

## CHEM 332 – TAKE-HOME EXAMINATION 3 – Spring 2021

**DATED: May 3, 2021**

**DUE: May 10, 2021**

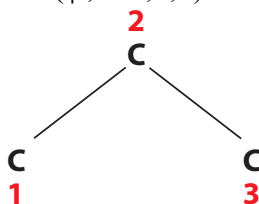
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### Question 1 (40 points)

- Look up the electron configuration of the  $V^{2+}$  ion and list the possible S values. (5 points)
- Consider a  $p^1, d^1$  configuration. What are the complete term symbols for this case? What is term symbol corresponding to the lowest energy level? (20 points)
- The highest occupied molecular orbitals for an excited state of the  $O_2$  molecule are  $(1\pi_g)^1, (3\sigma_u)^1$ . What are the molecular term symbols? Hint: the  $1\pi_g$  derives from  $2p_x$  or  $2p_y$  atomic orbitals and the  $3\sigma_u$  comes from 2s orbitals. (15 points)

### Question 2 (40 points)

In the neutral allyl system (shown below) comprising of 3 carbon atoms, each carbon contributes one  $\pi$  electron housed in their  $2p_z$  orbitals ( $\phi_i, i=1,2,3$ ).



- Write down the secular determinant for the  $\pi$ -system. (5 points)
- What are the energies of the various energy levels? (6 points)
- What are the corresponding normalized wavefunctions? (15 points)
- Calculate the charge on each carbon atom for the allyl cation. (9 points)
- Calculate the  $\pi$ -bond order for each bond for the allyl cation. (5 points)

### Question 3 (20 points)

What is the value for the overlap integral between the following two atomic orbitals?

$$\phi_1 = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left[2 - \frac{r}{a_0}\right] e^{-r/2a_0}$$

$$\phi_2 = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \cos(\theta)$$