

**CHEM 325**  
**Spring 2009**  
**Post-Exam 1**  
**Due March 6, 2009 at 5:00 PM**

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

**Instructions**

Fill in only the answers below. Attach your work to these cover pages, but do not include the questions. Sign the affidavit at the bottom of the second page. A link to the full contest rules is posted on the *Announcements* section of the class web page.

1a. \_\_\_\_\_

b. \_\_\_\_\_

2. \_\_\_\_\_

3. \_\_\_\_\_

4.

5a. \_\_\_\_\_

b. \_\_\_\_\_

c. \_\_\_\_\_

d. \_\_\_\_\_

6. \_\_\_\_\_

7. \_\_\_\_\_

8. \_\_\_\_\_

9. \_\_\_\_\_

By my signature below I attest that I have abided by all the rules set forth on the web page.

\_\_\_\_\_  
Signature

\_\_\_\_\_  
Date

**Instructor Use Only!**

Number correct	
Work included	
Instructions followed	
Total	

DO NOT TURN THESE QUESTIONS IN WITH THE ANSWER SHEET

- 1a. Is the integral  $\iiint (xy)(z)(x^2 - y^2) dx dy dz$  non-zero in  $D_{2d}$  symmetry?
- b. What irreducible representations are spanned by the direct product  $E \times E$  in  $D_{2d}$ ?
2. Is the transition from a state with  $A_1$  symmetry to a state with  $A_2$  symmetry electric dipole allowed in  $C_{2v}$  symmetry? If it is allowed, in what polarization is it allowed?
3. The rotational constant for  $^{12}\text{C}-^{16}\text{O}_2$  determined from rotational Raman spectroscopy is  $0.39021 \text{ cm}^{-1}$ . Determine the C–O bond length in picometers. The atomic mass of  $^{12}\text{C}$  is 12.0000 amu and the atomic mass of  $^{16}\text{O}$  is 15.9949 amu.
4. Draw a vector representation, using arrows to show the direction of the angular momentum vectors, of a rigid rotor's allowed orientations when  $\ell = 2$ . Indicate the magnitude of each vector and the different values of  $L_z$  on your picture.
- 5a. Determine the equation in terms of  $J$  and  $J-1$  that gives the splitting between the allowed molecular rotational transitions for a linear molecule when the centrifugal distortion is not zero.
- b. Given that the spacing of the lines in the rotational spectrum of  $^{35}\text{Cl}^{19}\text{F}$  is  $1.033 \text{ cm}^{-1}$  and the isotopic mass of  $^{35}\text{Cl}$  is 34.968853 amu and that of  $^{19}\text{F}$  is 18.99840 amu, what is the Cl–F bond length in  $^{35}\text{Cl}^{19}\text{F}$  in picometers?
- c. Calculate  $B$  for  $^{37}\text{Cl}^{19}\text{F}$ .
- d. Will the rotational transitions of  $^{37}\text{Cl}^{19}\text{F}$  occur at higher, at lower, or at the same wavenumbers as those of  $^{35}\text{Cl}^{19}\text{F}$ ?
6. The threshold frequency for the emission of a photoelectron from Na metal is  $43.9 \times 10^{13} \text{ s}^{-1}$ . What is the ionization energy of Na in kJ/mole?
7. Given that the Br–Br bond distance is 283.3 pm, what must a spectrometer's resolution be (in  $\text{cm}^{-1}$ ) to distinguish between the Stokes lines arising from the  $^{79}\text{Br}-^{81}\text{Br}$ ,  $^{79}\text{Br}-^{79}\text{Br}$  and  $^{81}\text{Br}-^{81}\text{Br}$  isotopomers in a rotational Raman spectrum? Assume that the resolution must be half of the smallest splitting that you seek to measure.
8. Naphthalene may be approximated as a  $4.00 \text{ \AA} \times 7.00 \text{ \AA}$  rectangular box. Calculate the expected wavenumber for the light absorbed to give the first excited state of naphthalene.
9. The lowest-lying excited state of a molecule is  $15.0 \text{ cm}^{-1}$  above the ground state in energy. To what temperature, in K, must a sample of this molecule be cooled so that 90.0% of the molecules in the sample are in the ground state? Assume both states are singly degenerate.