CHEM. 341 (DR. AQUINO) TEST #1 OCTOBER 22, 2010

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

Question 1 - (10 marks)

a) Using the VSEPR model, draw the structures and indicate the shape of ClO_2^-, ClO_3^-, and ClO_4^-. (6 marks)

b) The O-Cl-O angle in ClO_2^- is 105°, in ClO_3^- it is 107°, and in ClO_4^- it is 109°. Give a plausible reason to explain this trend. (4 marks)

Question 2 - (15 marks, 5 marks each)

List <u>all</u> of the symmetry elements and determine the point group of:

a) BrF_5 b) 1,4-dibromobenzene c) a beer bottle (without label)

Question 3 – (12 marks)

a) What is the symmetry label of each SALC above under C_{3v}? (Show how you determined it) (6 marks).

b) What orbital or orbitals, if any, on the central atom is (are) of correct symmetry to combine with these SALC's? (4 marks)

c) Which symmetry type(s) (of all the symmetry types) in C_{3v} is (are) both IR active *and* Raman active. (2 marks).

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 H_2O and HDO (one hydrogen is replaced by a deuteron). 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)

Sketch all the isomers of the following complex ions:

a) $[Cr(H_2O)_3IBrCl]^-$

b) $[Pt(en)_2Cl_2]^{2+}$