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

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**

Drusy Quartz on Barite

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

Crystal Systems

CRYSTAL SYSTEMS are divided into 6 main groups.

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

ISOMETRIC - Fluorite Crystals
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° 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  BASIC CRYSTAL SHAPES

- Octahedron
- Cube
- Cube with Pyritohedron Stirations
- Spinel
- Fluorite
- Pyrite
- Garnet
- Garnet - Dodecahedron
- Trapezohedron

Crystal Systems
● HEXAGONAL  CRYSTALS

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

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

HEXAGONAL Crystal Axes
Crystal Systems

- **HEXAGONAL CRYSTALS**

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

Two subsystems:
1. Hexagonal
2. Trigonal

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Crystal Systems

- **TETRAGONAL CRYSTALS**

**TETRAGONAL**

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

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

- **TETRAGONAL CRYSTALS**

  All hexagonal crystals have a single 3- or 6-fold axis = C

- **ORTHORHOMBIC CRYSTALS**

  **ORTHORHOMBIC**
  Three mutually perpendicular axes of different lengths.

  An alternative crystal axes orientation
  Each axis has symmetry, either 2-fold or m-normal
Crystal Systems

- **ORTHORHOMBIC CRYSTALS**

Topaz from Topaz Mountain, Utah.

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

- **ORTHORHOMBIC CRYSTALS**

STAUROLITE

- **MONOCLINIC CRYSTALS**

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”
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.
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 symmetry conforms to 32 point groups $\rightarrow$ 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

<table>
<thead>
<tr>
<th>Crystal System</th>
<th>No Center</th>
<th>Center</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>$\mathbb{1}$</td>
<td>$\mathbb{1}$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$2, \overline{2}$ ($= m$)</td>
<td>$2/m$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>222, 2mm</td>
<td>2/m 2/m 2/m</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>4, 4, 422, 4mm, $\overline{4}2m$</td>
<td>4/m, 4/m 2/m 2/m</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>3, 3, 3m</td>
<td>$\mathbb{3}, \mathbb{3} 2/m$</td>
</tr>
<tr>
<td>Isometric</td>
<td>23, 432, $\overline{4}3m$</td>
<td>2/m $\overline{3}, 4/m \overline{3} 2/m$</td>
</tr>
</tbody>
</table>
Six Crystal Systems

<table>
<thead>
<tr>
<th>3-D Lattice Types</th>
<th>Name</th>
<th>axes</th>
<th>angles</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Triclinic</td>
<td>( a \neq b \neq c )</td>
<td>( \alpha \neq \beta \neq \gamma \neq 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Monoclinic</td>
<td>( a \neq b \neq c )</td>
<td>( \alpha = \gamma = 90^\circ \beta \neq 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Orthorhombic</td>
<td>( a \neq b = c )</td>
<td>( \alpha = \beta - \gamma = 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Tetragonal</td>
<td>( a_1 = a_2 = c )</td>
<td>( \alpha = \beta = \gamma = 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Hexagonal</td>
<td>( a_1 = a_2 = a_3 \neq c )</td>
<td>( \beta = 90^\circ \gamma = 120^\circ )</td>
</tr>
<tr>
<td></td>
<td>Hexagonal (4 axes)</td>
<td>( a_1 = a_2 = a_3 \neq c )</td>
<td>( \alpha = \beta = \gamma = 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Rhombohedral</td>
<td>( a_1 = a_2 = a_3 )</td>
<td>( \alpha = \beta = \gamma = 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>Isometric</td>
<td>( a_1 = a_2 = a_3 )</td>
<td>( \alpha = \beta = \gamma = 90^\circ )</td>
</tr>
</tbody>
</table>

Axial convention: “right-hand rule”
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
\( \alpha \neq \beta \neq \gamma \neq 90^\circ \)

Monoclinic
\( \alpha = \gamma = 90^\circ, \beta \neq 90^\circ \)

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 \( c \).
Orthorhombic and Tetragonal

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.

Hexagonal

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

Crystal Axes

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

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 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 or 4bar. The b axis in monoclinic crystals is a 2-fold 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

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”)

<table>
<thead>
<tr>
<th></th>
<th>( a )</th>
<th>( b )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>unknown face</td>
<td>( \frac{1}{2} )</td>
<td>( 1 )</td>
<td>( \infty )</td>
</tr>
<tr>
<td>reference face</td>
<td>( \frac{1}{1} )</td>
<td>( 1 )</td>
<td>( \frac{1}{1} )</td>
</tr>
<tr>
<td>invert</td>
<td>( \frac{2}{1} )</td>
<td>( 1 )</td>
<td>( \frac{1}{\infty} )</td>
</tr>
<tr>
<td>clear of fractions</td>
<td>2</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Miller index of face \( y \) using \( x \) as the \( a-b \) reference face
What is the Miller Index of the reference face?

\[
\begin{array}{ccc}
\text{unknown face (x)} & a & b & c \\
\text{reference face (x)} & 1 & 1 & \infty \\
\text{invert} & 1 & 1 & 1 \\
\text{clear of fractions} & 1 & 1 & 0 \\
\end{array}
\]

Miller index of the reference face is always 1 - 1

---

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

\[
\begin{array}{ccc}
\text{unknown face (x)} & a & b & c \\
\text{reference face (y)} & 2 & 1 & \infty \\
\text{invert} & 1 & 1 & 1 \\
\text{clear of fractions} & 1 & 2 & 0 \\
\end{array}
\]

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?

axial ratio = \( a/b = 0.80 \)
axial ratio = \( a/b = 1.60 \)
What are the Miller Indices of all the faces if we choose \textit{x} as the reference?

Face \textit{Z}? 

The Miller Indices of face \textit{z} using \textit{x} as the reference

\[
\begin{array}{ccc}
\text{unknown face (z)} & \frac{1}{1} & \infty \quad \infty \\
\text{reference face (x)} & \frac{1}{1} & \frac{1}{1} \quad \frac{1}{1} \\
\end{array}
\]

invert

\[
\begin{array}{ccc}
1 & \frac{1}{1} & \frac{1}{1} \\
\end{array}
\]

clear of fractions

\[
\begin{array}{ccc}
1 & 0 & 0 \\
\end{array}
\]

Miller index of face \textit{z} using \textit{x} (or any face) as the reference face
Can you index the rest?
3-D Miller Indices (an unusually complex example)

unknown face \((XYZ)\)

reference face \((ABC)\)

inject

clear of fractions

\[
\begin{array}{ccc}
a & b & c \\
\frac{2}{1} & \frac{2}{4} & \frac{2}{3} \\
\frac{1}{2} & \frac{4}{2} & \frac{3}{2} \\
(1 & 4 & 3)
\end{array}
\]

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 MILLER INDICES

Hexagonal System

(hkil) where
\(i = -(h+k)\)
or\( h+k+i=0 \)
**Form** = a set of *symmetrically equivalent* faces
braces indicate a form \{210\}
**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
- Octahedron
- Dodecahedron

Halite
Magnetite
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).

Illustrated above are the stereographic projections for Triclinic point groups 1 and -1.
The 32 Point Groups

- **Triclinic**: \(1, \overline{1}\)
- **Monoclinic**: \(2, \overline{2}=m, 2/m\)
- **Orthorhombic**: \(222, 2mm, 2/m2/m2/m (=mmm)\)
- **Tetragonal**: \(4, \overline{4}, 4/m, \overline{4}2m, 422, 4mm, 4/m2/m2/m\)
- **Trigonal**: \(3, 3m, 32, \overline{3}, \overline{3}2/m\)
- **Hexagonal**: \(6, \overline{6}, 6/m, \overline{6}m2, 622, 6mm, 6/m2/m2/m\)
- **Cubic**: \(23, 2/m3, 432, \overline{4}3m, 4/m32/m\)

The Triclinic System
The Monoclinic System

The Orthorhombic System
The Trigonal Subsystem

3 \hspace{1cm} 3m \hspace{1cm} 32

The Trigonal Subsystem

\bar{3} \hspace{1cm} \bar{32} / m
The Tetragonal System

- Vesuvianite
- Scapolite
- Rutile

Diagram showing crystallographic symbols 4 and 42m.

The Tetragonal System

Diagram showing crystallographic symbols 4 and 4/m.
The Tetragonal System

The Hexagonal System
The Hexagonal System

beryl

6

6/m

The Hexagonal System

zincite

622
6mm
6/m2/m2/m
The Isometric System

23  \hspace{1cm} 2/m\overline{3}

The Isometric System

432  \hspace{1cm} \overline{4}3m  \hspace{1cm} 4/m\overline{3}2/m