CHEM. 341 (DR. AQUINO) TEST #1 OCTOBER 21, 2011

Answer all questions in the booklets provided. A point-group flow chart, character tables and a periodic table are provided. You have 50 minutes.

Question 1 - (10 marks)

a) Using the VSEPR model, draw and name the actual structure of ClO_3^-. (4 marks)

b) The O-Cl-O angle in ClO_3^- is 107°, the O-Br-O angle in BrO_3^- is 104° and the O-I-O angle in IO_3^- is 100°. Give two plausible reasons to explain this trend. (6 marks)

Question 2 - (10 marks, 5 marks each)

List all of the symmetry elements and determine the point group of:

a) Cyclohexane (chair conformation) b) SF_4

Question 3 – (12 marks)

(i) (ii) (iii)

a) What is the symmetry label of each SALC above under D_{3h}? (6 marks).

b) What orbital or orbitals, if any, on the central atom is (are) of correct symmetry to combine with these SALC's?

c) Which symmetry type(s) (of all symmetry types) in D_{3h} is (are) both IR active *and* Raman active.

Question 4 – (15 marks)

Molecules that contain H can often be identified by looking at the number of lines in their IR spectrum and comparing this to the IR of the same molecule in which one or more H is replace by D (deuteration). Using the Table below, determine the reducible representation for both NH_3 and NH_2D. Using the appropriate character table for each molecule, factor the reducible representation into a set of irreducible representations and subsequently into a set of irreducible representations corresponding to the vibrational modes only. Finally determine how many bands will be seen in the IR and Raman spectra of both molecules and give the labels of the IR and Raman active modes.

Symmetry Operation	**Character Contribution per Unshifted Atom**
E	3
i	-3
σ	1
C_2	-1
C_3	0
C_4	1
C_6	2
S_3	-2
S_4	-1
S_6	0

Question 5 – (8 marks)

Glycine has the structure NH_2CH_2COOH. It can lose a proton from the carboxyl group and form bidentate chelate rings bonded through both the N and one of the O atoms. Draw structures for all possible isomers of tris(glycinato)cobalt and assign the isomer (i.e. *cis, trans, fac, mer, delta, lambda, etc.*) You may use the abbreviation N O to represent a chelated glycinate.