

CRYSTAL MEASUREMENT AND AXIAL RATIO LABORATORY

George R. McCormick

Department of Geology
The University of Iowa
Iowa City, Iowa 52242
george_mccormick@uiowa.edu

Goals of the Exercise

This exercise is designed to help you understand relationships among external morphology of crystals (their shape and faces), internal structure (unit cell shape, edge measurements, and volume), Hermann-Mauguin notation for the 32 crystal classes, and Miller Indices of forms and faces. When you look up the information on any mineral in a standard reference or text book such as Dana's *Manual of Mineralogy* (Klein and Hurlbut, 1993) or *Introduction to the Rock Forming Minerals* (Deer, Howie, and Zussman, 1966) you will note that the following crystallographic information is given: crystal class in Hermann-Mauguin notation, axial ratios (relative unit cell lengths), absolute unit cell lengths (in Angstrom units), and common crystal forms present in terms of Miller Indices. Some references may also give Φ (Phi) and ρ (Rho) values for each form. These values have been determined by measurement of the external form of the crystal and can be used to plot the forms or faces on a Wulff stereographic projection. This exercise should help you to understand and use this standard mineralogical information.

Before proceeding with the exercise you should have an understanding of the symmetry elements present in the 32 crystal classes and how they are represented by Hermann-Mauguin notation. You should also understand the differences between the axial ratio and absolute cell lengths of a mineral, the meaning and use of Miller Indices, and how mineral faces and forms are plotted on a Wulff stereographic projection. These subjects are covered with examples in most mineralogy textbooks.

How Crystals are Measured

Each crystal face can be identified by two angular measurements, Φ (Phi) and ρ (Rho). The Rho angle is the angle measured along a great circle from the **c**-crystallographic axis to the **face pole** (a line perpendicular to the face). The Phi angle is the angle measured in the plane of the equator of the crystal from the + **b** axis to the great circle in which the face pole is located. These measurements are similar to the latitude and longitude of any geographic location on earth. Longitude is measured from the Greenwich meridian (a great circle passing through the north and south poles) in the plane of the equator to the great circle on which the geographic location is located. Latitude is measured along a great circle from the equator to the geographic location. Great circles are circles that pass through both the north and south pole (longitude in geographical terms); small circles are planes parallel to the equator (latitude in geographical terms).

Measurements are made by an instrument called a **goniometer**. These can range from very sophisticated two-circle models with microscope and telescope to a very simple one made with a protractor and ruler. All goniometers are designed to measure the interfacial angles between perpendiculars to faces (face poles). Examples of goniometers and how to use them are found in mineralogy textbooks such as *Manual of Mineralogy*, (Klein and Hurlbut, 1993).

Measurements on a goniometer are usually made in **zones**. All faces are said to be in a zone if they all lie parallel to one crystallographic direction, e.g. all faces parallel to a **c**-crystallographic axis are in the same zone. The sum of all angles measured between face poles in a zone should be 360° . If the total is not 360° a mistake has been made -- either a number was read wrong or an angle missed that should be measured.

Faces are grouped together in **forms**. Each face in a form has the same angular relationship to each of the crystallographic axes. The Form symbol chosen is that for the most positive face, e.g. for a cube there are 6 faces (001), (00 $\bar{1}$), (100), ($\bar{1}$ 00), (010), (0 $\bar{1}$ 0) and the form symbol chosen is {100}. Notice that braces are used to indicate forms.

The Wulff Stereographic Projection

Once a crystal has been measured and each face assigned Φ and ρ values, one can then plot the faces on a Wulff stereonet (also known as an equal angle net) to determine the symmetry of the crystal, and thus, to determine the crystal class to which it belongs. The description of the method of plotting faces on a Wulff projection are found in all mineralogy textbooks such as *Manual of Mineralogy* (Klein and Hurlbut, 1993).

Calculating the Axial Ratio

After you have measured a crystal, plotted all the faces on a stereographic projection, determined all the symmetry elements present, and determined the crystal system to which the crystal belongs, you are then ready to calculate the axial ratios. You first must choose a face that cuts all three crystallographic axes and arbitrarily give it the Miller Index (111). This is called a **parametral plane**. When more than one form cuts all three crystallographic axes it is customary to take the form with the larger faces as the parametral plane, however, either one could be chosen.

It is not necessary to calculate an axial ratio for an isometric crystal because all three crystallographic axes are the same length and all angles are 90° . However, it is possible to calculate axial ratios for a crystal in any of the other crystal systems. Axial ratio's for the tetragonal and hexagonal crystal systems are written **a:c** where **a = 1** (by convention) and the axial ratio's for the orthorhombic, monoclinic and triclinic crystal systems are written as **a:b:c** where **b = 1** (also by convention). This exercise deals only with crystals in the tetragonal and orthorhombic crystal systems to simplify the calculations needed. Calculations for other crystal systems are simplified by a matrix algebra approach (see Gibbs, this volume). The equations for **a** and **c** are as follows:

$$a = h (\cot \Phi) / k \qquad c = l (\tan \rho) (\cos \Phi) / k$$

where **h**, **k**, and **l** are from the Miller Index for the face (**hkl**) and are all one if the face is (111).

Calculation of Miller Indices

Once an axial ratio is determined for a crystal by the equations above, it is possible to calculate the Miller Index of each face or form on the crystal using the same equations in a slightly different form as shown below:

$$k / h = (\cot \Phi) / a \qquad k / l = (\tan \rho) (\cos \Phi) / c$$

Keep in mind that once an axial ratio is determined for a crystal, the same value for **a** and **c** should be used to calculate the Miller Index of each face. There are several exceptions: (1) Any face that cuts one axis and is parallel to two other axes can be indexed by inspection, e.g. (001), (010), or (00 $\bar{1}$); and (2) it is not possible to calculate the Miller Index for any face parallel to the **b**-axis as the angle $\Phi = 90^\circ$ and thus the cosine and cotangent values in the above formulas would be 0. A practical solution to the problem is to exchange the **a** and **b** values in the axial ratio, divide **a**, **b**, and **c** with the old **a** value, and use the new **a** and **c** values in the above equation for that face (**a:b:c** is **a:1:c = 1/a : 1/a : c/a**). (See the worked example.)

A Checklist for Crystal Measurement

- 1) Make a sketch of the mineral and label each face with a small letter such as a, b, c, etc. to identify the face.
 - 2) Measure all interfacial angles by zones and list the angles for each zone.
 - 3) Chose an orientation for the mineral and make an angle table of Φ and ρ values.
 - 4) Plot each face on a Wulff projection using the Φ and ρ values for each face.
 - 5) Determine the symmetry elements that are present from the arrangement of the faces, mark the symmetry on the net, from this determine the crystal class, and label your diagram with the Hermann-Mauguin notation for that class.
 - 6) Choose one face which cuts all three axes as the parametral plane and arbitrarily give it the Miller Index (1 1 1).
 - 7) Calculate the axial ratio.
 - 8) Group the faces into forms and make a Table of Forms.
 - 9) Calculate the Miller Index for each of the remaining forms.
-

References

- Klein, C. and Hurlbut, C.S., Jr., (1993) *Manual of Mineralogy*, 21st Edition: New York, John Wiley and Sons, 681p.
- Deer, W.A., Howie, R.A., and Zussman, J. (1966) *An Introduction to the Rock-Forming Minerals*: New York, John Wiley and Sons, 528p.

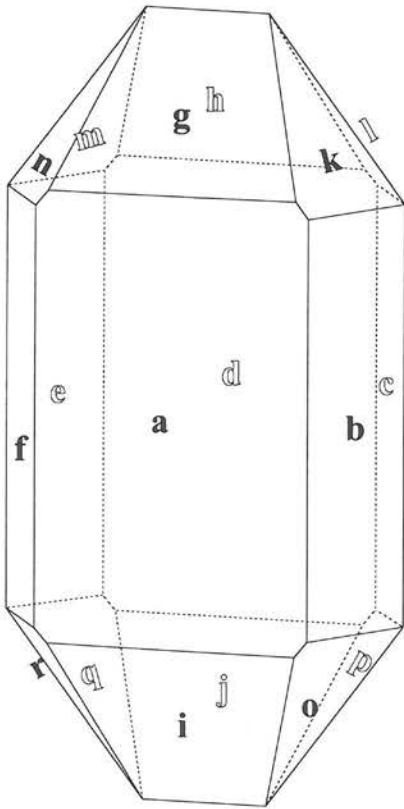
Notes for the Instructor

The example and four crystal measurement problems have been drawn using the computer program SHAPE (see both Brock and Velbel, this volume). Both a single drawing and stereo pair are given for each problem. The stereo pair drawings can be used with the normal stereoscope used to read air photographs. The interfacial angles were calculated by the SHAPE program. If you have access to SHAPE you can design other crystal problems or have students generate the crystal drawing on the computer and then make the calculations ask for in this exercise.

Some geology departments still have access to wooden crystal models (Krantz models). Students can make a simple goniometer with a plastic protractor and ruler and then measure the interfacial angles on the wooden models. They then can make the drawings and angle tables themselves rather than using the computer program.

Example of a Crystal Measurement and Calculation

The crystal drawing and interfacial table for a crystal are shown below:



Interfacial Angles

$$a \wedge b = 58.47^\circ$$

$$b \wedge c = 63.06^\circ$$

$$c \wedge d = 58.47^\circ$$

$$d \wedge e = 58.47^\circ$$

$$e \wedge f = 63.06^\circ$$

$$f \wedge a = 58.47^\circ$$

$$a \wedge g = 31.89^\circ$$

$$g \wedge h = 116.23^\circ$$

$$h \wedge d = 31.89^\circ$$

$$d \wedge i = 31.89^\circ$$

$$i \wedge j = 116.23^\circ$$

$$j \wedge a = 31.89^\circ$$

$$b \wedge k = 33.05^\circ$$

$$k \wedge m = 113.90^\circ$$

$$m \wedge e = 33.05^\circ$$

$$e \wedge q = 33.05^\circ$$

$$q \wedge o = 113.90^\circ$$

$$o \wedge b = 33.05^\circ$$

$$f \wedge n = 33.05^\circ$$

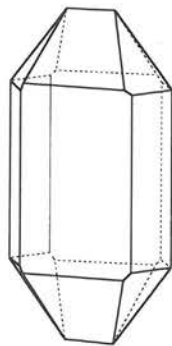
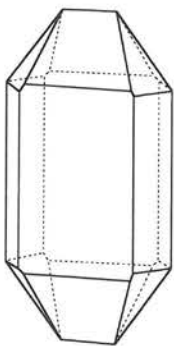
$$n \wedge l = 113.90^\circ$$

$$l \wedge c = 33.05^\circ$$

$$c \wedge p = 33.05^\circ$$

$$p \wedge r = 113.90^\circ$$

$$r \wedge f = 33.05^\circ$$

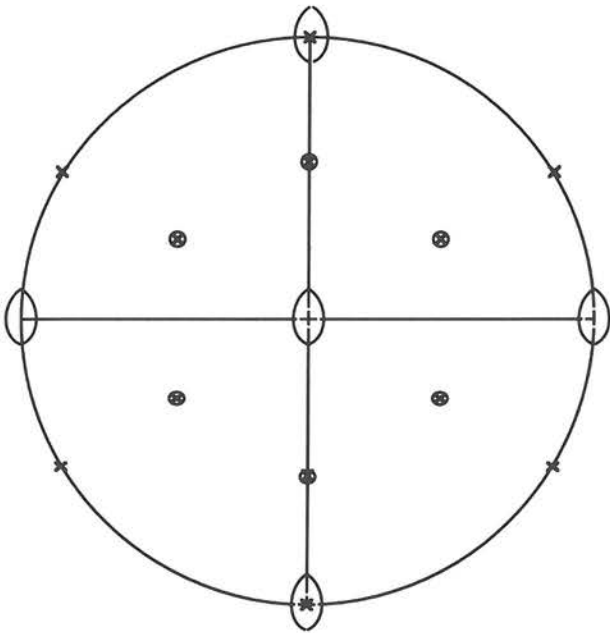


Orient the crystal so that the **a**, **b**, and **c** crystallographic axes are parallel to symmetry axes and calculate the Φ and ρ values for each face.

Angle Table:

<u>face</u>	<u>Φ</u>	<u>ρ</u>
a	90°	90°
b	31.53°	90°
c	-31.53°	90°
d	-90°	90°
e	-148.47°	90°
f	148.47°	90°
g	90°	58.12°
h	-90°	58.12°
i	90°	-58.12°
j	-90°	-58.12°
k	31.53°	56.95°
l	-31.53°	56.95°
m	-148.47°	56.95°
n	148.47°	56.95°
o	31.53°	-56.95°
p	-31.53°	-56.95°
q	-148.47°	-56.95°
r	148.47°	-56.95°

Wulff Projection of all Faces and Symmetry



Hermann-Mauguin symbol for the symmetry shown is $2/m 2/m 2/m$.

Table of Forms

<u>Form</u>	<u>Miller Index</u>	Φ	ρ
a,d	{100}	90°	90°
b,c,e,f	{110}	31.53°	90°
k,l,m,n,o,p,q,r	{111}	31.53°	56.95°
g,h,i,j	{201}	90°	58.12°

Calculation of the Axial Ratio

Use the Parametral plane (111) which you have arbitrarily chosen because it cuts all three crystallographic axes.

$$a = h (\cot \Phi) / k = 1 (\cot 31.53^\circ) / 1 = 1.63$$

$$c = l (\tan \rho) (\cos \Phi) / k = 1 (1.537) (0.852) / 1 = 1.31$$

$$a:b:c = 1.63:1:1.31$$

Calculation of the Miller Index for Each Form

{111} This is the parametral form and is arbitrarily chosen as (111).

{100} Each face in this form cuts only one axis and is parallel to the other two axes. The index is chosen by inspection.

{110} This form is parallel to the **c**-axis and cuts the **a**- and **b**-axes, thus, only one equation is needed.

$$k / h = (\cot \Phi) / a = 1.63 / 1.63 = 1 / 1; \text{ thus the Miller Index is (110)}$$

{201} Whenever a face has a Φ value of 90° the above equations will not work because the cotangent and cosine functions are 0 for 90°. A simple trick can be used to get rid of this $\Phi = 90^\circ$ problem by rotating the crystal 90° and making $\Phi = 0^\circ$.

$$a:b:c = 1.63:1:1.31$$

exchange the **a** and **b** axes thus **b:a:c** = 1:1.63:1.31

$$\text{Divide through by 1.63} \quad (1/1.63):(1.63/1.63):(1.31/1.63) = 0.613:1:0.804$$

Use the axial ratio **a:b:c** = **0.613:1:0.804** together with $\Phi = 0^\circ$ and the ρ value for the form to calculate the Miller Index.

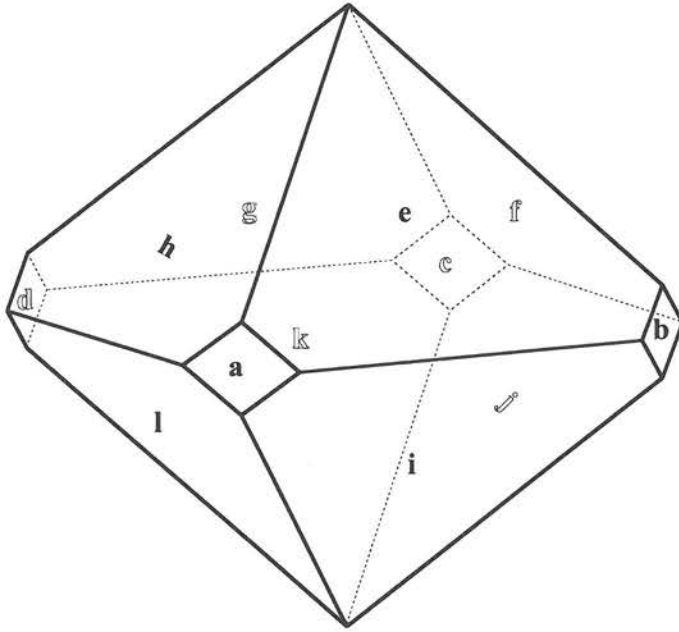
The faces of the form are all parallel to the new **a**-axis so the **h** value in the new Miller Index will be 0 and only the following equation need be used:

$$k / l = (\tan \rho)(\cos \Phi) / c = (\tan 58.12^\circ)(\cos 0^\circ) / 0.804 = (1.608)(1) / 0.804 = 2/1$$

The Miller Index would be (021), however, if the crystal is rotated back to its original position according to the original axial ratio (**a** exchanged for **b**), then the Miller Index is (201).

CRYSTAL MEASUREMENT EXERCISES

Crystal #1



Interfacial Angles

$$a \wedge b = 90^\circ$$

$$b \wedge c = 90^\circ$$

$$c \wedge d = 90^\circ$$

$$d \wedge a = 90^\circ$$

$$e \wedge i = 83.59^\circ$$

$$i \wedge k = 96.41^\circ$$

$$k \wedge g = 83.59^\circ$$

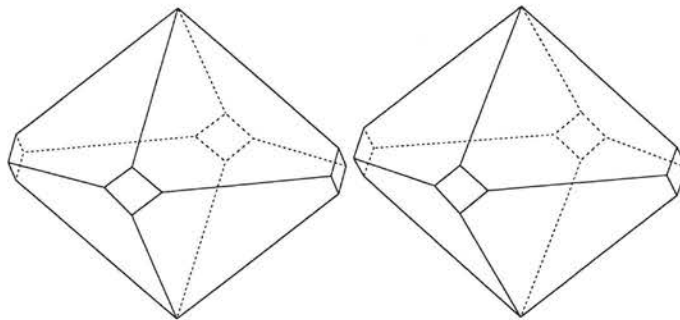
$$g \wedge e = 96.41^\circ$$

$$h \wedge l = 83.59^\circ$$

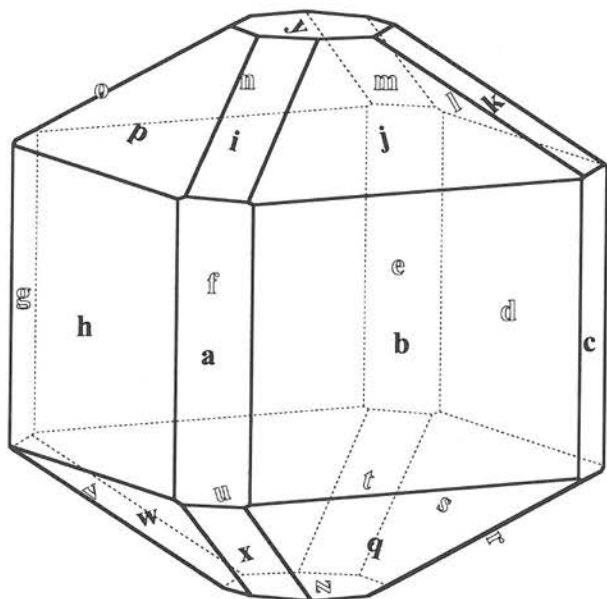
$$l \wedge j = 96.41^\circ$$

$$j \wedge f = 83.59^\circ$$

$$f \wedge h = 96.41^\circ$$



Crystal #2



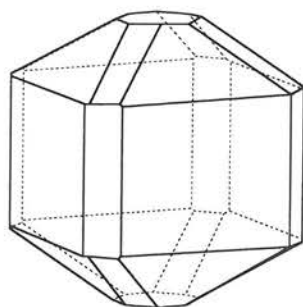
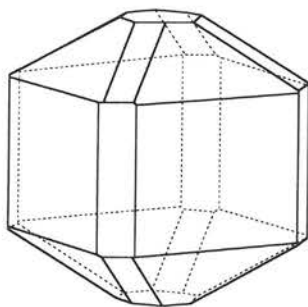
Interfacial Angles

- $a \wedge b = 45^\circ$
- $b \wedge c = 45^\circ$
- $c \wedge d = 45^\circ$
- $d \wedge e = 45^\circ$
- $e \wedge f = 45^\circ$
- $f \wedge g = 45^\circ$
- $g \wedge h = 45^\circ$
- $h \wedge a = 45^\circ$
- $y \wedge k = 29.98^\circ$
- $k \wedge c = 60.02^\circ$
- $c \wedge r = 60.02^\circ$
- $r \wedge z = 29.98^\circ$
- $z \wedge v = 29.98^\circ$
- $v \wedge g = 60.02^\circ$
- $g \wedge o = 60.02^\circ$
- $o \wedge y = 29.98^\circ$

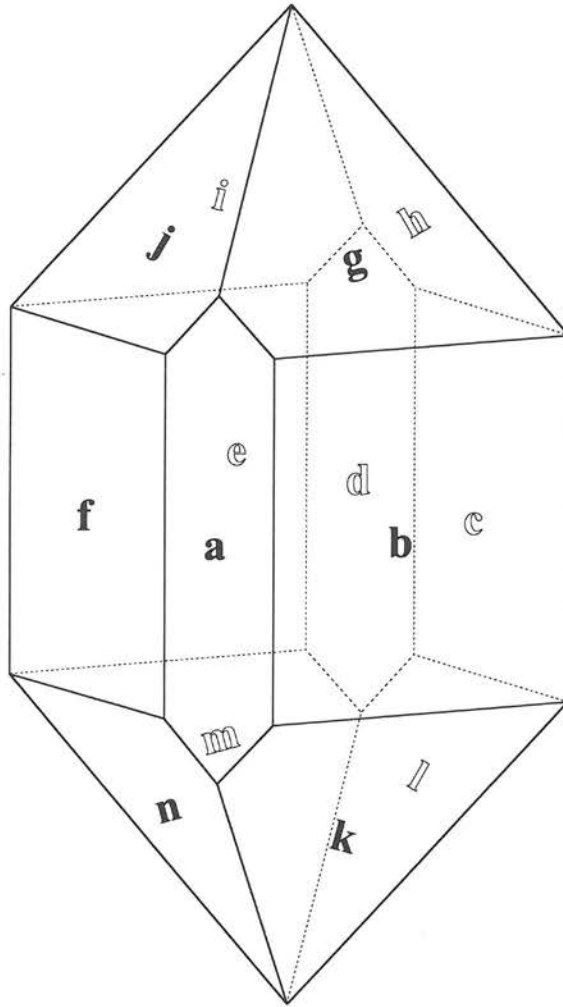
- $y \wedge j = 39.21^\circ$
- $j \wedge b = 50.79^\circ$
- $b \wedge q = 50.79^\circ$
- $q \wedge z = 39.21^\circ$
- $z \wedge u = 39.21^\circ$
- $u \wedge f = 50.79^\circ$
- $f \wedge n = 50.79^\circ$
- $n \wedge y = 39.21^\circ$

- $y \wedge p = 39.21^\circ$
- $p \wedge h = 50.79^\circ$
- $h \wedge w = 50.79^\circ$
- $w \wedge z = 39.21^\circ$
- $z \wedge s = 39.21^\circ$
- $s \wedge d = 50.79^\circ$
- $d \wedge l = 50.79^\circ$
- $l \wedge y = 39.21^\circ$

- $y \wedge i = 29.98^\circ$
- $i \wedge a = 60.02^\circ$
- $a \wedge x = 60.02^\circ$
- $x \wedge z = 29.98^\circ$
- $z \wedge t = 29.98^\circ$
- $t \wedge e = 60.02^\circ$
- $e \wedge m = 60.02^\circ$
- $m \wedge y = 29.98^\circ$



Crystal # 3

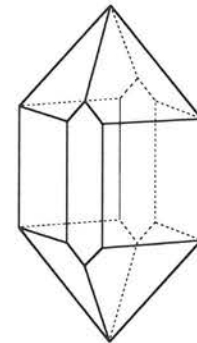
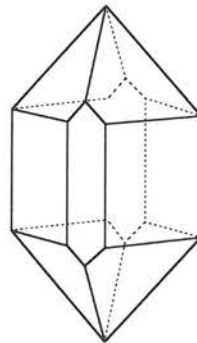


Interfacial Angles

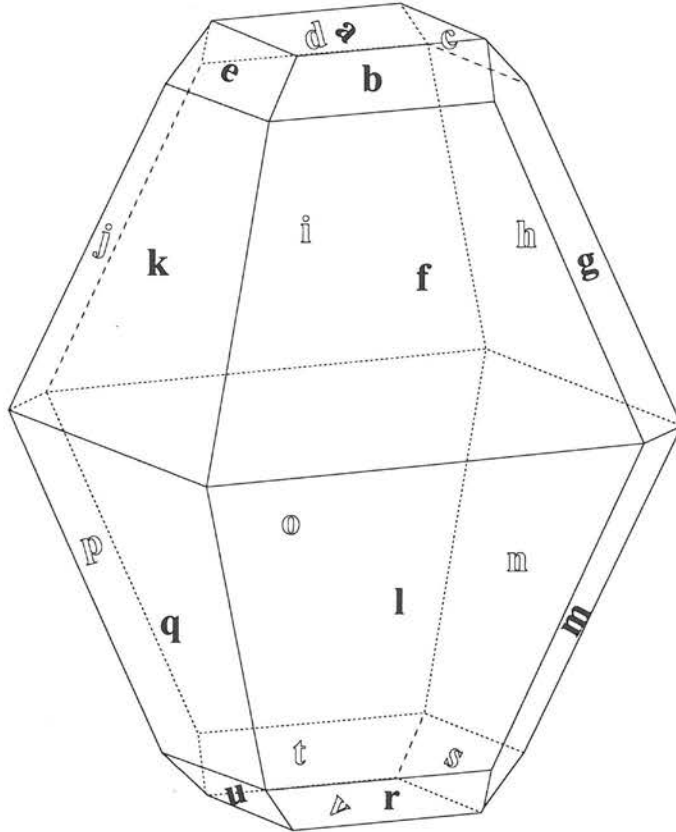
- $a \wedge b = 43.47^\circ$
- $b \wedge c = 93.06^\circ$
- $c \wedge d = 43.47^\circ$
- $d \wedge e = 43.47^\circ$
- $e \wedge f = 93.06^\circ$
- $f \wedge g = 43.47^\circ$

- $g \wedge b = 32.02^\circ$
- $b \wedge k = 32.02^\circ$
- $k \wedge m = 115.95^\circ$
- $m \wedge e = 32.02^\circ$
- $e \wedge i = 32.02^\circ$
- $i \wedge g = 115.95^\circ$

- $j \wedge f = 32.02^\circ$
- $f \wedge n = 32.02^\circ$
- $n \wedge l = 115.95^\circ$
- $l \wedge c = 32.02^\circ$
- $c \wedge h = 32.02^\circ$
- $h \wedge j = 115.95^\circ$



Crystal # 4



Interfacial Angles

- $a \wedge g = 64.54^\circ$
- $g \wedge m = 50.93^\circ$
- $m \wedge v = 64.54^\circ$
- $v \wedge p = 64.54^\circ$
- $p \wedge j = 50.93^\circ$
- $j \wedge a = 64.54^\circ$

- $a \wedge b = 42.85^\circ$
- $b \wedge f = 27.38^\circ$
- $f \wedge l = 39.53^\circ$
- $l \wedge r = 27.38^\circ$
- $r \wedge v = 42.85^\circ$
- $v \wedge t = 42.85^\circ$
- $t \wedge o = 27.38^\circ$
- $o \wedge i = 39.53^\circ$
- $i \wedge d = 27.38^\circ$
- $d \wedge a = 42.85^\circ$

- $a \wedge e = 42.85^\circ$
- $e \wedge k = 27.38^\circ$
- $k \wedge q = 39.53^\circ$
- $q \wedge u = 27.38^\circ$
- $u \wedge v = 42.85^\circ$
- $v \wedge s = 42.85^\circ$
- $s \wedge n = 27.38^\circ$
- $n \wedge h = 39.53^\circ$
- $h \wedge c = 27.38^\circ$
- $c \wedge a = 42.85^\circ$

$h/n \text{ edge} \wedge f/l \text{ edge} = 82.02^\circ$

