Week 9 Worksheet

Chem 11200-2: Section 33

March 8, 2022

Problem 1: Lets consider the Born-Oppenheimer approximation.

- a) Explain what the Born-Oppenheimer approximation is and why it is a valid approximation.
- b) Calculate the de Broglie wavelength of a hydrogen atom (a single proton) at 300K. Compare the de Broglie wavelength to the diameter of a hydrogen atom, 1Å. What can you conclude about quantum effects?
- c) In the previous part, you must have also calculated the velocity of the hydrogen atom. Compare this to the average velocity of an electron in a molecule, about 2200 km/s. At what temperature would the hydrogen atom have to be at to be moving at around the same speed as an electron? Is this a realistic temperature?
- d) Based on the previous parts, does your analysis support or illustrate a flaw in the Born-Oppenheimer approximation? Explain.

Problem 2: Consider the molecule GaBr₃.

- a) Draw the 2D Lewis Dot structure.
- b) Draw the 3D VSEPR structure
- c) Using valence bond theory, determine the hybridization of the orbitals on the central atom in GaBr₃. Use noble gas shortcut orbital diagrams to show any electron promotions / hybridizations.

Problem 3: Use valence bond theory to explain why formation of hybrid orbitals in PBr_3 does not require the promotion of an electron to a higher energy orbital, but formation of hybrid orbitals in PBr_5 does.

Problem 4: Consider the molecule N_2 .

- a) Draw the 2D Lewis Dot structure.
- b) Draw the 3D VSEPR structure.
- c) Using an MO diagram, determine the bond order for a molecule of N_2 .
- d) How many σ bonds does N₂ have? π bonds? Label each bond.
- e) Which of the following should be diamagnetic: N_2 , N_2^+ , N_2^- ? Why?

Problem 5: Draw the MO diagram for CO. Furthermore, draw a representation of each MO.

The following problems are written by Professor Mcleod or Head TA Miah Turke. They may mimic homework problems closely, but will be highly beneficial for the midterms and final.

Problem 6: If an electron is removed from the fluorine molecule, an F_2^+ molecular ion forms.

- a) Construct the correlation diagram and give the molecular electron configurations for F_2 and F_2 $^+.$
- b) Give the bond order of each species.
- c) Predict which species should be paramagnetic.
- d) Predict which species has the greater bond dissociation energy.

Problem 7:

- a) Draw the molecular orbital diagram for NO. Next to each energy level for both the atomic and molecular orbitals, draw a representation of the orbital or bond (or antibond).
- b) Write out the valence electron configuration for this molecule.

Problem 8:

- a) Draw the Lewis structure of HCN.
- b) What is the hybridization of the central atom? How many of these hybrid orbitals does the central atom have?
- c) Draw the molecule showing the hybridized orbitals of the central atom, and the atomic orbitals of the end atoms. Label each orbital and bond type, and each of the bonds that are formed.
- d) What are the relevant bond angles in the molecule?