

Mid-Term 2

Do all questions. If you think that you may wish to have the test re-graded, it must be done in permanent ink. No liquid paper/white-out or other such correction tools should be used in the spaces provided for your answers - if an answer is wrong, just put a line through it. You may use a calculator, a ruler, character tables and molecular models; no additional material may be used. Answer all questions on the test - if more space is required, use the back of the page and indicate that your answer is not complete.

Question #1 [30 points]

(a) What does the word “point” indicate in the term “point group”? [2]

(b) In the molecule HF, what is the overlap integral for the combination of the 1s orbital on H and the $2p_x$ orbital on F? Provide an equation, a reasonable numerical value and a drawing showing the overlap of the orbitals: [8]

(c) In a molecule containing N number of atoms, why are there usually $3N-6$ vibrational modes? [2]

(d) Write acceptable LCAO's for the molecular orbitals in the molecule H_2 : [6]

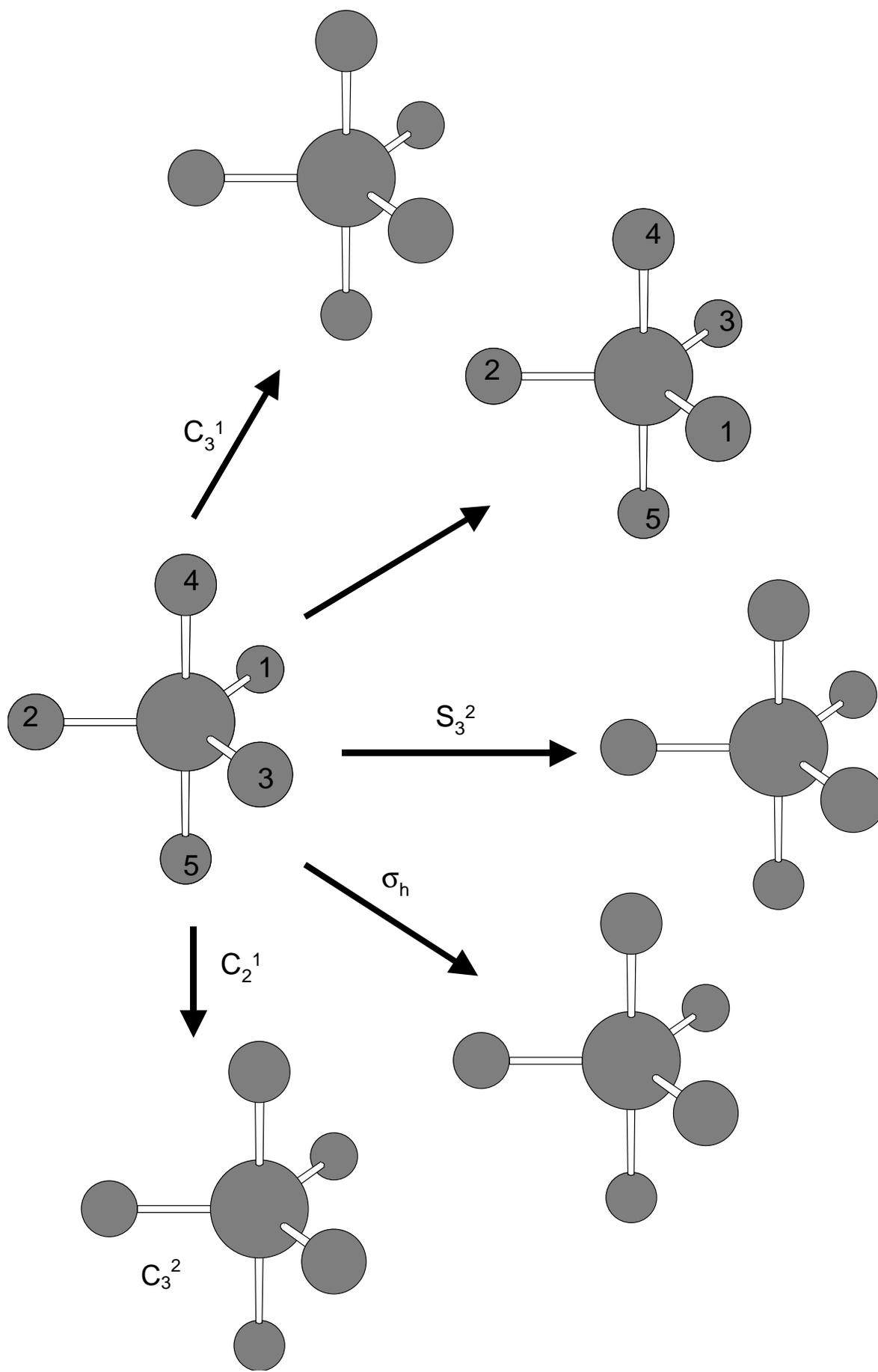
(e) What is the point group of $AsBr_3$? [4]

(f) What is the point group of $SnCl_4$? [4]

(g) What is the point group of the inorganic benzene analogue : [4]

Question #2 [15 points]

Fill in the blanks (operations or numbers) for the following operations on this D_{3h} molecule:



Question #3 [25]

Pentaphenylantimony (SbPh_5) has a square-based pyramidal geometry. (a) Assuming a point group of C_{4v} , use the appropriate character table to determine the orbitals on Sb that are used in the σ bonding. Hint: you only have to consider the bonds of the SbC_5 fragment. [20] (b) Comment **very briefly** on the similarities and differences between the orbitals that you have determined and those that are used to make a trigonal bipyramidal molecule.[5]

Question #4 [20]

(a) Draw and label a VALENCE molecular orbital diagram for the diatomic molecule BF. Note that the molecule is diamagnetic and the HOMO is of σ symmetry. **Be sure to provide labels for each MO and AO and indicate the HOMO and the LUMO.** [15]

(b) What is the predicted bond order in the BF molecule? [1]

(c) Draw a reasonable picture of an anti-bonding molecular orbital that has π symmetry [2]

(d) What is the electron configuration of the BF molecule? [2]

Question #5 [5 points]

In the table below insert the correct symbols for the elements:

Gallium, Neon, Manganese, Lithium, Carbon.

If you choose to fill in the symbols for all the first 36 elements, be sure to emphasize the symbols of the elements that were required.

Look at a periodic table to find the answers for this question!