January 16, 2007

LECTURE #01

Notation: Introduction to the Stereogram
Rotation axes

\[ C_2(2) \]

\[ C_3(3) \]

\[ C_4(4) \]

\[ C_6(6) \]

Inversion through a center

\[ i(\bar{1}) \]

Rotatory inversion axes

\[ i(\bar{1}) = \text{inversion} \]
\[ \sigma(2) = \text{mirror plane} \]

Mirror plane

\[ \sigma(m) \]

Looking parallel perpendicular

Fig. 1-2 The point symmetry operations and the symbols used to designate them. Hands are used to show the effect for several symmetry operations.

Crystal Structure Database

http://serc.carleton.edu/research/education/crystallography/f/e1databases.html

http://www.ics.ac.uk/eg/3pg3/atomic.html

http://www.newbert.net


Crystal Structure Applets

http://home3.netcarrier.com/~chan/SOLIDSTATE/CRYSTAL

Other interesting Applets

http://www.falstad.com/
Notes on the conventions used by Burns.

- Left and Right handed images (mirror) are enantiomorphic images of one another.

  Example 🤔

- + Any general object above plane of the paper
- − or below plane

- Point symmetry operations:
  - inversion: \( i \)
  - horizontal plane: \( C_n \)
  - vertical plane contains principle axis: \( \sigma_d \)
  - rotation through a plane: \( \sigma \)
  - unit operation (identity): \( E \)

- Plane bisects the angle between the \( n \) fold axes perpendicular to the principle axis.

  \( D_n \) implies that there are \( n \) two-fold axes perpendicular to the \( n \) fold rotational axis.

  \( S_n \) improper rotation — (rotation by \( \frac{2\pi}{n} \) followed by a reflection in the plane perpendicular to the axis).

As a consequence:

\[
\begin{align*}
S_n &= \sigma_h C_n \quad S_4(x,y,z) \rightarrow (y,-x,-z) \\
S_2 &= i \quad S_3^3 = \sigma_h \quad S_3^6 = E
\end{align*}
\]

(This is the Shoentflies' notation for denoting symmetries.)
3-5 Hermann–Mauguin notation

In the Hermann–Mauguin system the point groups are designated by combinations of the symbols for symmetry elements. Some of the elements of the group are, therefore, immediately apparent from the symbol, and a few conventions make it possible to deduce the entire group structure. This system is preferred by crystallographers because it is easily extended to include translational symmetry elements and because it specifies the directions of the symmetry axes.

The Schoenflies and the Hermann–Mauguin symbols for the thirty-two crystallographic point groups are given in Table 3-1, and many of the features of the Hermann–Mauguin notation will be revealed by comparison with the Schoenflies symbols. The following summary should further clarify the meanings of the symbols:

1. Each component of a symbol refers to a different direction. The terms 2/m, 4/m, and 6/m are single components and refer to only one direction. In 4/mmm, for example, the 4/m (read “four over m”) indicates that there is a mirror plane perpendicular to a fourfold rotation axis.

2. The position of an m in a symbol indicates the direction of the normal to the mirror plane.

3. In the orthorhombic system, the three directions are mutually perpendicular. If we label our axes x, y, z, the symbol mm2 indicates that mirror planes are perpendicular to x and y, and a twofold rotation axis is parallel to z. The 2 in this case is redundant since we have seen that two perpendicular mirror planes inevitably generate a twofold axis. Note that such symbols as m2m and 2mm correspond to renaming the axes.

4. If in the tetragonal system the 4 or 4 axis is in the z direction, the second component of the symbol refers to mutually perpendicular x and y axes, and the third component refers to directions in the xy plane that bisect the angles between the x and y axes.

5. In the trigonal and hexagonal systems, a second component in the symbol refers to equivalent directions (120° or 60° apart) in the plane normal to the 3, 3, 6, or 6 axis.

6. A third component in the hexagonal system refers to directions that bisect the angles between the directions specified by the second components.

7. A 3 in the second position always denotes the cubic system and refers to the four body diagonals of a cube. The first component of cubic symbol refers to the cube axes, and a third component refers to the face diagonals of the cube.
The stereographic projection of the points of a sphere onto the horizontal plane (see the previous page for the definition)
a) shows the method
b) shows the view of the plane from the north pole.