Homework 10 – Molecular Symmetry

Name: _____

Excercise 10A.4(a) (10 points)

List the symmetry elements of the following molecules and name the point groups to which they belong:

(i) NO_2

(ii) PF_5

(iii) $CHCl_3$

(iv) 1,4-difluorobenzene

Exercise 10B.5(a) (10 points)

By inspection of the character table for D_{3h}, state the symmetry species of the $3p$ and $3d$ orbitals located on the central Al atom in AlF_3

Exercise 10B.7(a) (5 points)

What is the maximum possible degree of degeneracy of the orbitals in benzene?

Exercise 10C.1(a) (5 points)

Use symmetry properties to determine whether or not the integral $\int p_x z p_z \mathrm{d}\tau$ is necessarily zero in a molecule iwth symmetry C_{2v}

Exercise 10C.2(a) (5 points)

Is the transition $A_1 \rightarrow A_2$ forbidden for electric dipole transitions in a C_{3v} molecule?

Exercise 10C.4(a) (10 points)

Consider the C_{2v} molecule OF_2; take the molecule to lie in the yz-plane, with z directed along the C_2 axis; the mirror plane σ_v' is the yz-plane, and σ_v is the xz-plane. The combination $p_z(A) + p_z(B)$ of the two F atoms spans A_1, and the combination $p_z(A) - p_z(B)$ of the two F atoms spans B_2. Are there any valence orbitals of the central O atom that can have a non-zero overlap with these combinations of F orbitals? How would the situation be different in SF_2, where $3d$ orbitals might be available?

Exercise 10C.6(a) (5 points)

The ground state of NO_2 is A_1 in the group C_{2v}. To what excited states may it be excited by electric dipole transitions, and what polarization of light is it necessary to use?