonal		
Hexagonal (4 axes)	$a_1 = a_2 = a_3 \neq c$	$\beta = 90^\circ$ $\gamma = 120^\circ$
Rhombohedral	$a_1 = a_2 = a_3$	$\alpha = \beta = \gamma \neq 90^\circ$
Isometric	$a_1 = a_2 = a_3$	$\alpha = \beta = \gamma = 90^\circ$



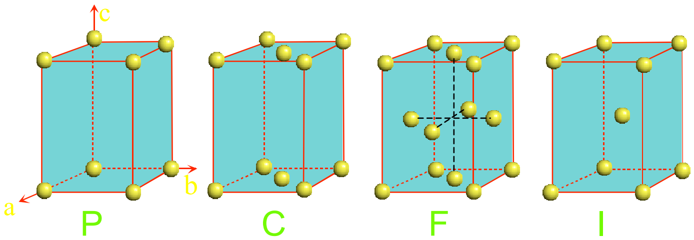
Axial convention:
“right-hand rule”



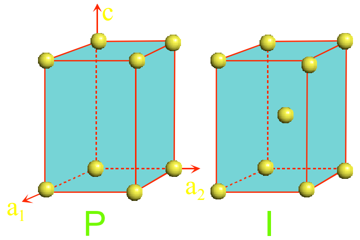
P
Triclinic
$\alpha \neq \beta \neq \gamma$
a ≠ b ≠ c



P I = C
Monoclinic
$\alpha = \gamma = 90^\circ \neq \beta$
a ≠ b ≠ c

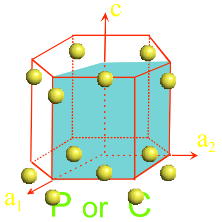


P C F I
Orthorhombic
$\alpha = \beta = \gamma = 90^\circ$ a ≠ b ≠ c



Tetragonal

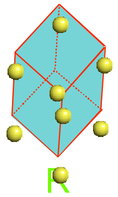
$\alpha = \beta = \gamma = 90^\circ$ $a_1 = a_2 \neq c$



Hexagonal

$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

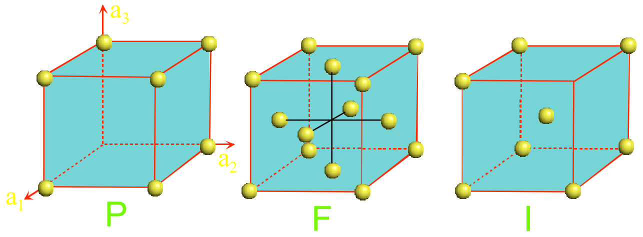
$a_1 = a_2 \neq c$



Rhombohedral

$\alpha = \beta = \gamma \neq 90^\circ$

$a_1 = a_2 = a_3$



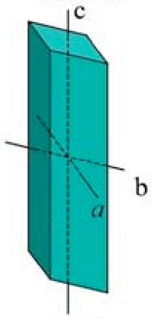
Isometric

$\alpha = \beta = \gamma = 90^\circ$ $a_1 = a_2 = a_3$

Triclinic and Monoclinic

Crystal Axes

Triclinic

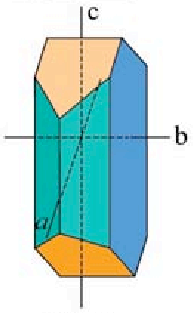


$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90$

The axes are chosen as parallel to the principal face intersections. There are no symmetric restrictions to the choice of ***a***, **b**, and **c**, but, by convention, the most pronounced zone is oriented vertically and the zone axis is **c**.

Monoclinic



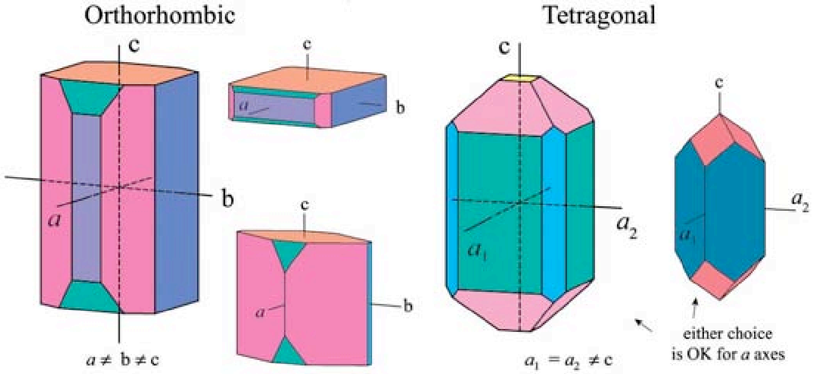
$a \neq b \neq c$

$\alpha = \gamma = 90, \beta \neq 90$

The axes are chosen as parallel to the principal face intersections. **b** is selected as || to the 2-fold axis or ⊥ to the mirror. The most pronounced zone is oriented vertically and the zone axis is **c**. ***a*** slopes down and forward so that β is typically > 90.

Orthorhombic and Tetragonal

Crystal Axes



$a \neq b \neq c$

$\alpha = \beta = \gamma = 90$

The axes are mutually perpendicular and || to 2-fold axes (conventionally **c** < ***a*** < **b**). When crystals are elongated (as above left) **c** is chosen as the direction of elongation. When crystals are flattened (top insert), **c** is chosen as normal to the predominant plane.

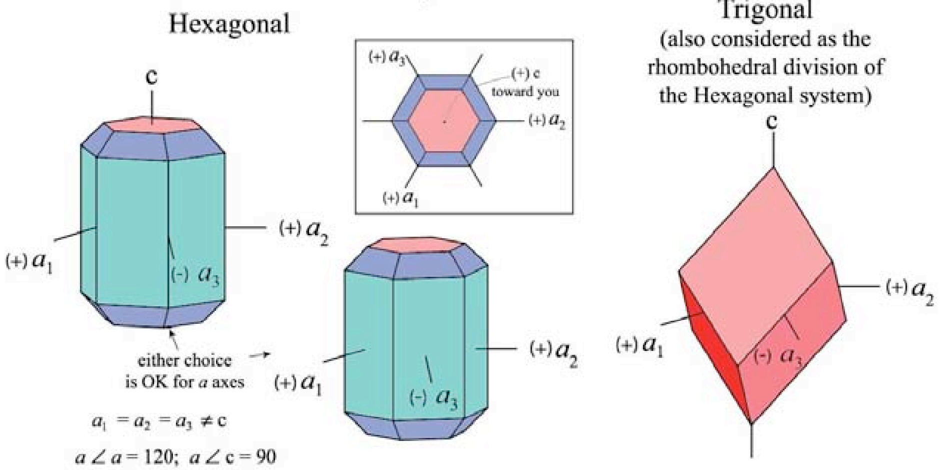
$a_1 = a_2 \neq c$

$\alpha = \beta = \gamma = 90$

The axes are mutually perpendicular and **c** is chosen || to the 4-fold axis. Due to the 4-fold symmetry, the other two axes are equal. $\boldsymbol{a_1}$ is oriented toward the front and $\boldsymbol{a_2}$ to the right.

Hexagonal

Crystal Axes

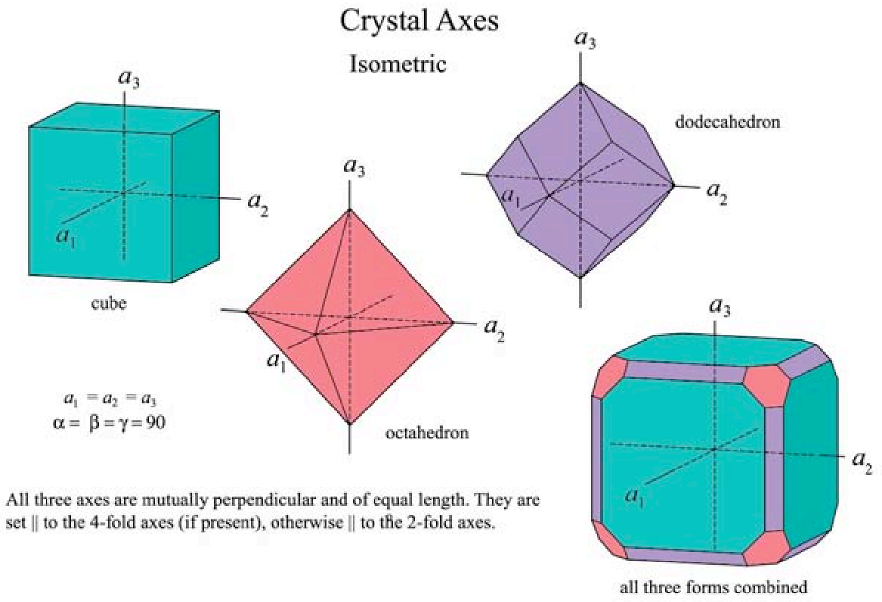


$a_1 = a_2 = a_3 \neq c$

$a \angle a = 120;\ a \angle c = 90$

The Hexagonal system (and Trigonal sub-system) typically has four axes, three are of equal length at 120 degrees to one another, and all ⊥ to **c**, which is || to either the 3-fold or 6-fold rotation. The conventional choice of the three ***a*** axes is shown in the inset.

Isometric

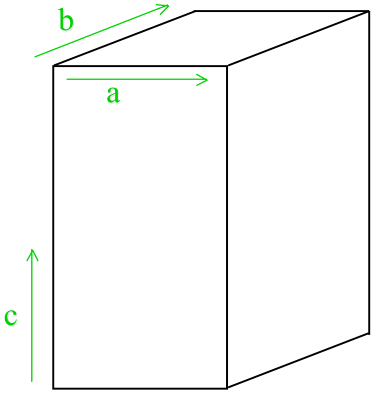


All three axes are mutually perpendicular and of equal length. They are set || to the 4-fold axes (if present), otherwise || to the 2-fold axes.

Crystal Morphology

Crystal Axes: generally taken as parallel to the edges (intersections) of prominent crystal faces

halite



Crystal Morphology

Crystal Axes:

Symmetry also has a role: c = 6-fold in hexagonal, 4-fold in tetragonal, and 3-fold in trigonal. The three axes in isometric are 4 o 4bar. The b axis in monoclinic crystals is a 2fold or m-normal.

The crystallographic axes determined by x-ray and by the face method nearly always coincide. This is not coincidence!!

Crystal Morphology

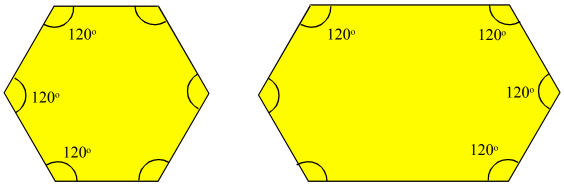
How do we keep track of the faces of a crystal?

Crystal Morphology

How do we keep track of the faces of a crystal?

Remember, face sizes may vary, but angles can't

Note: “interfacial angle” = the angle between the faces measured like this



Miller Indices of Crystal Faces

How do we keep track of the faces of a crystal?

Remember, face sizes may vary, but angles can't

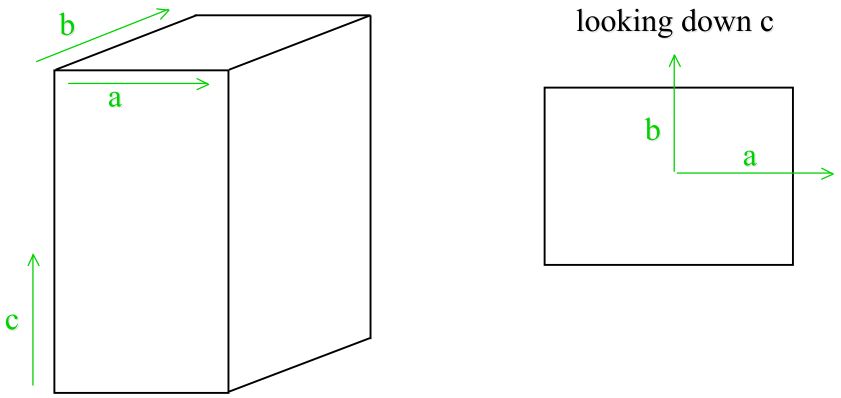
Thus it's the orientation & angles that are the best source of our indexing

Miller Index is the accepted indexing method

It uses the relative intercepts of the face in question with the crystal axes

Crystal Morphology

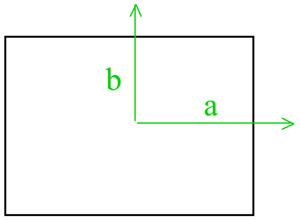
Given the following crystal:



2-D view
looking down c

Crystal Morphology

Given the following crystal:

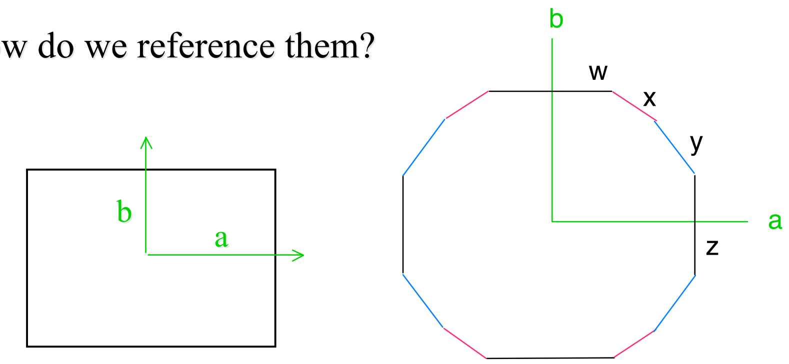


How reference faces?
- a face?
- b face?
- -a and -b faces?

Crystal Morphology

Suppose we get another crystal *of the same mineral* with 2 other sets of faces:

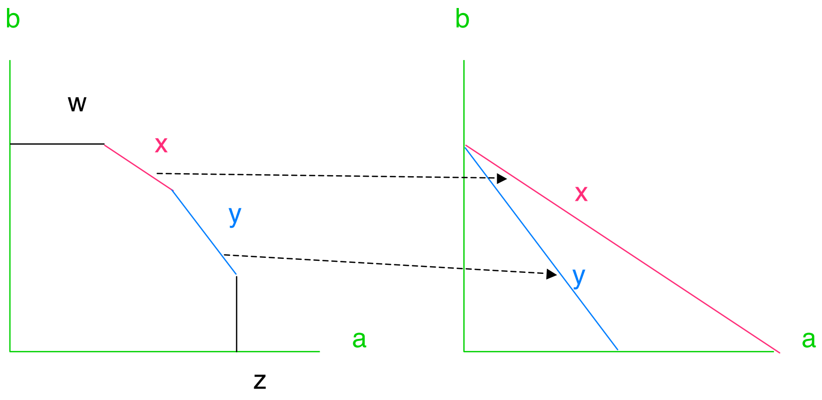
How do we reference them?



Miller Index uses the *relative* intercepts of the faces with the axes

Pick a reference face that intersects both axes

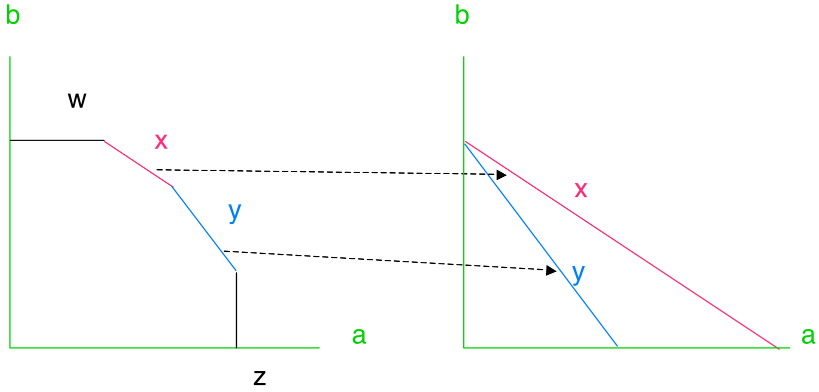
Which one?



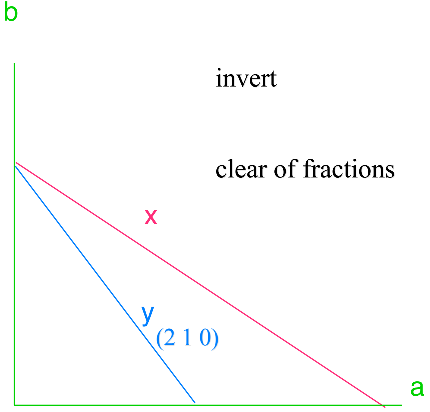
Which one?

Either x or y. The choice is arbitrary. Just pick one.

Suppose we pick x

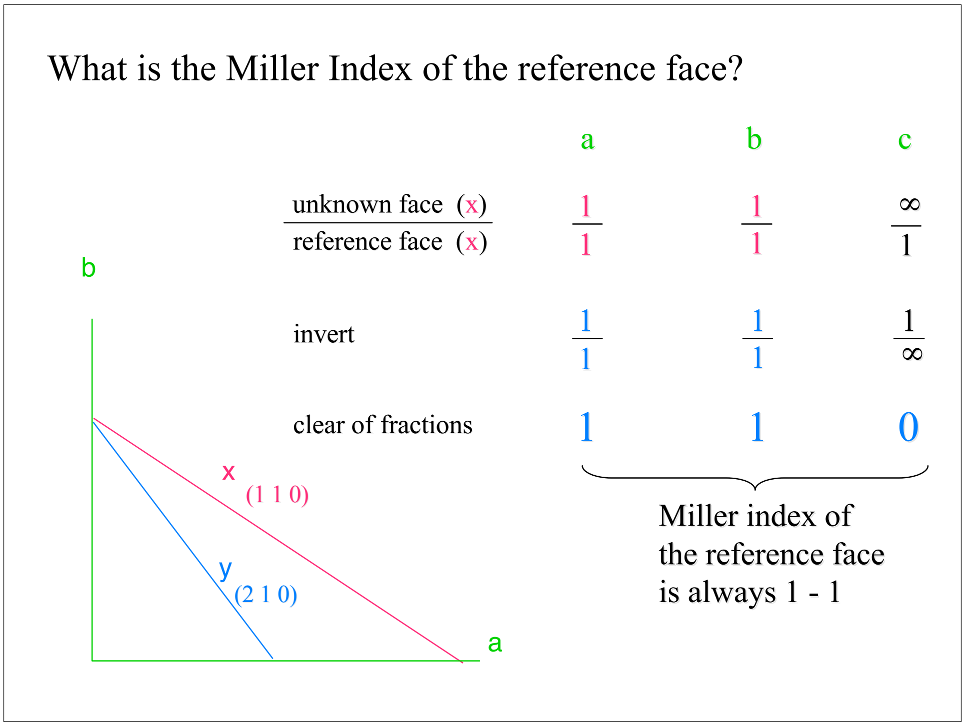


MI process is very structured (“cook book”)



	a	b	c
$\frac{\text{unknown face (y)}}{\text{reference face (x)}}$	$\frac{1}{2}$	$\frac{1}{1}$	$\frac{\infty}{1}$
invert	$\frac{2}{1}$	$\frac{1}{1}$	$\frac{1}{\infty}$
clear of fractions	2	1	0

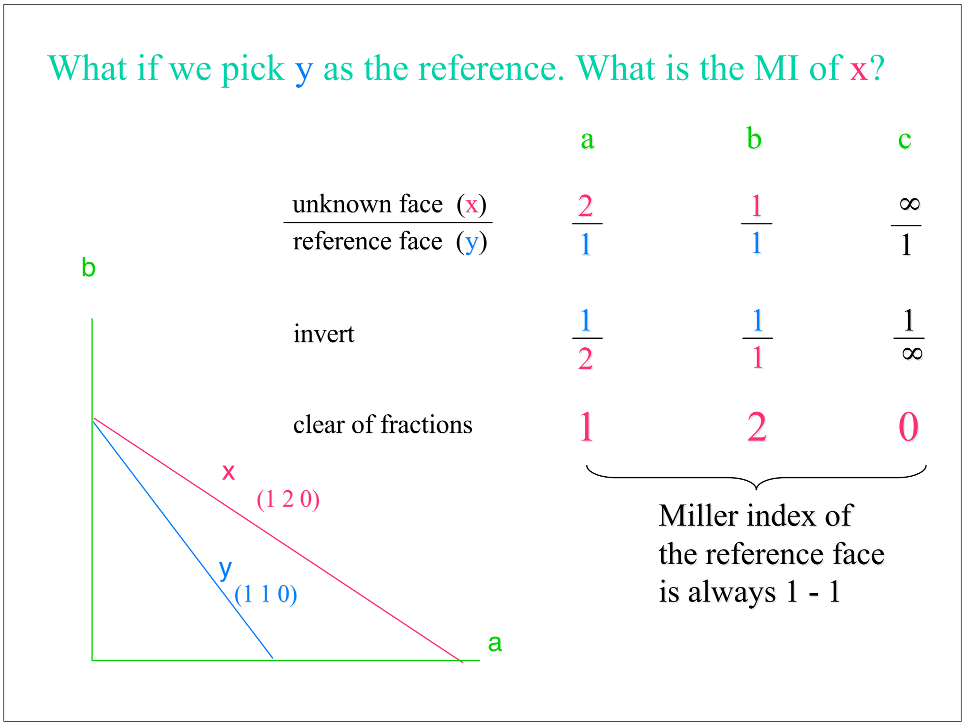
Miller index of
face y using x as
the a-b reference face



What is the Miller Index of the reference face?

	a	b	c
$\frac{\text{unknown face (x)}}{\text{reference face (x)}}$	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{\infty}{1}$
invert	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{\infty}$
clear of fractions	1	1	0

Miller index of the reference face is always 1 - 1

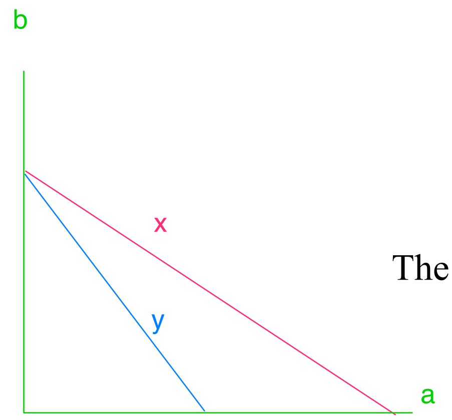


What if we pick y as the reference. What is the MI of x?

	a	b	c
$\frac{\text{unknown face (x)}}{\text{reference face (y)}}$	$\frac{2}{1}$	$\frac{1}{1}$	$\frac{\infty}{1}$
invert	$\frac{1}{2}$	$\frac{1}{1}$	$\frac{1}{\infty}$
clear of fractions	1	2	0

Miller index of the reference face is always 1 - 1

Which choice is correct?



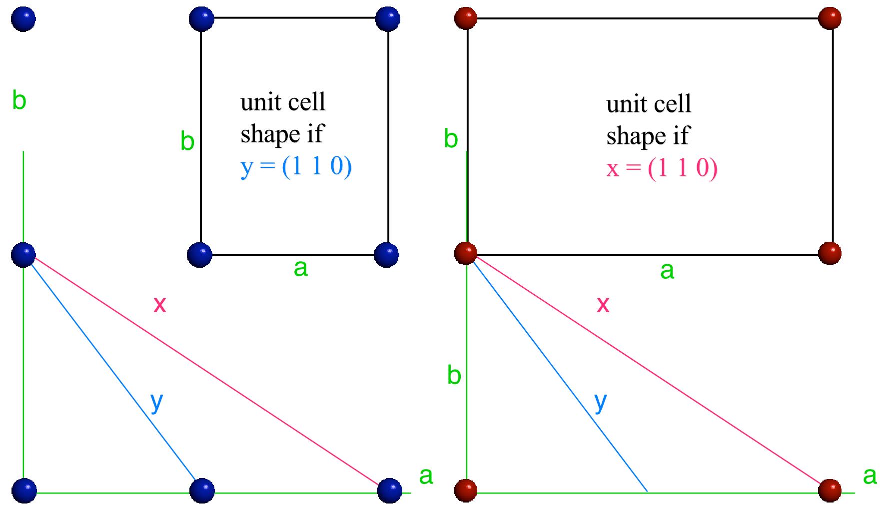
1) $x = (1\ 1\ 0)$
   $y = (2\ 1\ 0)$

2) $x = (1\ 2\ 0)$
   $y = (1\ 1\ 0)$

The choice is arbitrary

What is the difference?

What is the difference?

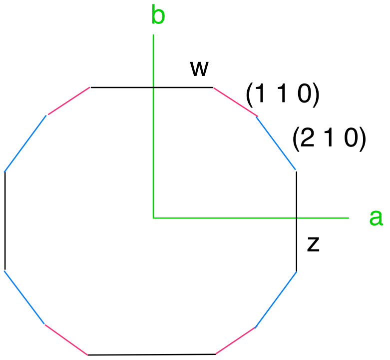


axial ratio = a/b = 0.80

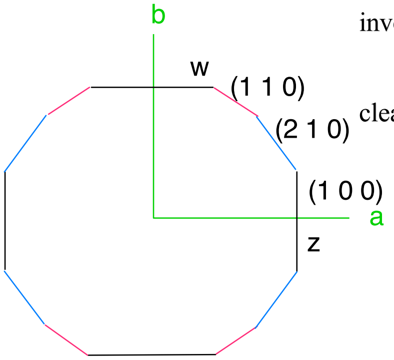
axial ratio = a/b = 1.60

What are the Miller Indices of all the faces if we choose x as the reference?

Face Z?



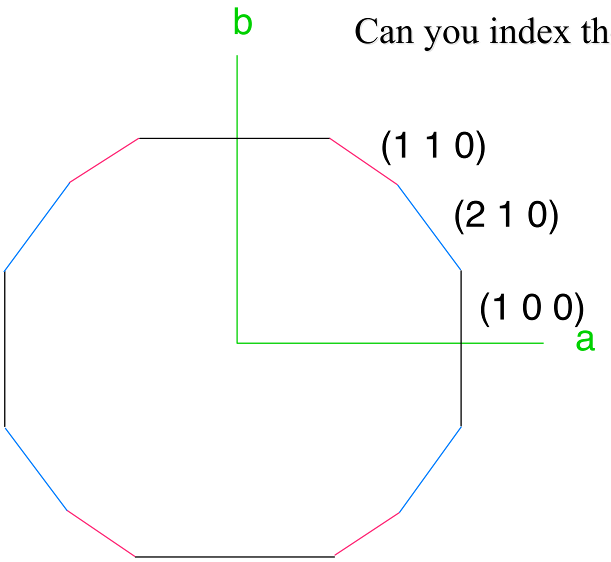
The Miller Indices of face z using x as the reference

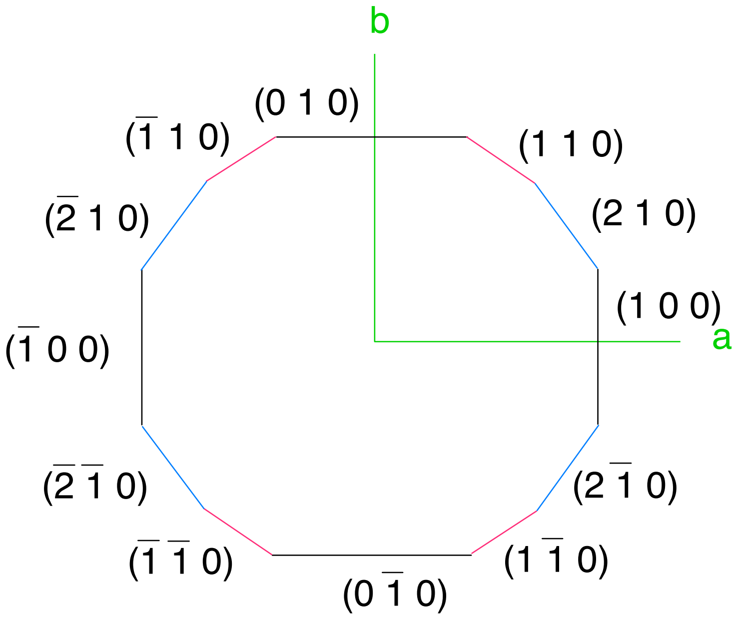


	a	b	c
$\frac{\text{unknown face (z)}}{\text{reference face (x)}}$	$\frac{1}{1}$	$\frac{\infty}{1}$	$\frac{\infty}{1}$
invert	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{\infty}$
clear of fractions	1	0	0

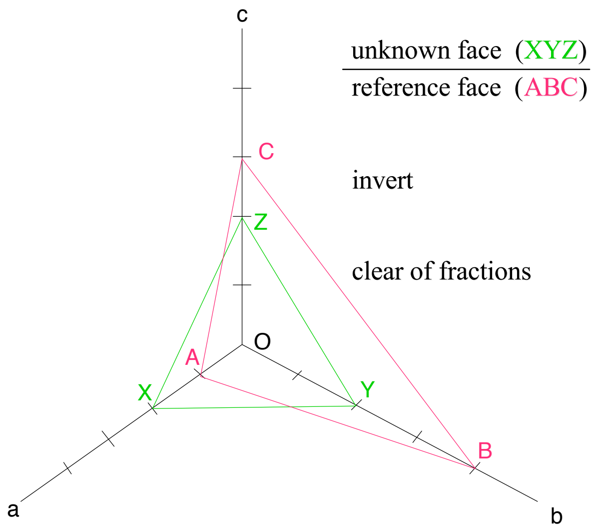
Miller index of face z using x (*or any face*) as the reference face

Can you index the rest?





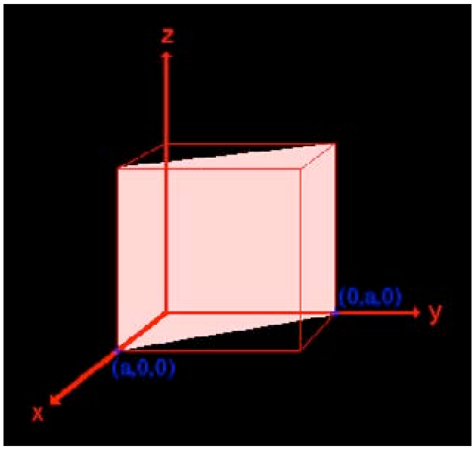
3-D Miller Indices (an unusually complex example)



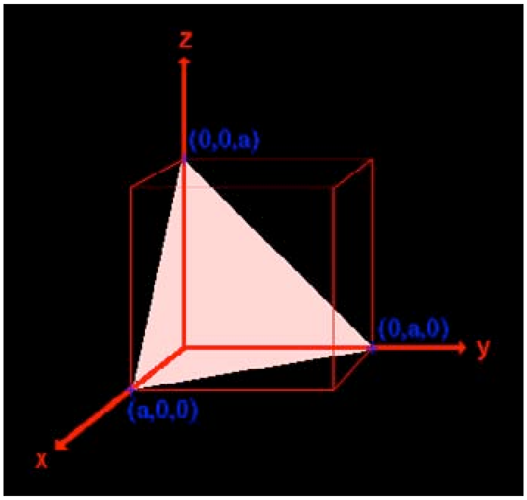
	a	b	c
unknown face (XYZ) / reference face (ABC)	$\frac{2}{1}$	$\frac{2}{4}$	$\frac{2}{3}$
invert	$\frac{1}{2}$	$\frac{4}{2}$	$\frac{3}{2}$
clear of fractions	(1	4	3)

Miller index of face XYZ using ABC as the reference face

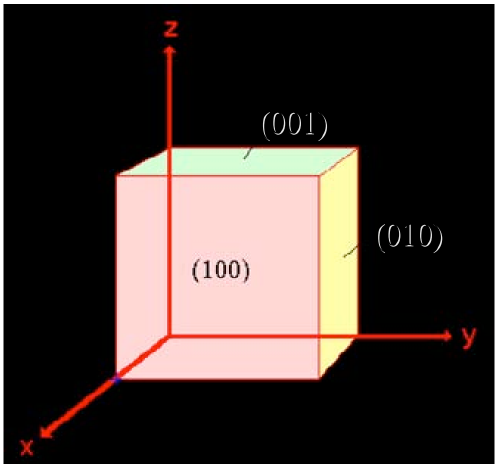
Example: the (110) surface



Example: the (111) surface

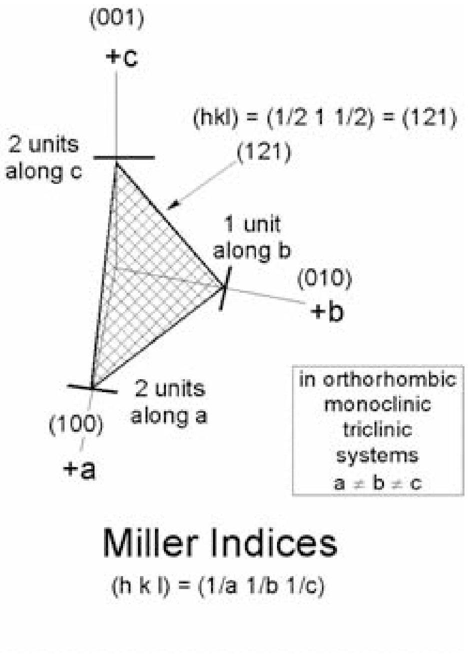


Example: (100), (010), and (001)



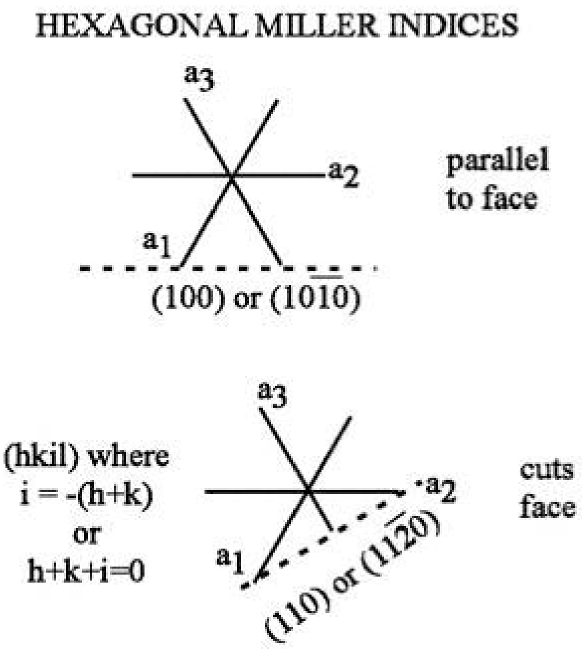
For the isometric system, these faces are equivalent (=zone)

Miller Indices - 3 axes



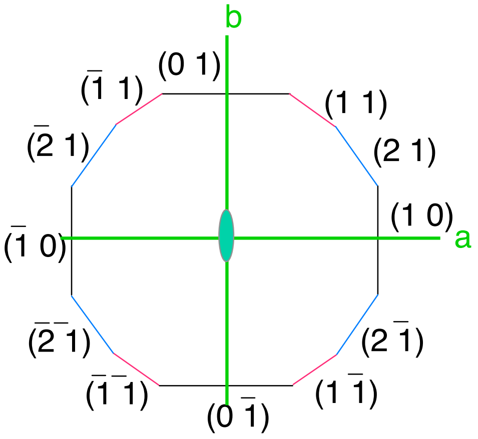
Miller - Bravais Indices

Hexagonal System



Form = a set of symmetrically equivalent faces

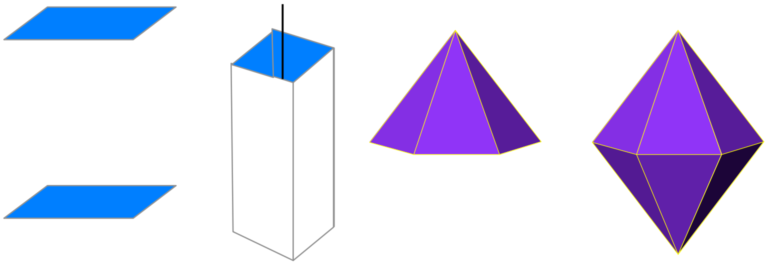
braces indicate a form {210}



Form = a set of symmetrically equivalent faces

braces indicate a form {210}

pinacoid prism pyramid dipryamid



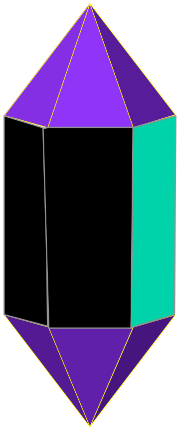
related by a mirror
or a 2-fold axis

related by n-fold
axis or mirrors

Form = a set of symmetrically equivalent faces

braces indicate a form {210}

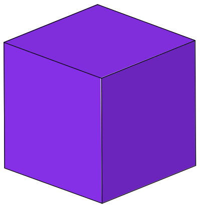
Quartz = 2 forms:
  Hexagonal prism (m = 6)
  Hexagonal dipyramid (m = 12)



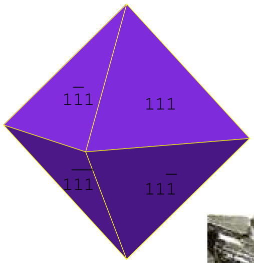
Isometric forms include

Cube

halite

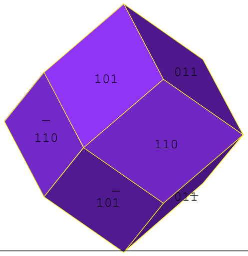


Octahedron



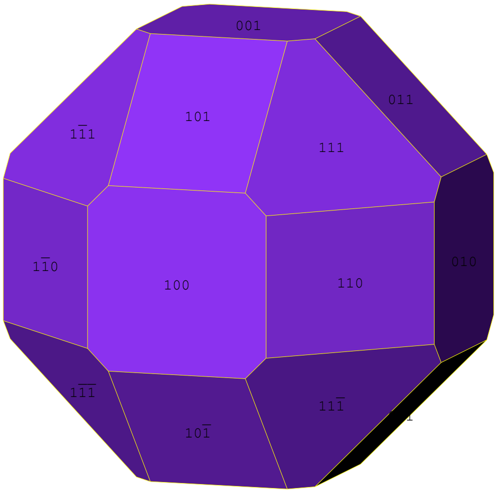
magnetite

Dodecahedron



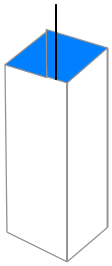
garnet

All three combined:



Zone

Any group of faces || a common axis

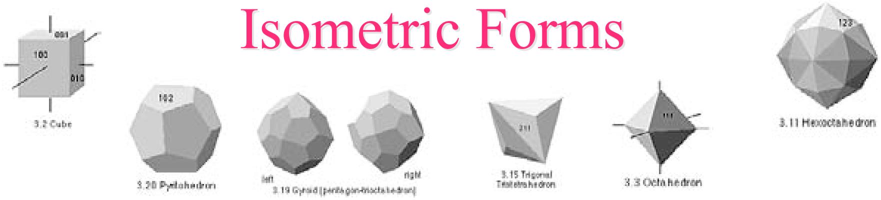


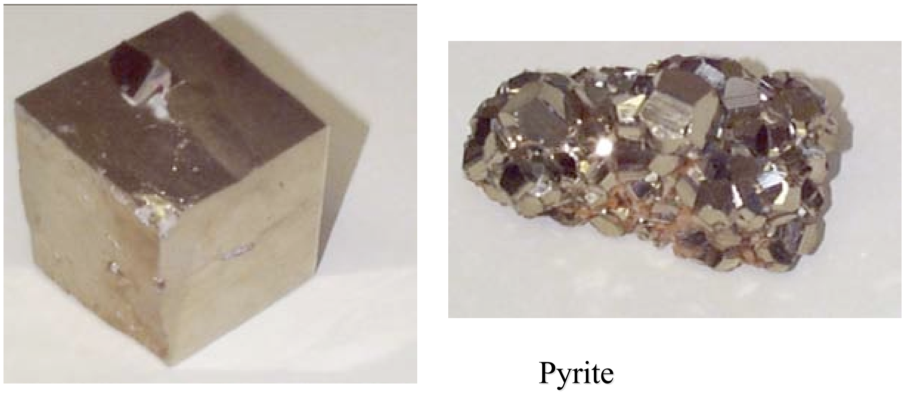
Use of h k l as variables for a, b, c intercepts

(h k 0) = [001]

If the MI’s of 2 non-parallel faces are added, the result = MI of a face between them & in the same zone

Isometric Forms



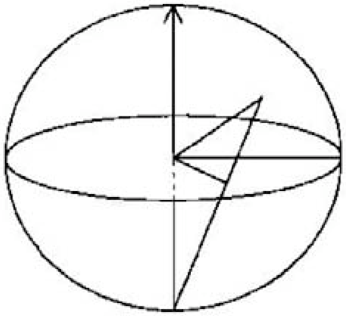


Pyrite

The Cubic Form of Native Copper

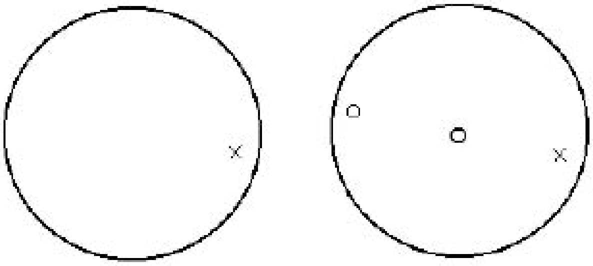
Stereographic Projections

- Used to display crystal morphology.
- X for upper hemisphere.
- O for lower.



- We will use stereographic projections to plot the perpendicular to a general face and its symmetry equivalents (general form *hkl*).

Stereographic Projections

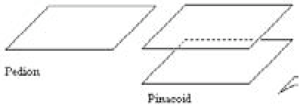


Illustrated above are the stereographic projections for Triclinic point groups 1 and -1

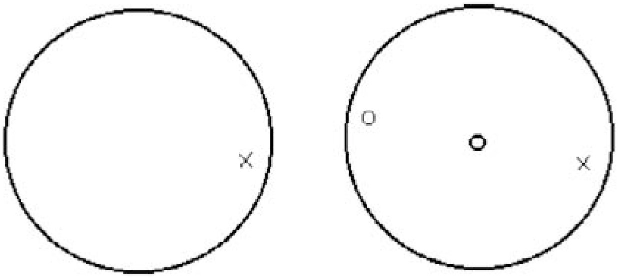
The 32 Point Groups

- **Triclinic**: 1, $\bar{1}$
- **Monoclinic**: 2, $\bar{2}=m$, $2/m$
- **Orthorhombic**: 222, $2mm$, $2/m2/m2/m$ ($=mmm$)
- **Tetragonal**: 4, $\bar{4}$, $4/m$, $\bar{4}2m$, 422 $4mm$ $4/m2/m2/m$
- **Trigonal**: 3, $3m$, 32, $\bar{3}$, $\bar{3}2/m$
- **Hexagonal**: 6, $\bar{6}$, $6/m$, $\bar{6}m2$, 622, $6mm$, $6/m2/m2/m$
- **Cubic**: 23, $2/m\bar{3}$, 432, $\bar{4}3m$, $4/m\bar{3}2/m$

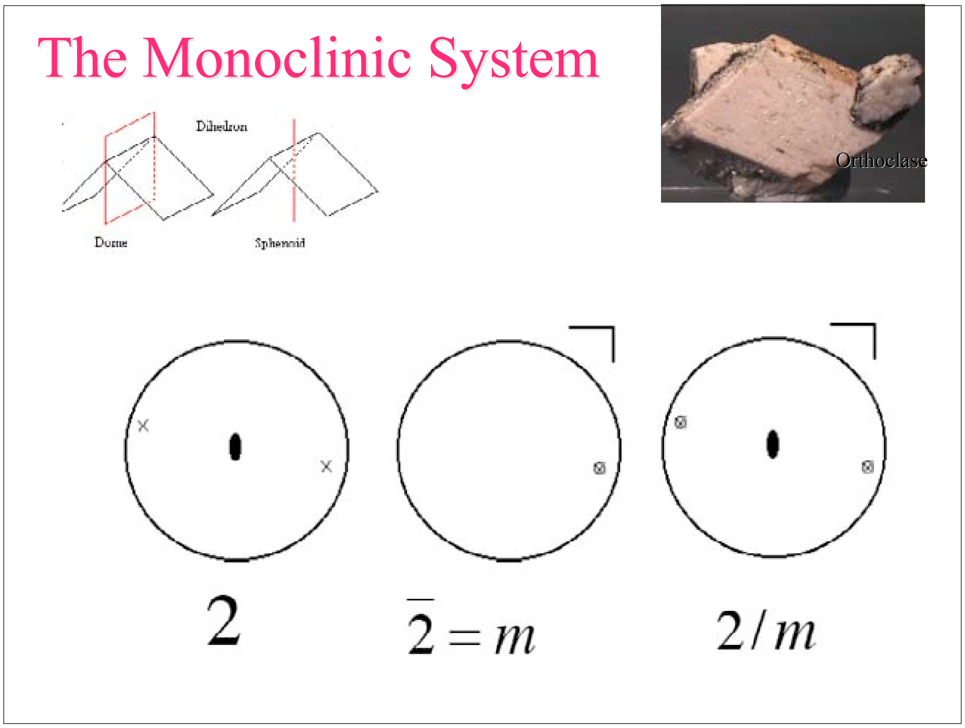
The Triclinic System



microcline

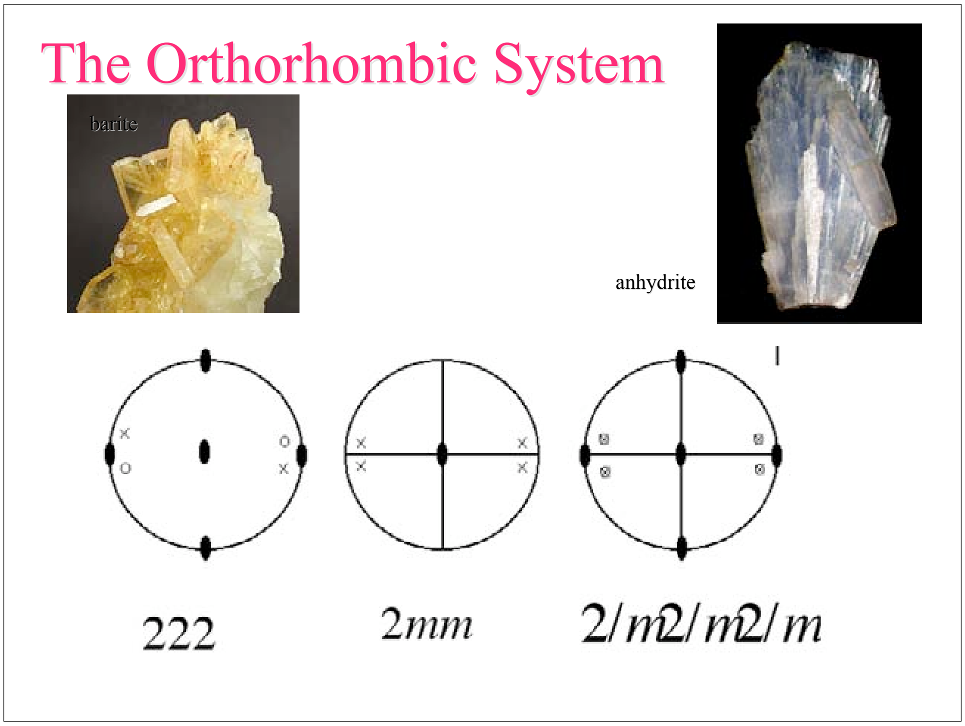


1 $\bar{1}$



The Monoclinic System

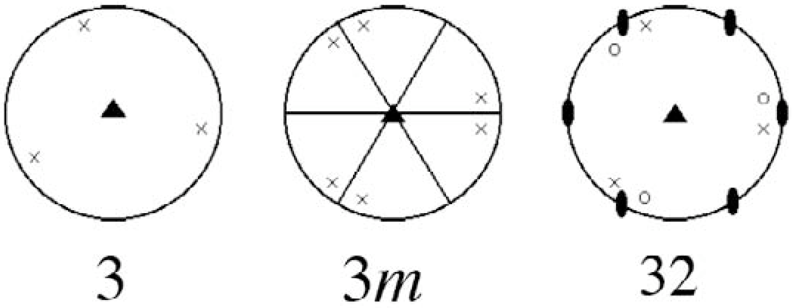
2 $\quad$ $\bar{2} = m$ $\quad$ $2/m$



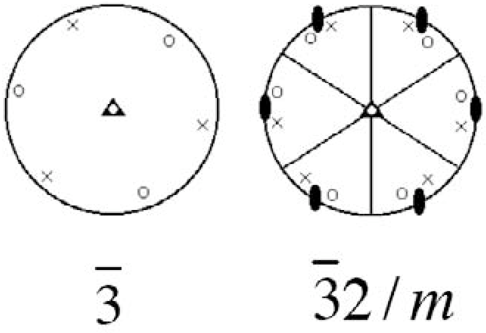
The Orthorhombic System

222 $\quad$ $2mm$ $\quad$ $2/m2/m2/m$

The Trigonal Subsystem



The Trigonal Subsystem

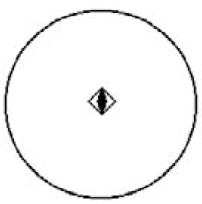


Tourmaline on quartz

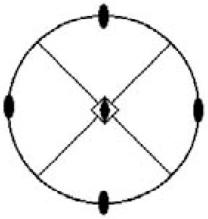
The Tetragonal System

vesuvianite

scapolite



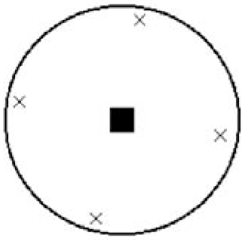
$\bar{4}$



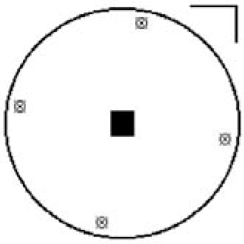
$\bar{4}2m$

The Tetragonal System

rutile

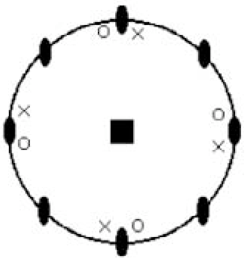


4

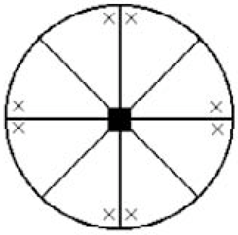


$4/m$

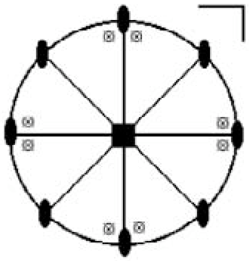
The Tetragonal System



422

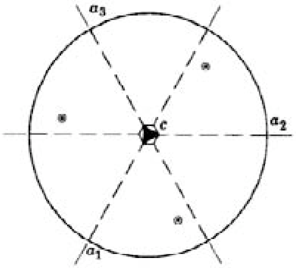


$4mm$

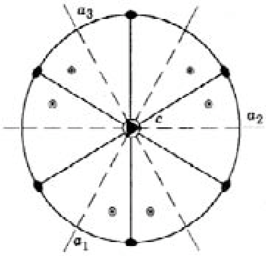


$4/m2/m2/m$

The Hexagonal System

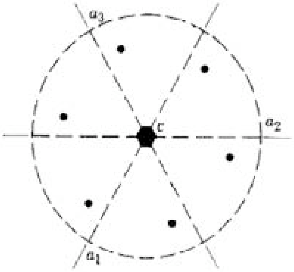


$\bar{6}$

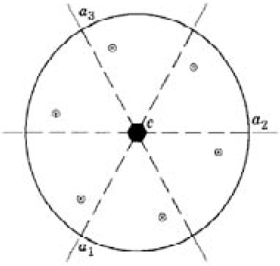


$\bar{6}m2$

The Hexagonal System

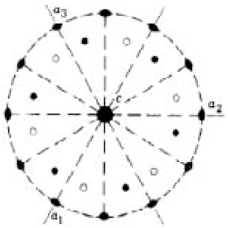


6

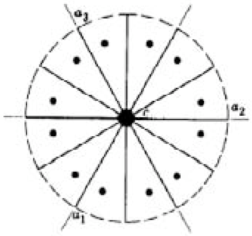


$6/m$

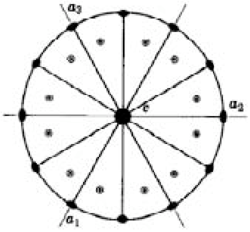
The Hexagonal System



622

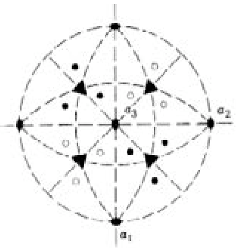


$6mm$

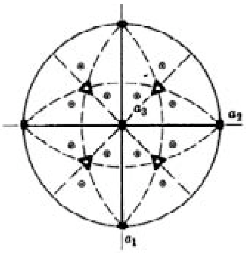


$6/m2/m2/m$

The Isometric System

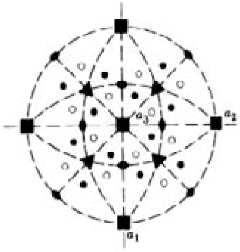


23

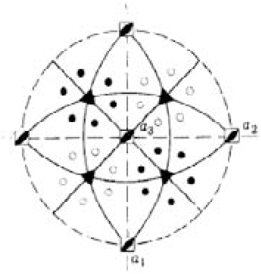


$2/m\bar{3}$

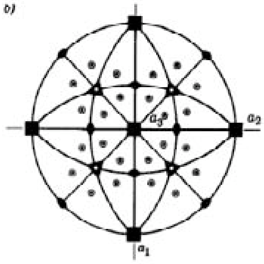
The Isometric System



432



$\bar{4}3m$



$4/m\bar{3}2/m$