

APPENDIX A: *Introduction to Crystallography and Mineral Crystal Systems*

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Part 1: Introduction

Crystallography is a fascinating division of the entire study of mineralogy. Even the non-collector may have an appreciation for large well-developed beautifully symmetrical individual crystals, like those of pyrite from Spain, and groups of crystals, such as quartz from Arkansas or tourmaline from California, because they are esthetically pleasing. To think that such crystals come from the ground "as is" is surprising to many. The lay person simply hasn't had the opportunity to learn about crystals and why they are the way they are; however, neither have many rockhounds and hobbyists.

We hope to bring you to a greater appreciation of natural mineral crystals and their forms by giving you some background and understanding into the world of crystallography. **CRYSTALLOGRAPHY** is simply a fancy word meaning "the study of crystals". At one time the word crystal referred only to quartz crystal, but has taken on a broader definition which includes all minerals with well expressed crystal shapes.

Crystallography may be studied on many levels, but no matter how elementary or in-depth a discussion of the topic we have, we confront some **geometry**. Oh no, a nasty 8-letter word! Solid geometry, no less. But stop and think about it, you use geometry every day, whether you hang sheetrock, pour concrete, deliver the mail, or work on a computer. You just don't think of it as geometry. Geometry simply deals with spatial relationships. Those relationships you are familiar with are not intimidating. The key word here is "familiar". We want this series of articles to help you become more familiar, and, therefore more comfortable, with the geometry involved with the study of crystal forms.

Crystallography is easily divided into 3 sections -- geometrical, physical, and chemical. The latter two involve the relationships of the crystal form (geometrical) upon the physical and chemical properties of any given mineral. We will cover the most significant

geometric aspects of crystallography and leave the other topics for later. We do not intend for this series to be a replacement for a mineralogy textbook, but instead an introduction to the study of crystallography. During and after reading these articles, you will probably want to examine one or two textbooks for more detail about individual subjects. I recommend two: *Klein and Hurlbut's Manual of Mineralogy* (20th edition, 1985) and *Ford's Textbook of Mineralogy* (4th edition, 1932). Both of these are based on E. S. Dana's earlier classic publications.

In any type of study, there exists special words used to summarize entire concepts. This is the special language of the "expert", whether you speak of electrical engineering, computer science, accounting, or crystallography. There's no real way to get around learning some of these basic definitions and "laws" so we might as well jump right into them. ***Get Ready!***

First, let's define what we're dealing with. A **CRYSTAL** is a regular polyhedral form, bounded by smooth faces, which is assumed by a chemical compound, due to the action of its interatomic forces, when passing, under suitable conditions, from the state of a liquid or gas to that of a solid. WOW, what a mouthful! Let's dissect that statement. A polyhedral form simply means a solid bounded by flat planes (we call these flat planes **CRYSTAL FACES**). "A chemical compound" tells us that all minerals are chemicals, just formed by and found in nature. The last half of the definition tells us that a crystal normally forms during the change of matter from liquid or gas to the solid state. In the liquid and gaseous state of any compound, the atomic forces that bind the mass together in the solid state are not present. Therefore, we must first crystallize the compound before we can study its geometry. Liquids and gases take on the shape of their container, solids take on one of several regular geometric forms. These forms may be subdivided, using geometry, into six systems.

But before we can begin to discuss the individual systems and their variations, let's address several other topics which we will use to describe the crystal systems. There's also some laws and rules we must learn.

Way back in 1669, Nicholas Steno, a Danish physician and natural scientist, discovered one of these laws. By examination of numerous specimens of the same mineral, he found that, when measured at the same temperature, the angles between similar crystal faces remain constant regardless of the size or the shape of the crystal. So whether the crystal grew under ideal conditions or not, if you compare the angles between corresponding faces on various crystals of the same mineral, the angle remains the same.

Although he did not know why this was true (x-rays had not yet been discovered, much less x-ray diffraction invented), we now know that this is so because studies of the atomic structure of any mineral proves that the structure remains within a close set of given limits or geometric relationships. If it doesn't, then by the modern definition of a mineral, we are not comparing the same two minerals. We

might be comparing polymorphs, but certainly not the same mineral! (Polymorphs being minerals with the same chemistry, like diamond and graphite or sphalerite and wurtzite, but having differing atomic structure and, therefore, crystallizing in different crystal systems) Steno's law is called the **CONSTANCY OF INTERFACIAL ANGLES** and, like other laws of physics and chemistry, we just can't get away from it.

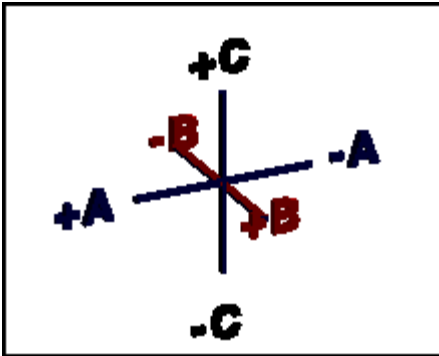
Now, some of you may be thinking: I have a mineral crystal that does not match the pictures in the mineral books. What you may have is a distorted crystal form where some faces may be extremely subordinate or even missing. Distorted crystals are common and result from less-than-ideal growth conditions or even breakage and recrystallization of the mineral. However, remember that we must also be comparing the angles between similar faces. If the faces are not present, then you cannot compare them. With many crystals we are dealing with a final shape determined by forces other than those of the interatomic bonding.

During the process of crystallization in the proper environment, crystals assume various geometric shapes dependent on the ordering of their atomic structure and the physical and chemical conditions under which they grow. If there is a predominant direction or plane in which the mineral forms, different habits prevail. Thus, galena often forms equate shapes (cubes or octahedrons), quartz typically is prismatic, and barite tabular.

To discuss the six crystal systems, we have to establish some understanding of solid geometry. To do this, we will define and describe what are called **CRYSTALLOGRAPHIC AXES**. Since we are dealing with 3 dimensions, we must have 3 axes and, for the initial discussion, let's make them **all equal and at right angles** to each other. This is the simplest case to consider. The axes pass through the center of the crystal and, by using them, we can describe the intersection of any given face with these 3 axes.

Mineralogists had to decide what to call each of these axes and what their orientation in each crystal was so that everyone was talking the same language. Many different systems arose in the early literature. Then, as certain systems were found to have problems, some were abandoned until we arrived at the notational system used today. There exists two of these presently in use, complimentary to each other. One uses number notation to indicate forms or individual faces and the other uses letters to indicate forms. But let's get back to our 3 axes and we'll discuss these two systems later.

We are going to draw each axis on a sheet of paper and describe its orientation. All you need for this exercise is a pencil and paper. Make the first axis vertical, and we'll call it the c axis. The top is the + end and the bottom is the - end. The second axis, the b axis, is horizontal and passes through the center of the c axis. It is the same length as the c axis. The right end is the +, and the left is the -. The third axis is the a axis and passes at a right angle through the join of the b and c axes.

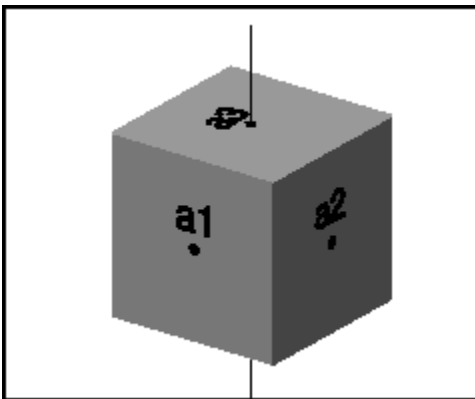


It is somewhat tricky to draw because, even though the a axis is the same length as the c and b axes, because it goes from front to back it **appears** shorter. It is hard to represent a 3-dimensional figure on the 2-dimensional surface of paper, but you can do it. You have to use a sense of perspective, as an artist would say. The front end of a, which appears to come out of the paper, is the + and the back end the - (appears to be in the background or behind the paper).

This all sounds complicated, but look at Figure 1 if you are having problems with drawing the final axis. We always refer to the axes in the order - a, b, c in any type of notation. The point of intersection of the three axes is called the **AXIAL CROSS**.

Perspective is a key to drawing 3 dimensional objects on a flat 2D piece of paper. Perspective is what makes railroad tracks look like they come together in the distance. It is also what causes optical illusions when trying to draw axial crosses, or line drawings of crystal models. Perhaps you've looked at these lines and tried to decide which one comes forward, and which one recedes, and then have the illusion flip-flop so that it looks the other way. That's why they are labeled + and -. It can be confusing, so don't feel like the lone ranger.

We have now reached the point in our discussion that we can actually mention the six large groups or crystal systems that all crystal forms may be placed in. We will use our crystallographic axes which we just discussed to subdivide all known minerals into these systems. The systems are:



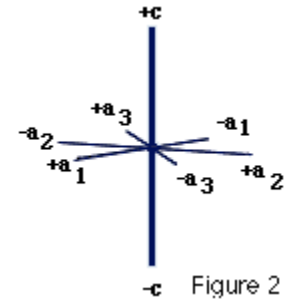
(1) **CUBIC** (aka **ISOMETRIC**) - The three crystallographic axes are all equal in length and intersect at right angles (90 degrees) to each other. This is exactly what you drew to obtain Figure 1. However, we now will rename the axes a1, a2, and a3 because they are the same length (a becomes a1, b becomes a2, and c becomes a3).

(2) **TETRAGONAL** - Three axes, all at right angles, two of which are equal in length (a and b) and one (c) which is different in length (shorter or longer). Note: If c was equal in length to a or b, then we would be in the cubic system! Discussed in part 4.

(3) **ORTHORHOMBIC** - Three axes, all at right angles, and all three of different lengths. Note: If any axis was of equal length to any other, then we would be in the tetragonal system!

Discussed in part 5.

(4) **HEXAGONAL** - Four axes! We must define this situation since it can not be derived from our Figure 1. Three of the axes fall in the same plane and intersect at the axial cross at 120 degrees between the positive ends. These 3 axes, labeled a_1 , a_2 , and a_3 , are the same length. The fourth axis, termed c , may be longer or shorter than the a axes set. The c axis also passes through the intersection of the a axes set at right angle to the plane formed by the a set. Look at Figure 2 to see these relationships more clearly. Discussed in part 6.



(5) **MONOCLINIC** - Three axes, all unequal in length, two of which (a and c) intersect at an oblique angle (not 90 degrees), the third axis (b) is perpendicular to the other two axes. Note: If a and c crossed at 90 degrees, then we would be in the orthorhombic system! Discussed in part 7.

(6) **TRICLINIC** - The three axes are all unequal in length and intersect at three different angles (any angle but 90 degrees). Note: If any two axes crossed at 90 degrees, then we would be describing a monoclinic crystal! Discussed in part 8.

As was stated earlier, all known crystal forms fit into the above six crystal systems. But why don't all crystals in a given set look the same? Or, stated differently, why can't I learn six crystal shapes and know all I need to know? Well, crystals, even of the same mineral, have differing **CRYSTAL FORMS**, depending upon their conditions of growth. Whether they grew rapidly or slowly, under constant or fluctuating conditions of temperature and pressure, or from highly variable or remarkably uniform fluids or melts, all these factors have their influence on the resultant crystal shapes, even when not considering other controls.

We must touch on a type of notation often seen in mineral literature known as **Miller Indices**. Before William H. Miller (1801-1880) devised this mathematical system for describing any crystal face or group of similar faces (forms), there existed a considerable amount of confusion due to the many different descriptive systems. Some of these systems used letter symbols to denote crystal faces and forms. Also different mineralogical "schools" existed as to how a given crystal should be viewed or oriented before assigning the crystallographic axes and then describing the various faces and forms present. If you were of the German school, you had one view; from the English school another thought; from the French school, still another opinion.

So the problem was really one of how to bring order to the literature's chaos. To the problem, Miller (University of Cambridge) applied relatively simple mathematics - the Universal Language. To the lettering systems, Miller described the a, b, c (for hexagonal crystals his notation is four numbers long) intercepts of each planar crystal form as numbers and also made note of the form letter. His

numbering system became widely accepted and is known as Miller indices. The numbers are presented as whole numbers (fractions are not allowed) and are the reciprocal of the actual intercept number, all whole numbers being reduced by their lowest common denominator. Here's a couple of simple examples from the cubic system.

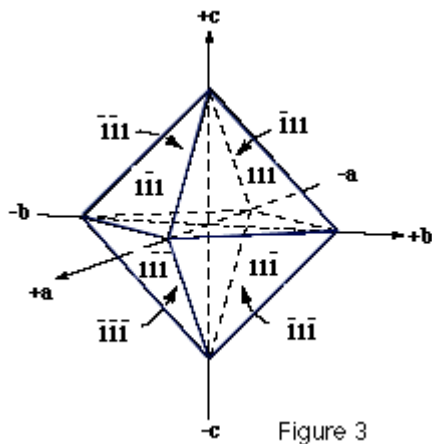


Figure 3

Let us first describe a face of an octahedron and later a cube using Miller's indices. First, we should realize that an octahedron is an eight-sided crystal form that is the simple repetition of an equilateral triangle about our 3 crystallographic axes. The triangle is oriented so that it crosses the a_1 , a_2 , and a_3 axes all at the same distance from the axial cross. This unit distance is given as 1. Dividing 1 into the whole number 1 (it's a reciprocal, remember?) yields a value of 1 for each Miller number. So the Miller indices is (111) for the face that intercepts the positive end of each of the 3 axes. See Figure 3 for all possible numbers for the 8 faces. Note: A bar over the number tells me that the intercept was across the negative end of the particular crystallographic axis. The octahedral form is given the letter designation of "o".

Now to the cube face. A cube face that intercepts the a_3 (vertical) axis on the + end will not intercept the a_1 and a_2 axes. If the face does not intercept an axis, then we assign a mathematical value of infinity to it. So we start with Infinity, Infinity, 1 (a_1 , a_2 , a_3). Infinity divided into 0 = 0 (any number divided into zero equals zero). So the Miller indices of the + a_3 intercept face equals (001). See the drawing for all possible Miller indices for the 6 faces of a cube (Figure 4).

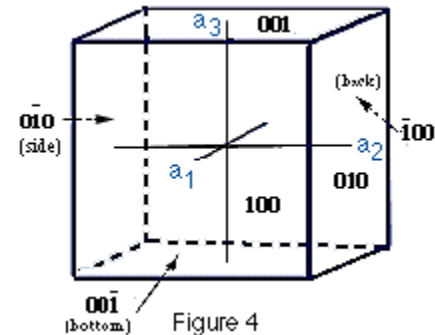
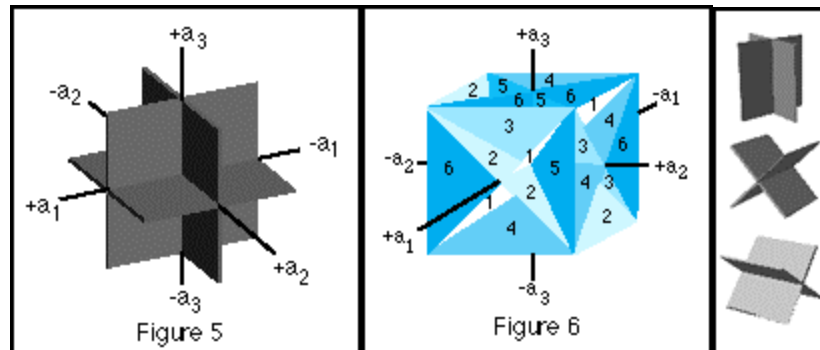


Figure 4

I think we should briefly mention cleavage at this point. **CLEAVAGE** is the preferred planar direction of breakage that many minerals possess. It is due to planes of weakness that exist in some minerals because the bonding strength between the atoms or molecules is not the same in every direction. Because crystals are composed of orderly arrangements of atoms or molecules, we really should expect cleavage to be present in many crystals. The notation that denotes cleavage is derived in much the same manner as Miller indices, but is expressed in braces. So a cubic crystal, say diamond, no matter whether it exhibits cubic {001} or octahedral {111} crystal form, has an octahedral cleavage form that is given as {111}.

Note: The Miller indices when used as face symbols are enclosed in parentheses, as the (111) face for example. Form symbols are enclosed in braces, as the {111} form for example. Zone symbols are enclosed in brackets, [111] for example and denote a zone axis in the crystal. So in the discussion of cleavage (above), you must use braces to denote cleavage. Cleavage is analogous to form as cubic, octahedral, or pinacoidal cleavage and does not refer to just one face of a form.

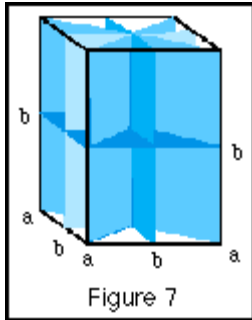
Now we are ready to discuss **ELEMENTS OF SYMMETRY**. These include **PLANES OF SYMMETRY**, **AXES OF SYMMETRY**, and **CENTER OF SYMMETRY**. These symmetry elements may be or may not be combined in the same crystal. Indeed, we will find that one crystal class or system has only one of these elements!



Huh? These parts, when put together, make the planes in figure 6.

Any two dimensional surface (we can call it flat) that, when passed through the center of the crystal, divides it into two symmetrical parts that are **MIRROR IMAGES** is a **PLANE OF SYMMETRY**. I repeat: any plane of symmetry divides the crystal form into two mirror images. Planes of symmetry are often referred to as mirror image planes. Let's discuss a cube again. A cube has 9 planes of symmetry, 3 of one set and 6 of another. We must use two figures to easily recognize all of them.

In Figure 5 the planes of symmetry are parallel to the faces of the cube form, in Figure 6 the planes of symmetry join the opposite cube edges. The second set corresponds to the octahedral crystal form. Planes of symmetry are **always** possible crystal forms. This means that, although not always present on many natural crystals, there exists the possibility that other crystal faces may be expressed. So even though a cube form does not present an octahedral face, it is always possible that it could have formed under the right conditions.



The typical human has two hands, right and left. Place them together palms facing away from you and the tips of the thumbs touching. Assuming that you have the same number of fingers on each hand, you will note that your right hand is the mirror image of your left and vice versa. The average person is symmetrical, having binary symmetry vertically from the head to the feet when viewed from the front or back (bilateral symmetry).

You can have a lot of laughs with friends and a long mirror using this symmetry element. You need at least one other person to do this so you both can view the results! Using Figures 5 and 6 as guides, take a wood or plastic cube and see if you can draw with a marker all the planes of symmetry that are present. Refer to the two figures for help.

It is sometimes convenient to designate planes of symmetry as axial, diagonal, principle, or intermediate. Figure 7 is an example of the 5 planes of symmetry of the tetragonal system and the proper abbreviated notation.

AXES OF SYMMETRY can be rather confusing at first, but let's have a go at them anyway. Any line through the center of the crystal around which the crystal may be rotated so that after a definite angular revolution the crystal form appears the same as before is termed an axis of symmetry. Depending on the amount or degrees of rotation necessary, four types of axes of symmetry are possible when you are considering crystallography (some textbooks list five). Given below are all possible rotational axes:

When rotation repeats form every 60 degrees, then we have sixfold or **HEXAGONAL SYMMETRY**. A filled hexagon symbol is noted on the rotational axis.

When rotation repeats form every 90 degrees, then we have fourfold or **TETRAGONAL SYMMETRY**. A filled square is noted on the rotational axis.

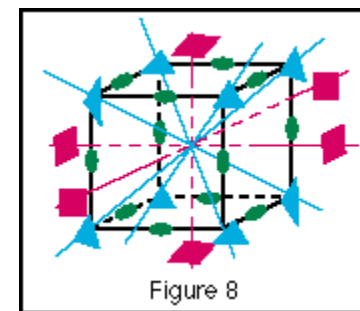
When rotation repeats form every 120 degrees, then we have threefold or **TRIGONAL SYMMETRY**. A filled equilateral triangle is noted on the rotational axis.

When rotation repeats form every 180 degrees, then we have twofold or **BINARY SYMMETRY**. A filled oval is noted on the rotational axis.

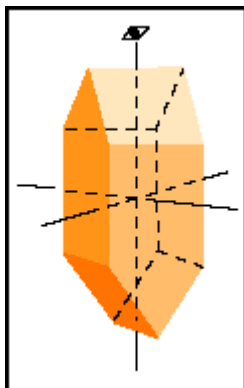
When rotation repeats form every 360 degrees, then we use a filled circle as notation. This one I consider optional to list as almost any object has this symmetry. If you really want to know the truth, this means **NO SYMMETRY!!**

Note that rotational axes may be on the plane of the face, on the edge of where two faces meet, or on the point of conjunction of three or more faces. On a complete crystal form, the axis must pass through the center of the crystal and exist at the equivalent site on the opposite side of the crystal as it entered.

Take a solid cube, made of wood or plastic (a clear plastic cube box works well for this exercise). Mark, using the rotational notation, every four-, three-, and two-fold axis of rotation that you can find. I think you will be surprised how many there are! Examine Figure 8 (the cube from *hades!*) to see how many symbols you can draw on your cube.



Now I'm sorry that this is not all there is to rotational axes, but there is another situation that we must consider -- **AXES OF ROTARY INVERSION**. This is where the twisted mind has one up on the rest of us (there's a pun in there somewhere!). We will consider a couple of simple examples.



First, let's examine a crystal as drawn in Figure 9a at left. Use a piece of "2 by 2" board and make this crystal form by cutting off the ends so the wood block looks like the drawing. Hold the block in your left hand with your thumb on the top and in the center of the 2-face edge join (long axis) and your index finger on the same join on the underside. Your palm will be toward your body. Align your two fingers so that you are looking straight down on your thumb and can not see end of your index finger. The top of the block will appear as 2 equal-sized faces, sloping away from you. If you rotate the block 180 degrees, the faces will appear back in the same position (2-fold axis of rotation), but here's the tricky part -- rotate the specimen 90 degrees and then turn your wrist where your index finger is on top (easiest done by turning your wrist counterclockwise). You will see that the block's faces appear in the original position in the original position. You have discovered an axis of rotary inversion!

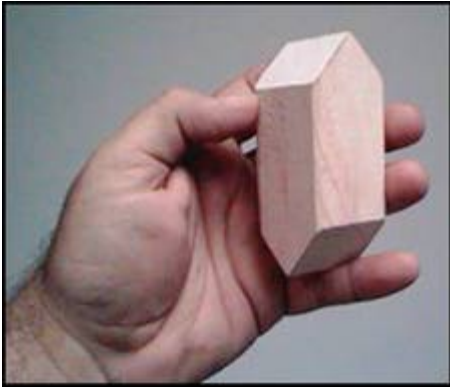


Fig 9b: Wooden or plastic models are known in a mineralogy class as 'idiot blocks'.



Fig 9c:



Fig 9d: Block rotated 90 degrees around the axis shown by the dot

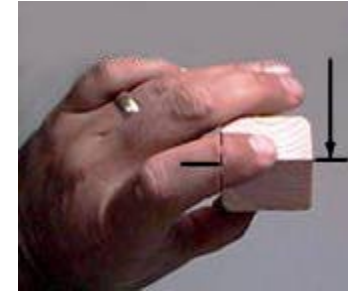
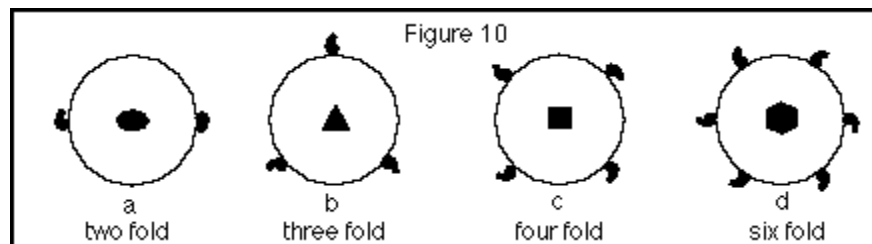


Fig 9e: Block rotated counterclockwise 180 degrees on the axis shown by the arrow.

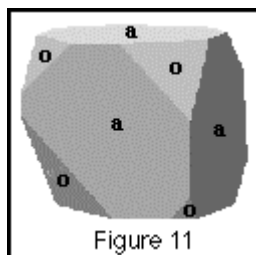
See the series of photos (Figures 9 b-9 e) if you get confused. Some textbooks term these axes rotary reflection axes or rotoinversion axes. There may be 1-, 2-, 3-, 4-, and 6-fold rotary inversion axes present in natural crystal forms, depending upon the crystal system we are discussing. I refer you to Klein and Hurlbut's *Manual of Mineralogy* (after J. S. Dana) if you want to sharpen your axes of rotary inversion skills. With axes of rotation, there is a graphical notation used which looks like a very bold type-face comma. For axes of rotary inversion, the same symbol is used, but appears dashed.

Both types of symmetrical rotational axes (discussed above) are commonly plotted on a circle (representing the complete cycle of one 360 degree rotation). The simple axes of rotation symbol for a face is plotted at the center of the circle and the axes of rotation and rotary inversion are plotted on the circle's boundary at whatever rotational angle is appropriate. See Figure 10 for examples.



We have finally come to our last topic of geometric crystallography -- the **CENTER OF SYMMETRY**. Most crystals have a center of symmetry, even though they may not possess either planes of symmetry or axes of symmetry. Triclinic crystals usually only have a center of symmetry. If you can pass an imaginary line from the surface of a crystal face through the center of the crystal (the axial cross) and it intersects a similar point on a face equidistance from the center, then the crystal has a center of symmetry. We may discuss this in a little more detail in the article about the triclinic system.

We now have to consider the relation of geometrical symmetry to **CRYSTALLOGRAPHIC SYMMETRY**. The crystal face arrangement symmetry of any given crystal is simply an expression of the internal atomic structure. This internal structure is generally alike in any parallel direction. But we must keep in mind that the relative size of a given face is of no importance, only the **angular relationship** or position to other given crystal faces. Refer back to Steno's law concerning the **CONSTANCY OF INTERFACIAL ANGLES**.



Let's consider a crystal in the cubic system with both cube $\{001\}$ and octahedral $\{111\}$ forms represented (Figure 11). In our figure, we have used the letter designation of -a- for the cube faces and -o- for the octahedral faces. Despite the initial observation that both the various cube and octahedral faces are unequal in size, the example displays all the symmetry elements and relationships of a crystal from the cubic system. I hope you now begin to grasp the difficulty of learning crystallography using natural crystals. Due to a variety of factors, many natural crystals have some degree of distortion to their growth, causing the faces to vary in size and sometimes shape. In college mineralogy, this problem was resolved by requiring the classroom use of a set of crystal forms, sometimes made of wood or plastic. These sets were not-so-fondly termed "idiot blocks" by exasperated students. Once you mastered the various forms and understood symmetry planes, rotational axes, and form names, then you became recognized as a "complete idiot" and could go on to examine real minerals!

Depending upon what elements of symmetry are present, all crystals may be divided into 32 distinct groups called **CLASSES OF SYMMETRY**. Remember, we concern ourselves with the symmetry elements we learned above, not the malformed crystal shapes of most minerals. Only forms which belong to the same class can occur in combination together in nature. We can not find a cube face on a hexagonal crystal. Likewise, we will never discover the rhombic dipyramid termination of a hexagonal crystal on a tetragonal crystal. So our laws, rules, and symmetry elements previously discussed prevent chaos in our beautifully symmetrical world of crystallography. Certainly, when dealing with real crystals, distortion problems can arise! Think of capillary pyrite. Here you have a cubic crystal which, due to a growth phenomenon, has one axis nearing infinity in length in relation to the other two. But this is caused by special conditions during growth, not the crystallography.

There are graphical methods of plotting all possible crystal faces and symmetry elements on a type of diagram called a stereo net. Stereo nets give a way to represent three-dimensional data on a two-dimensional surface (a flat sheet of paper). A discussion of stereo nets is out of the scope of this paper because to present it adequately would require much graphing, mathematics, and that each reader possess stereo-net paper. If you wish to attempt any exercises with stereo nets, I refer you to the previously mentioned textbooks. You can purchase the graph paper at most major college and university bookstores.

Well, if your faces are all shining, your symmetry now in order, and your axes properly aligned, then stay tuned for the next article when we consider crystal forms and the 32 symmetry classes. Then we will have the background necessary to discuss the six crystal systems!