January 16, 2007

LECTURE #01

Notation: Introduction to the Stereogram

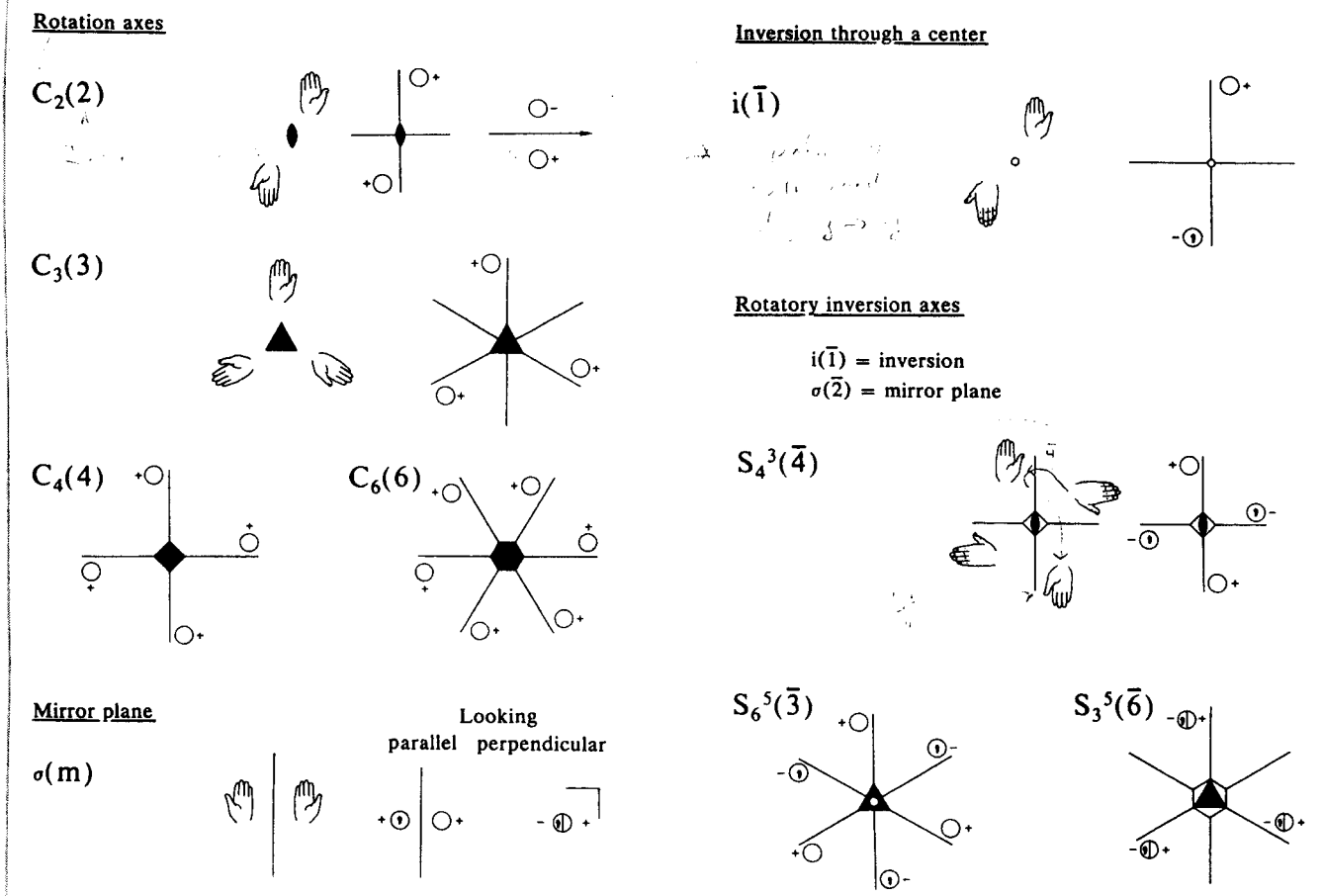


Fig. 1-2 The point symmetry operations and the symbols used to designate them. Hands are used to show the effect for several symmetry operations.

The letter notation is Schoenflies, that in brackets international (Herman-Maugin)

Crystal Structure Data Base

http://serc.carlton.edu/research_education/crystallography/xldatabases.html

// www.le.ac.uk/eg/3pg3/atomic.html

// www.newbert.net

// cst-www.nrl.navy.mil/lattice/

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 <u>enantiomorphic</u> images of one another

Example 

- $\pm$ Any general object above / below plane (of the paper)

- $\oplus$ above plane / below plane or $\ominus$

- Point symmetry operations

E, i, C_n, σ (σ_h, σ_v, σ_d)

E: unit operation (identity)

i: inversion

C_n: n-fold rotation around an axis

σ: reflection through a plane

σ_h: horizontal plane

σ_v: vertical plane contains principle axis

σ_d: plane bisects the angle between the 2fold axes ⊥'r the principle axis

D_n - implies that there are n-two fold axes ⊥'r to the n-fold rotational axis

S_n - improper rotation - (rotation by $2\pi/n$ followed by a reflection in the plane ⊥'r to the axis)

As a consequence

$S_n = \sigma_h C_n$, $S_4(x, y, z) \rightarrow (y, -x, -z)$

$S_2 = i$, $S_3^3 = \sigma_h$, $S_3^6 = E$

(This is the Shoenflies notation for denoting symmetries)

(Taken From Sands, Crystalography)

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.

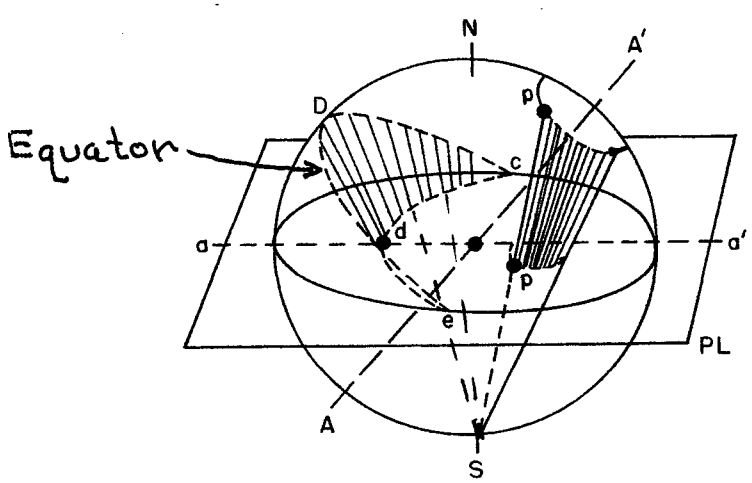
The Schoenflies and the Hermann–Mauguin symbols for the thirty-two crystallographic point groups are given in Table 3-1, and many of the features of the Hermann–Mauguin notation will be revealed by comparison with the Schoenflies symbols. The following summary should further clarify the meanings of the 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 rotati 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 $\bar{4}$ 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, $\bar{3}$, 6, or $\bar{6}$ 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.

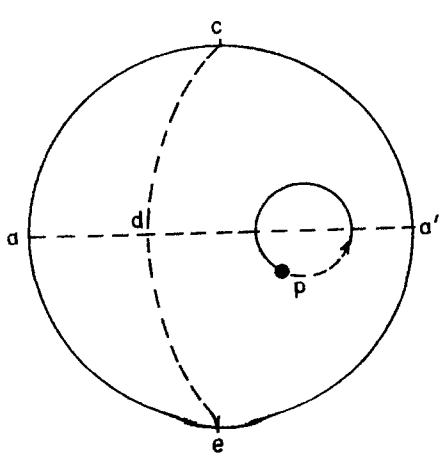
The stere graphic projection of the points of a sphere onto the horizontal plane (see the previous page for the definition)

a) shows the method

b) shows the view of the plane from the north pole.



(a)



(b)