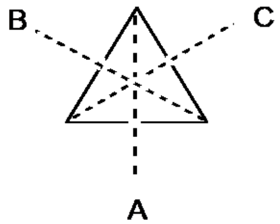
Chemistry 6330 - AU19 ***Problem Set 2***

(1) Consider the group {E,A,B,C,D,F} derived from the equilateral triangle discussed in class.



D: cw rotation by $2\pi/3$
F: ccw rotation by $2\pi/3$

(a) Construct the group multiplication table and verify the rearrangement theorem.
(b) Find all the subgroups of the group
(c) Divide the operations of the group into classes

(2) Consider the following set of matrices:

$$\underline{\underline{M}}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \underline{\underline{M}}_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \underline{\underline{M}}_3 = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$\underline{\underline{M}}_4 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix} \qquad \underline{\underline{M}}_5 = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix} \qquad \underline{\underline{M}}_6 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

(a) Use matrix multiplication to construct a multiplication table and to verify that the matrices comprise a group.
(b) Divide the matrices into classes.
(c) The trace of a matrix is defined as the sum of its diagonal elements. What do you observe about the trace of the matrices that belong to the same class?
(d) Are the groups discussed in Problems 1 and 2 isomorphic?

(3) Write down the multiplication table for the cyclic group of order 5. Show by trial and error that no other one is possible.

(4) You are told that there is a point group that is uniquely defined by an $S_4(z)$ and a $C_2(x)$.
(a) Using closure, generate all of the other symmetry elements of this point group. What is its order?
(b) What is the class structure of the group?
(c) For each operation in the group, generate the matrix describing the transformation of a general cartesian point (x,y,z).
(d) Do the matrices from part (c) form a representation of the group? If so, is reducible or irreducible?
(e) We can also generate matrices based upon the transformation products of x, y, and z. For example, consider the transformation of the product xy. If a certain operation transforms $x \rightarrow y$ and $y \rightarrow x$, then the product xy is transformed into itself, $xy \rightarrow xy$. Similarly, if $x \rightarrow -x$ and $y \rightarrow y$, then $xy \rightarrow -xy$, and so forth. Generate the 5 x 5 matrices that describe the transformation of (z^2, x^2-y^2, xy, xz, yz) under each of the operations of the group.

(f) Do the matrices from part (e) form a representation of the group? If so, is it reducible or irreducible?

(g) Show that the irreducible representations you have generated obey the great orthogonality theorem.

(h) Do you think there are other representations for this group?