Chemistry 410A **Exam 4** **Spring 2008**

NAME:

Instructions:

1. Keep this exam closed until instructed to begin. Please write your name on this page but not on any other page.
2. Please silence any noisy electronic devices you have.
3. Attached sheet(s) provide potentially useful constants and equations. You may detach these from the exam if you prefer.
4. To receive full credit for your work, please
   (a) show all your work, using the back of this sheet if necessary,
   (b) specify the correct units, if any, for your final answers,
   (c) stop writing and close your exam immediately when time is called.

Other notes:

- **Your 4 best scores of the 5 problems will constitute your total score.**
- Partial credit is available for all problems, so try each problem and do not erase any of your work.
- Each question is worth 25 points, but they are not intended to be equally easy.

1. The *sp* hybrid orbital defined below has the correct ratio of $(2s)$ and $(2p_z)$ but is not yet normalized. Find the normalization constant A_{a}, and then write the expression for the normalized hybrid orbital $(sp)_{\mathrm{b}}$ that accompanies $(sp)_{\mathrm{a}}$.

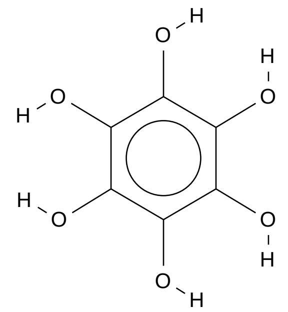
$$(sp)_{\mathrm{a}} = A_{\mathrm{a}} \left[(2s) + \frac{1}{\sqrt{3}}(2p_z) \right]$$

$$A_{\mathrm{a}} =$$

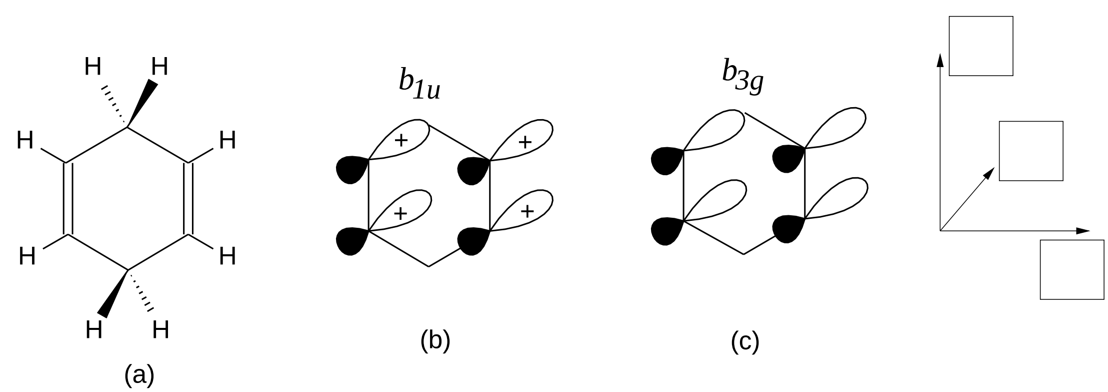
$$(sp)_{\mathrm{b}} =$$

2. Write the name of the *smallest* point group that contains the operators $\hat{C}_5$ and $\hat{I}$.

3. Find the point group of this hexahydroxybenzene. This conformation is planar.



4. The structure of 1,4-cyclohexadiene is shown below in (a). All of the atoms lie in one plane except for the CH_2 hydrogens, which are all equivalent. One MO for the π bonding orbitals, having b_{1u} symmetry, is shown in (b), with the phases of the carbon p orbitals labelled. Fill in the phases for the p orbitals in (c) and label the coordinates on the Cartesian axes to obtain a new molecular orbital for 1,4-hexadiene that has b_{3g} symmetry.



5. Find the symmetry representations of all of the states accessible by an *allowed Raman transition* from the B_{1u} excited state of benzene.