## CHM 330 - Worksheet 5 Prof. Andrew J. Pounds Spring 2022

Name\_\_\_\_\_

Section\_\_\_\_\_

- 1. Derive the Hamiltonian operator for the  ${\rm H_2}^-$  molecular system.
  - (a) Draw a box around the terms that go to zero in the Born-Oppenheimer approximation.
  - (b) Draw a circle around the term(s) that make the solution unsolvable in a closed analytic form?
- 2. Using the valence electrons of the nitrogen atomic orbitals, s and p, sketch the electron correlation diagram for the orbitals to form the N<sub>2</sub> molecule. Be sure to include all labels and electron populations.
  - (a) Which species has the longer bond length,  $\mathrm{N_2}$  or  $\mathrm{N_2}^+$
  - (b) Which species has the longer bond length,  $\mathrm{N}_2$  or  $\mathrm{N}_2^{-}$
  - (c) Which species is affected by a magnetic field, circle all that apply:  $N_2^+$ ,  $N_2$ ,  $N_2^-$
- 3. Using the valence electrons of the carbon and oxygen atomic orbitals, s and p, sketch the electron correlation diagram for the orbitals to form the CO molecule. Be sure to include all labels and electron populations.
  - (a) Which species has the longer bond length, CO or CO<sup>+</sup>
  - (b) Which species has the higher bond enthalpy, CO or CO<sup>-</sup>
  - (c) Which species is affected by a magnetic field, circle all that apply: CO<sup>+</sup>, CO, CO<sup>-</sup>
  - (d) An electron in CO makes a  $\pi \to \pi^*$  transition. How will the bond length of the exicited state be different than that of the ground state?