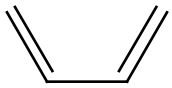
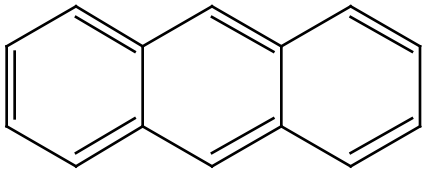
Examination 3 - Chemistry 262 **November 15, 1999**

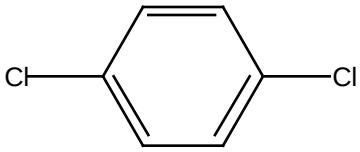
Name:_____ **Dr. Jay H. Baltisberger**

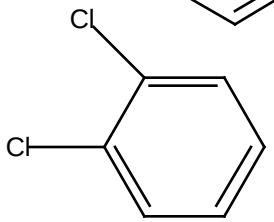
Please answer any 6 questions, showing all calculations - 25 points each, 150 total.

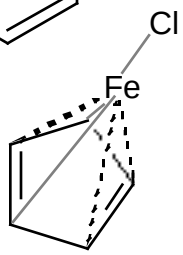
1. List the symmetry elements of the following molecules and name the point groups to which they belong: (a) Z,Z–butadiene, (b) anthracene, (c) p-dichlorobenzene, (d) m-dichlorobenzene, (e) cyclopentadieneyl iron (II) chloride.





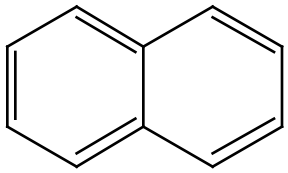






2. Treat naphthalene as belonging to the C_{2v} point group with the C_2 axis perpendicular to the plane of the molecule . Classify the irreducible representation spanned by the ten carbon $2p_z$ orbitals.

C_{2v}, 2mmm	*E*	*C_2*	σ_v	σ_v'	*h = 4*
A_1	+1	+1	+1	+1	z, z^2, x^2, y^2
A_2	+1	+1	–1	–1	xy, R_z
B_1	+1	–1	+1	–1	x, xz, R_y
B_2	+1	–1	–1	+1	y, yz, R_x



3. Consider the molecule NO_2 which is in the C_{2v} point group. Derive the irreducible representation of the 9 degrees of freedom of this molecule. Show which are Raman, IR active and which modes correspond to rotation and translation. Does this point group allow this molecule to have a dipole moment?

4. Write out a group multiplication table for the C_{2v} point group.

5. Write out a Hückel determinant for π orbitals (made from carbon $2p_z$ orbitals) for the molecule naphthalene.

6. Which of the following triatomic molecules are expected to be linear. Give reasons in each case: (a) NO_2^-, (b) SO_2, (c) H_2O^{2+}.

7. Show that the sp^2 hybrid orbital $(s + 2^{1/2} p) / 3^{1/2}$ is normalized to 1 if the s and p orbitals are normalized to 1.

8. Write the possible ground state electronic configurations for the V^{2+} ion. What are the possible values for S and M_S in each case? What are the possible term symbols for one of the configurations (your choice)?

9. Calculate the commutator between d/dx and $(d/dx + x^2)$.

10. Determine which of the following functions are eigenfunctions of the inversion operator *i* (converts x into –x): (a) $x^3 – kx$, (b) cos(kx), (c) $x^2 + 3x – 1$. State the eigenvalue when relevant.