

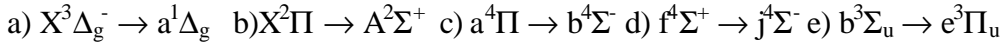
## Homework #10 (due Wednesday Nov. 30)

1. (10 Pts) Making use of the diatomic electronic selection rules:

$$\Delta S = 0; \Delta \Lambda = 0 \pm 1; (g \leftrightarrow u \text{ allowed, but } g \leftrightarrow g \text{ and } u \leftrightarrow u \text{ forbidden});$$

$$(\Sigma^+ \leftrightarrow \Sigma^+ \text{ \& } \Sigma^- \leftrightarrow \Sigma^- \text{ allowed but } \Sigma^+ \leftrightarrow \Sigma^- \text{ is forbidden})$$

State whether the following transitions are allowed or forbidden:



2. (9 Pts) For the planar molecule  $N_2O_4$  draw a "stick diagram" of the molecule and show the 3  $C_2$  axes. (note this molecule is composed of two  $NO_2$  groups forming an N-N bond).

3. (18 Pts) For  $NO_3$  a planar molecule with  $D_{3h}$  symmetry label the oxygen atoms as #1,#2,#3. Illustrate via stick-ball diagram the initial  $NO_3$  molecule and after application of:

a) a  $C_3$  operation

b) a  $C_3^2$  operation

c) a  $C_2', C_2'', C_2'''$  operations (3 different illustrations corresponding to rotations about each axis)

d) a  $\sigma_h$  operation

e) a  $\sigma_v, \sigma_v', \text{ and } \sigma_v''$  operations (3 different illustrations corresponding to reflections through each plane)

f) a  $S_3$  operation

g) a  $S_3^2$  operation

i) a  $S_3^3$  operation

j) an  $E$  operation

4. (16 Pts) If the electron configuration of  $H_2O$  ground state is:  $(1a_1)^2(2a_1)^2(1b_1)^2(3a_1)^2(1b_1)^2$  and that of the first excited state is:  $(1a_1)^2(2a_1)^2(1b_1)^2(3a_1)^2(1b_1)^1(4a_1)^1$ , what is the electronic symmetry of the **total electronic molecular wavefunction** in each state.

5. (16 Pts) Show what irreducible representations in  $C_{3v}$  are spanned by the reducible representation

(you need to understand section 12-7 or my lecture notes to attempt this problem)

E	2C <sub>3</sub>	3C <sub>2v</sub>
5	2	1