

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

Dr. Jay H. Baltisberger

Please answer all 6 questions, showing all calculations - 25 points each, 150 total.

$$h = 6.626 \times 10^{-34} \text{ J s}$$

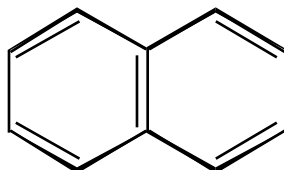
$$c = 2.998 \times 10^8 \text{ m/s}$$

$$N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$$

$$MW_H = 1.00794$$

$$MW_O = 15.9994$$

- Using pictures and words describe the similarities and differences between  $g$ ,  $u$ ,  $g$ , and  $u$  types of molecular orbitals in diatomic molecules.
- Write out the Hückel matrix for naphthalene, describing each variable. In words describe how this matrix may be used to calculate the electronic energies of each  $\pi$ -type orbital and indicate the number of  $\pi$ -type orbitals will be filled. (5 bonus points if you correctly identify the point group for naphthalene.)



- For  $N_2$  describe the difference between calculating the ionization energy and the dissociation energy using SCF-HF methods.
- Describe how a four energy level laser system works and describe briefly two uses for a laser in chemistry.
- Using a 500 nm laser and given that the rotational constant ( $B$ ) for HCl is  $10.5 \text{ cm}^{-1}$ , calculate the position of the four lines in a rotational Raman spectrum nearest to the Rayleigh scattering at  $20,000 \text{ cm}^{-1}$ .
- Calculate the force constant for an O—H bond, given that the O—H stretch appears at approximate  $3500 \text{ cm}^{-1}$ .