

**Examination 3 - Chemistry 262**

**November 18, 1998**

**Name:** \_\_\_\_\_

**Dr. Jay H. Baltisberger**

**Please answer 3 of 4 questions, showing all calculations - 35 points each, 105 total.**

1. In your own words, describe how the Born-Oppenheimer approximation is used to simplify the quantum mechanical calculations for a  $\text{BeH}_2$  molecule.
1. Draw a pictorial representation of a  $\sigma_g$ ,  $\sigma_u$ ,  $\pi_g$  and  $\pi_u$  molecular orbital. Which of these in general is lower in energy? Which of these in general is higher in energy? Explain.
3. Write out the complete secular determinant used to solve for the energies and coefficients of the molecular orbitals for HF (use the H1s, F1s, F2s, F2p<sub>x</sub>, F2p<sub>y</sub> and F2p<sub>z</sub> orbitals as a basis set). Describe the meaning of each  $\alpha$ ,  $\beta$  and S term in the determinant. Describe a reasonable approximation for which terms may be safely ignored in such a calculation.
4. For each species NF, NF<sup>+</sup>, and NF<sup>-</sup>, use the MO method to A) write the valence-electron configuration; B) find the bond order; C) decide whether the species is paramagnetic.

**BONUS TIME (10 points)**

5. In homonuclear diatomic molecules, all  $u$  MOs are anti-bonding, true or false? Explain.