CIRCLE YOUR ANSWERS AND KEY INTERMEDIATE RESULTS
STAPLE YOUR PAPERS TOGETHER
INCLUDE ALL COMPUTER PRINTOUTS

Levine Problems: (Levine 6^{th} Ed)
13.14 – atomic units
13.24 – review MO diagrams and relative stability
Levine Problems: (Levine 5^{th} Ed)
13.14 – atomic units
13.28 – review MO diagrams and relative stability

Additional Problems:

1) Atomic emission spectroscopy can be used to detect the presence of certain metals at very low concentration. The basic concept is simple enough, and you may have even done this in some form or another in a chemistry lab: heat the sample until it is hot enough to emit light and see what color the flame is glowing. Sodium makes the flame glow yellow because of an electronic transition from the (3p) $^2P_{3/2}$ to the (3s) $^2S_{1/2}$ level. Calculate the percentage of atoms in the relative populations of these levels in thermal equilibrium in flames at temperatures of 1500, 2500 and 3500K.

2) Choose a MO wave-function for the H_2^+ ground state using 1s-like orbitals with the exponent (nuclear charge) as the variational parameter (Levine 5^{th} edition eqns 13.43 and 13.44). Set up the coordinate system as suggested in lecture so that you won't need to learn confocal elliptical coordinates.

2A) Evaluate the overlap integral (S) for the H_2^+ MO wave function.

2B) Evaluate the Coulomb (H_{aa}) and Exchange (H_{ab}) integrals for H_2^+ MO wave function.

2C) Using your results from 2 and 3, plot minimized E (as a function of the variational parameter, k) as a function of R for the H_2^+ ion for the bonding and antibonding molecular orbitals. Optional: Plot E vs R for the orbitals with k=1.

2D) Use your calculation to find the equilibrium bond length, and the dissociation energy, of the H_2^+ molecule. Use your calculation to find the energy required to excite the molecule from the n=0 to n=1 vibrational level.

Tips: Make sure you use the 'assume' command to tell the computer everything you know about parameters such as a_0 , R_{AB} (are they positive, real, etc.) or you won't get a correct answer.