Symmetry Elements

Further discussion of crystallography requires the introduction of the concepts of symmetry. Among the key ideas that will be explained are:

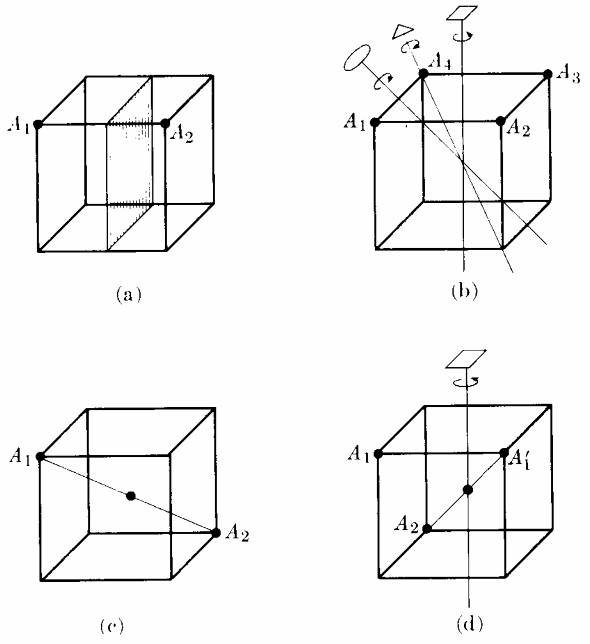
- The requirements for a crystal system (such as a = b = c) are incomplete since the atomic/molecular arrangements must also meet the minimum symmetry criteria for that given system.
- Further classification of crystals is possible by introducing microscopic and macroscopic symmetry operations, which are known as point and space groups, respectively.

Basic Operations

The possession of a minimum set of symmetry elements is a fundamental property of each crystal system. A symmetry element is an operation that when performed on the body will bring it into coincidence with itself. Macroscopic symmetry can be described by the following four elements:

- reflection: symmetry across a reflecting (or mirror) plane
- rotation: symmetry about an axis of rotation (line)
- inversion: symmetry about a point
- rotation-inversion: combination of rotation and inversion (Rotation-reflection can be used instead, which will lead to the same operations.) Rotation-inversion is the commonly used term.)

We can consider these symmetry elements (or operations) in the schematic below:



(a) (b)

(c) (d)

Fig. 2–6 Some symmetry elements of a cube. (a) Reflection plane. A_1 becomes A_2. (b) Rotation axes. 4-fold axis: A_1 becomes A_2; 3-fold axis: A_1 becomes A_3; 2-fold axis: A_1 becomes A_4. (c) Inversion center. A_1 becomes A_2. (d) Rotation-inversion axis. 4-fold axis: A_1 becomes A_1'; inversion center: A_1' becomes A_2.

Axes of symmetry: a rotation about a certain axis brings a lattice into a position indistinguishable from itself. *Symmetry about a line.*

Symmetry plane: equivalent points are brought into coincidence by reflection across the pane (mirror). *Symmetry about a plane.*

Center of inversion: every point on one side of the center is matched by an equivalent point on the other side, located on the same line through the center and at the same distance from the center. *Symmetry about a point.*

Rotation-inversion axis: equivalent points are brought into self-coincidence by a combined rotation and inversion.

Based upon symmetry operations, rather than lattice parameters and axes angles, we can describe the minimal requirements for our seven crystal systems:

Crystal System	Minimum Symmetry Elements
Triclinic	None
Monoclinic	One 2-fold rotation or rotation-inversion axis
Orthorhombic	Three 2-fold rotation or rotation-inversion axes
Tetragonal	One 4-fold rotation or rotation-inversion axis
Cubic	Four 3-fold rotation or rotation-inversion axes
Trigonal (Rhombohedral)	One 3-fold rotation or rotation-inversion axis
Hexagonal	One 6-fold rotation or rotation-inversion axis

Now, we can readily see that the case of "base centered cubic" that we discussed above does not satisfy the three-fold rotation axis requirement of cubic but does have the single four-fold axis characteristic of tetragonal.

Point Groups - Three Dimensions

A point group is a representation of the ways that the macroscopic symmetry elements (operations) can be self-consistently arranged around a single, immobile geometric point. There are 32 unique manners in which this can be done and, thus, 32 point groups.

To briefly review (and then expand), a point symmetry element describes an operation by which equivalent points are brought into coincidence. The operation is specified with respect to a fixed point in space.

Symmetry Elements

Rotations, also known as symmetry axes

Rotation axes are of five different types based upon the fraction of a full circle the rotation occurs.

Name	Alias	Rotation (°)	Symbol
monad	one-fold	360	● (or none)
diad	two-fold	180	⧫
triad	three-fold	120	▲
tetrad	four-fold	90	◆
hexad	six-fold	60	⬢

Symmetry about a line!!

Examples of the five rotation axes:

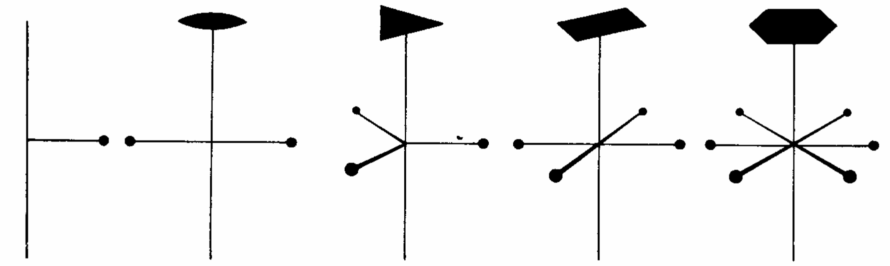
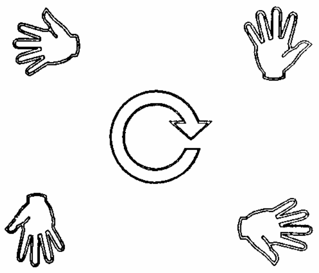


Fig. 1-10 Rotation axes of symmetry: one-, two-, three-, four-, and sixfold.

Four-fold rotation symmetry:

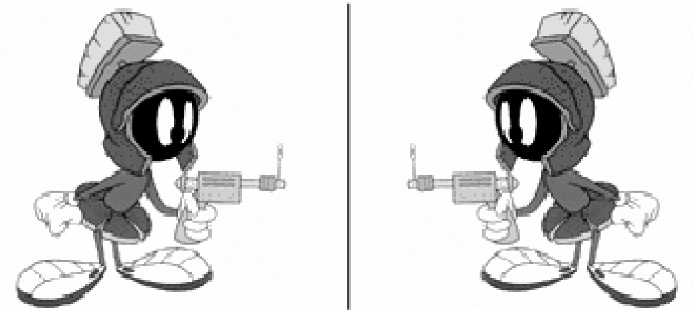


Note: Only certain rotations are possible because all lattice sites generated by the symmetry element must be equivalent.

Symmetry (mirror) Plane

Equivalent points are brought into coincidence by reflection across the plane. Symmetry about a plane!

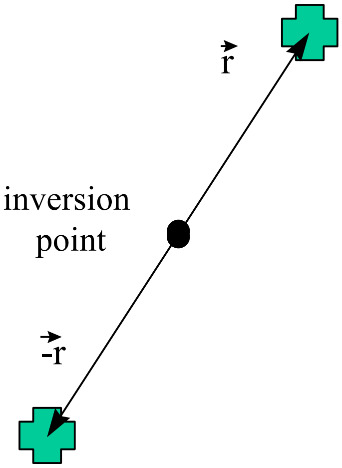
An example of a mirror plane:



The symbol for a mirror plane is “m.” When the mirror plane is normal to an axis of rotation, an “m” is placed in the denominator and a 1, 2, 3, 4, or 6 is in the numerator.

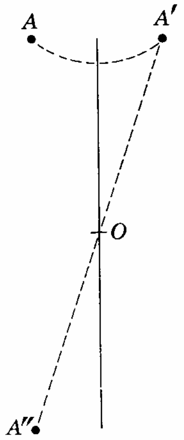
Center of Inversion or Inversion Point

All features are matched by an equivalent feature on the opposite side of the inversion point. Symmetry about a point. For example:



Rotation-Inversion (roto-inversion)

Combine rotation and inversion to have a hybrid element. (The same symmetry figures can be obtained by combining rotation and reflection, but roto-inversion appears to be the preferred terminology and symbolism.) For example:



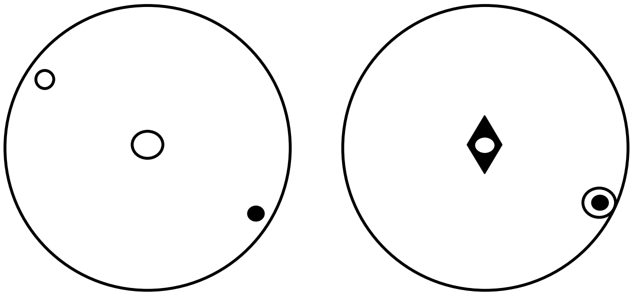
Name	Rotation (°)	Symbols
inverse monad	360 + inversion	○ $\bar{1}$
inverse diad	180 + inversion	⧫ $\bar{2}$
inverse triad	120 + inversion	▲ $\bar{3}$
inverse tetrad	90 + inversion	◈ $\bar{4}$
inverse hexad	60 + inversion	⬢ $\bar{6}$

We now have the basic macroscopic symmetry operations. Shall we do the stereograms to illustrate them?

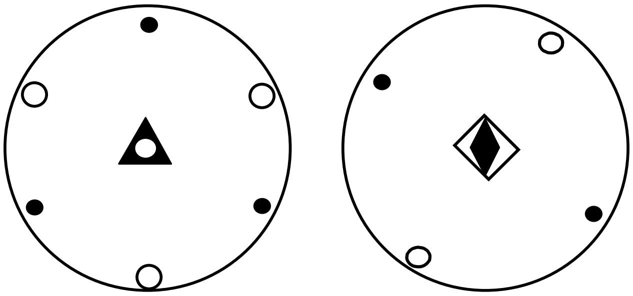
Starting from the standard circle (looking down from the north pole) for the rotation axes, one can easily draw monad, diad, triad, tetrad, and hexad.

Rotation inversion axes:

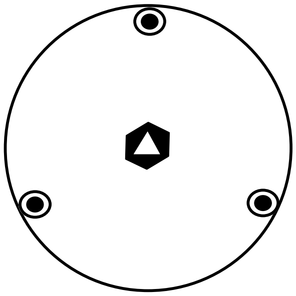
Inverse monad and inverse diad ($\bar{2}$ is also known as “m”)



Inverse triad and tetrad:



Inverse hexad:



So far, we have 10 of the 32 point groups!

While using points does offer ease of drawing, there is an addition consideration in rotation: properness. By this, we mean, “Does the figure change handedness with each operation?” All of the roto-inversion axes are improper rotations.

Multiple Symmetry Operations and Polyaxial Groups

Our next area of discussion must be, “How do we combine multiple symmetry operations about a point?”

As has been said before, crystallographers demand consistency. Thus, symmetry operations cannot be combined so as to violate one of the other symmetry elements - self-consistency. It is obvious that the placement of a mirror plane can seldom be random. (It would look quite odd if the plane of bilateral symmetry in people was not in the center.)

By placing a mirror plane perpendicular to the 2-, 4-, and 6-fold rotation axes, we get three additional point groups. The apparent point groups $\frac{1}{m} = m = \bar{2}$ and $\frac{3}{m} = \bar{6}$ add nothing new and, therefore, are not used. We can place mirror planes parallel to the rotation axis and add the point groups 2mm, 3m, 4mm, and 6mm. The term 3mm is not used since the second “m” would arise from the combination of the triad and the first mirror. We are now up to 17/32 done. At this point, you should be able to draw the stereograms for these point groups.

We must now consider the 6 permissible polyaxial groups using a figure from Schwartz and Cohen:

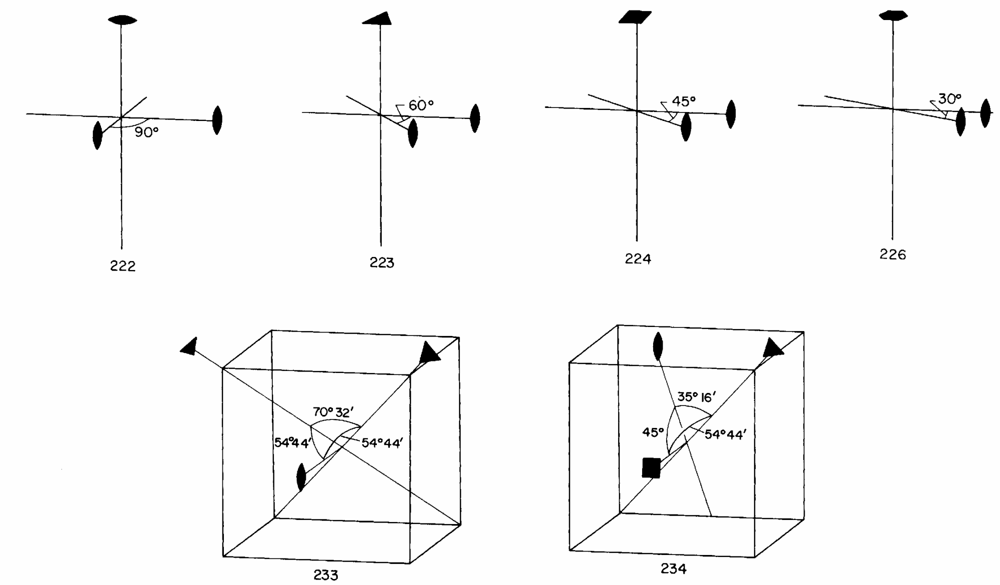


FIG. 1-19. The six permissible polyaxial point groups. (After Buerger, M. J., “Elementary Crystallography.” Copyright © 1956, John Wiley & Sons. Reprinted by permission of John Wiley & Sons, Inc.)

Stereograms of Point Groups

Now we have all 32 point groups:

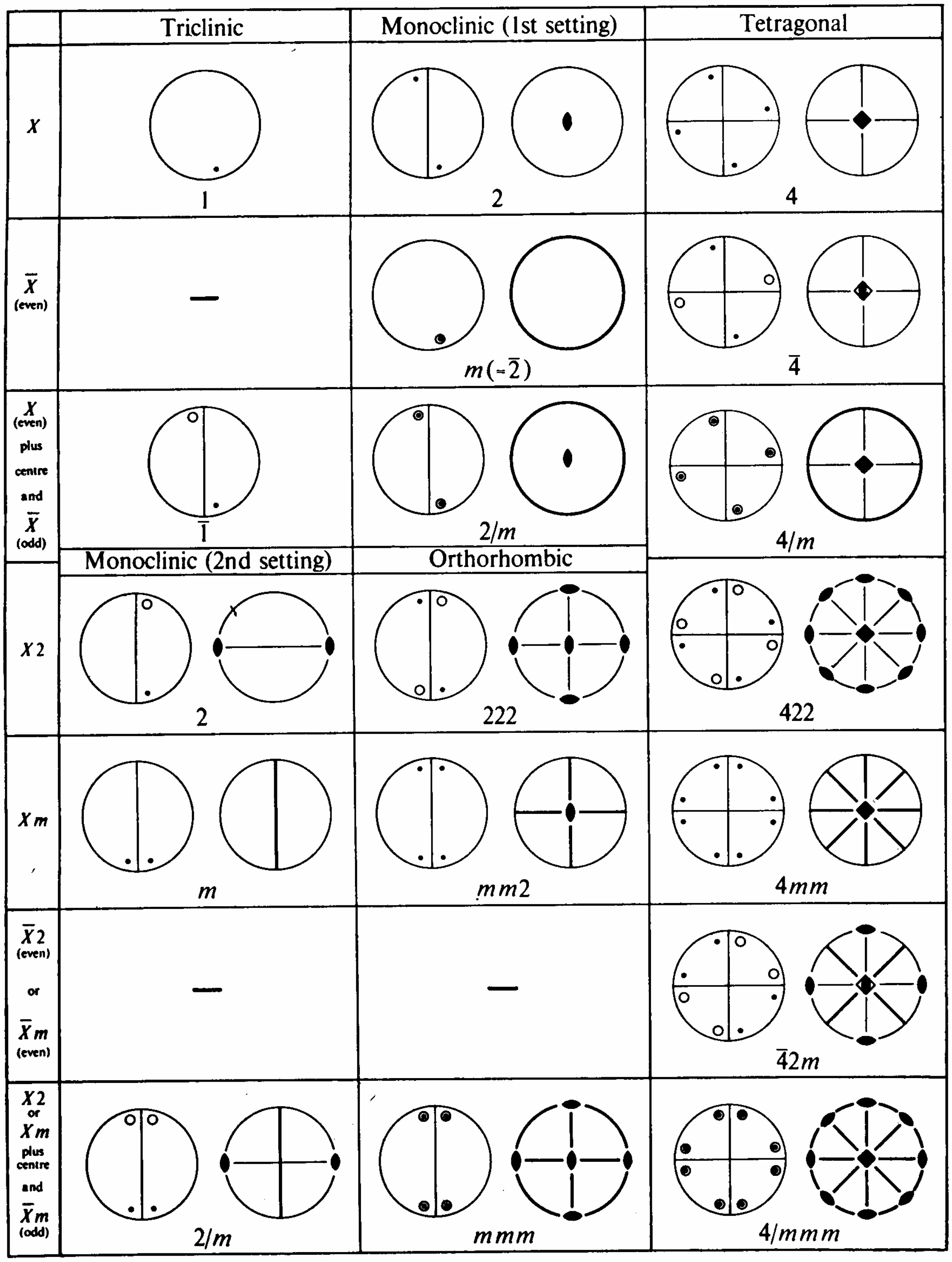


FIG. 1-22. The 32 point groups or crystal classes. On the right of each pair of figures are given the symmetry elements, on the left the molecular arrangements. (From "International Tables for X-Ray Crystallography." Vol. I, 3rd ed. Kynoch Press, Birmingham, England, 1969.)

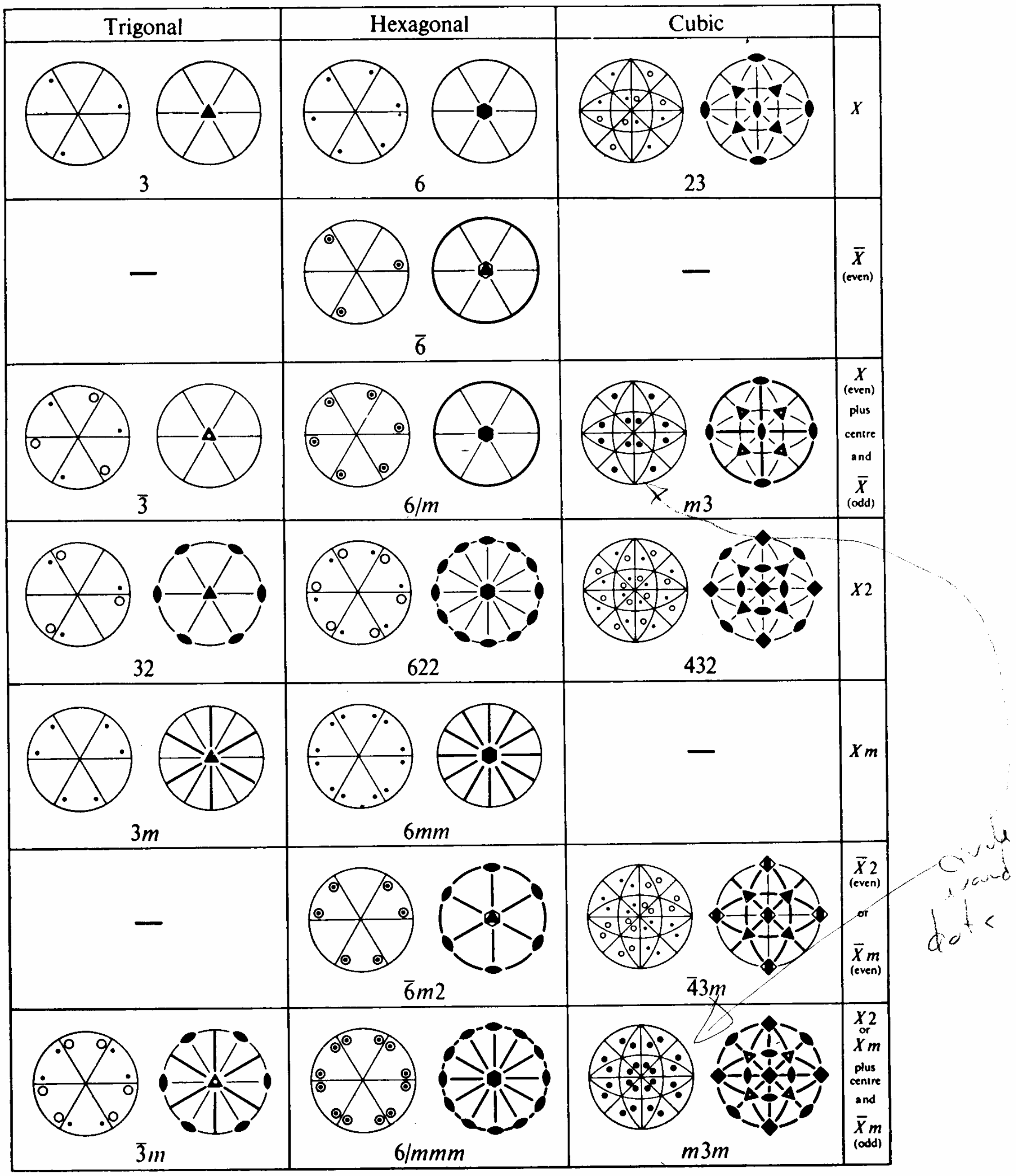


FIG. 1-22. (Continued.)

Point Groups and Crystal Systems

Given these symmetry operations, we can now classify the 32 point groups by the seven crystal systems:

Crystal System	Hermann-Mauguin (International) Symbol	
	Full	Abbreviated
Cubic	23 2/m $\bar{3}$ $\bar{4}$3m 432 4/m $\bar{3}$ 2/m	23 m3 $\bar{4}$3m 432 m3m
Tetragonal	4 $\bar{4}$ 4/m $\bar{4}$2m 4mm 422 4/m 2/m 2/m	4 $\bar{4}$ 4/m $\bar{4}$2m 4mm 422 4/mmm
Orthorhombic	mm2 222 2/m 2/m 2/m	mm 222 mmm
Rhombohedral	3 $\bar{3}$ 3m 32 $\bar{3}$ 2/m	3 $\bar{3}$ 3m 32 $\bar{3}$m
Hexagonal	6 $\bar{6}$ 6/m $\bar{6}$2m 6mm 622 6/m 2/m 2/m	6 $\bar{6}$ 6/m $\bar{6}$2m 6mm 622 6/mmm
Monoclinic	m 2 2/m	m 2 2/m
Triclinic	1 $\bar{1}$	1 $\bar{1}$

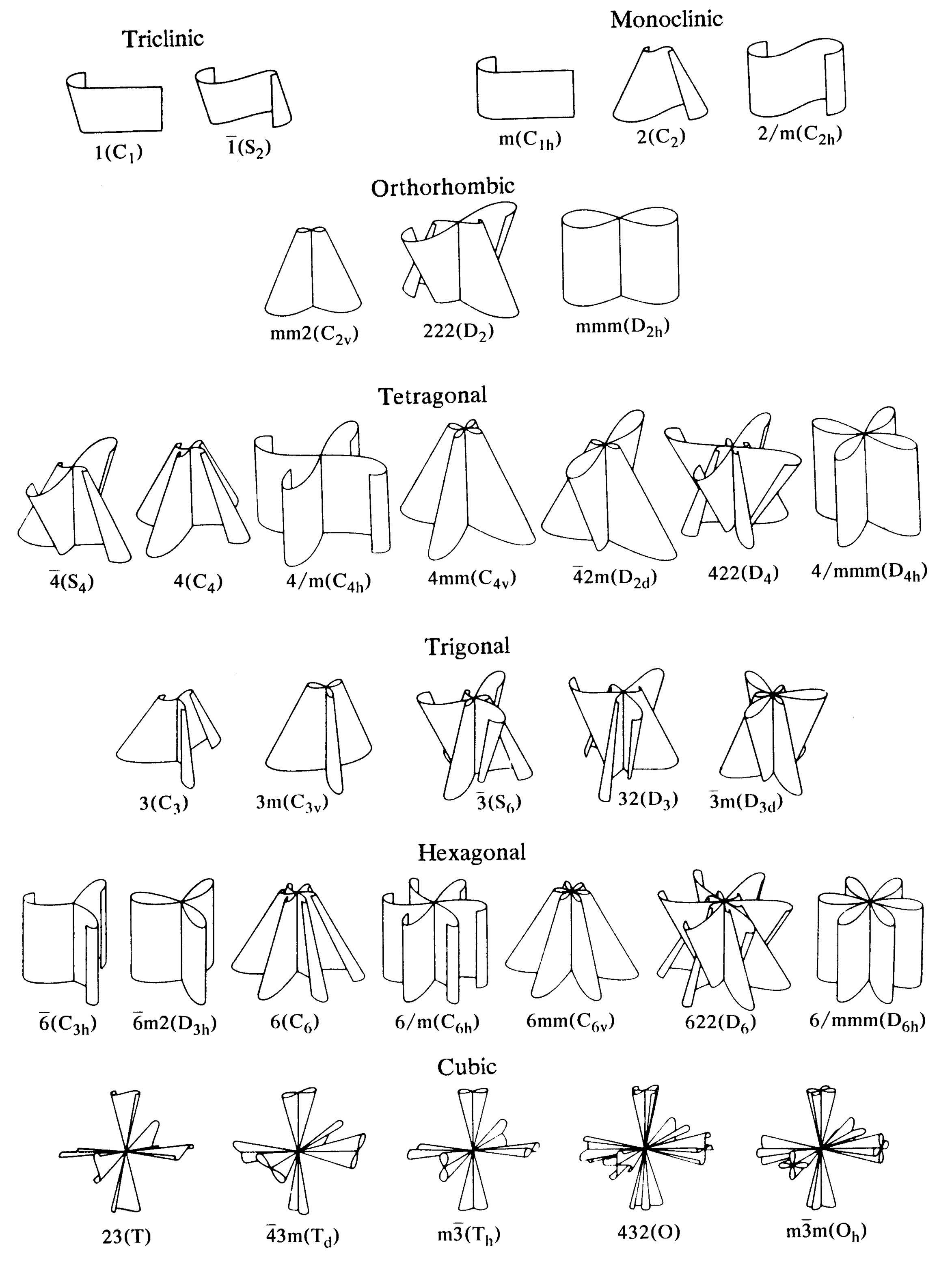
There is a convention on the order of indices in the International designations:

Crystal System	Order of Indices*			Axes and Symmetry Elements
	1st	2nd	3rd	
Cubic	$\begin{Bmatrix}[100] \\ {[010]} \\ {[001]}\end{Bmatrix}$	$\begin{Bmatrix}[111] \\ {[1\bar{1}\bar{1}]} \\ {[\bar{1}1\bar{1}]} \\ {[\bar{1}\bar{1}1]}\end{Bmatrix}$	$\begin{Bmatrix}[1\bar{1}0] & {[1\bar{1}0]} \\ {[01\bar{1}]} & {[011]} \\ {[\bar{1}01]} & {[101]}\end{Bmatrix}$	a, b, and c // to 4 or $\bar{4}$
Tetragonal	[001]	$\begin{Bmatrix}[100] \\ {[010]}\end{Bmatrix}$	$\begin{Bmatrix}[1\bar{1}0] \\ {[110]}\end{Bmatrix}$	c // to 4 or $\bar{4}$
Orthorhombic	[100]	[010]	[001]	a, b, and c // to 2 or $\bar{2}$
Rhombohedral (Hexagonal axes)	[001]	$\begin{Bmatrix}[100] \\ {[010]} \\ {[\bar{1}\bar{1}0]}\end{Bmatrix}$		c // to 3 or $\bar{3}$
Rhombohedral (Rhombohedral axes)	[111]	$\begin{Bmatrix}[1\bar{1}0] \\ {[01\bar{1}]} \\ {[\bar{1}01]}\end{Bmatrix}$		a b c // to 3 or $\bar{3}$
Hexagonal	[001]	$\begin{Bmatrix}[100] \\ {[010]} \\ {[\bar{1}\bar{1}0]}\end{Bmatrix}$	$\begin{Bmatrix}[1\bar{1}0] \\ {[120]} \\ {[\bar{2}\bar{1}0]}\end{Bmatrix}$	c // to 6 or $\bar{6}$
Monoclinic (unique c-axis	[001]			c // to 2 or $\bar{2}$
Monoclinic (unique b-axis	[010]			b // to 2 or $\bar{2}$
Triclinic	None			none

*Directions in the same set of equivalent symmetry directions are enclosed in braces. The first entry is generally taken as the representative case.

Thus, we can identify the crystal system instantly when examining the full designation.

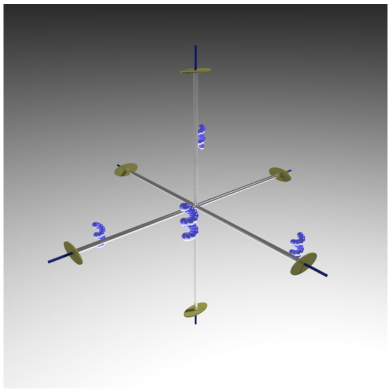
Point Group Visualizations



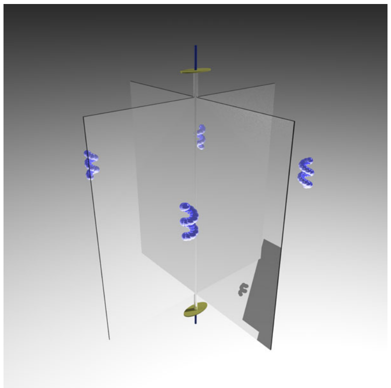
There are many neat ways to visualize the point groups. An excellent site (Marc DeGraef of Carnegie-Mellon) that has both movies and still images is:

Example of his figures for the orthorhombic point groups are:

222:



mm2:



mmm: