

**CHEM 325**  
**Spring 2008**  
**Post-Exam 2**  
**Due May 8, 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. Normal modes in  $D_{\infty h}$ : \_\_\_\_\_

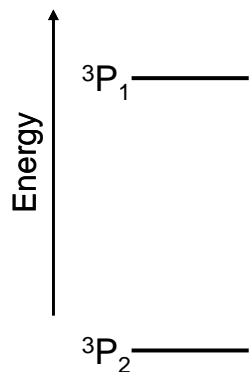
b. Normal modes in  $C_{\infty v}$ : \_\_\_\_\_

2a. Value of  $J$  for  $^1D$  term: \_\_\_\_\_

b. Lowest energy term arising from the  $[\text{He}] 2s^2 2p^3 3s^1$  configuration: \_\_\_\_\_

c.

$^3P_0$  \_\_\_\_\_



H →

d. Relative population equals \_\_\_\_\_

3. Wavenumber of indicated transition: \_\_\_\_\_

4a.  $\tilde{\nu} =$  \_\_\_\_\_  $x_e \tilde{\nu} =$  \_\_\_\_\_

b. Force constant for the N–N bond = \_\_\_\_\_

c.  $D_e =$  \_\_\_\_\_

d.  $D_o =$  \_\_\_\_\_

5. Peak assignments (write wavenumber of transition in the space provided)

${}^2B_2 \rightarrow {}^2A_1$ : \_\_\_\_\_

${}^2B_2 \rightarrow {}^2B_1$ : \_\_\_\_\_

${}^2B_2 \rightarrow {}^2E$ : \_\_\_\_\_

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

\_\_\_\_\_  
Signature

\_\_\_\_\_  
Date

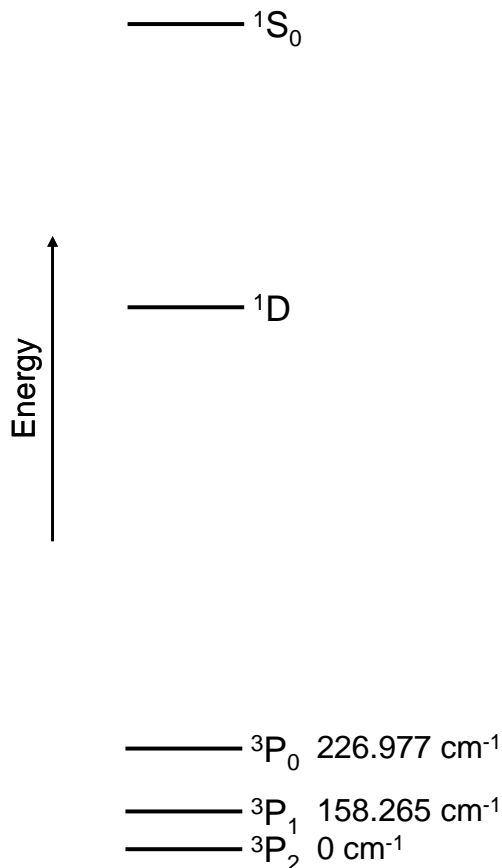
**Instructor Use Only!**

Number correct	
Work included	
Instructions followed	
Total	

DO NOT TURN THESE QUESTIONS IN WITH THE COVER PAGES

1. For a linear triatomic molecule with  $D_{\infty h}$  symmetry the molecular displacement vectors span the following irreducible representations:  $\Sigma_g^+$ ,  $\Sigma_u^+$ ,  $\Sigma_g^-$ ,  $2 \Pi_u$  and  $\Pi_g$ . The molecular displacement vectors for a linear triatomic molecule with  $C_{\infty v}$  symmetry span the irreducible representations  $3 \Sigma^+$  and  $3 \Pi$ . What are the normal modes for the molecules?

2. A partial energy level diagram for the oxygen atom is shown below.



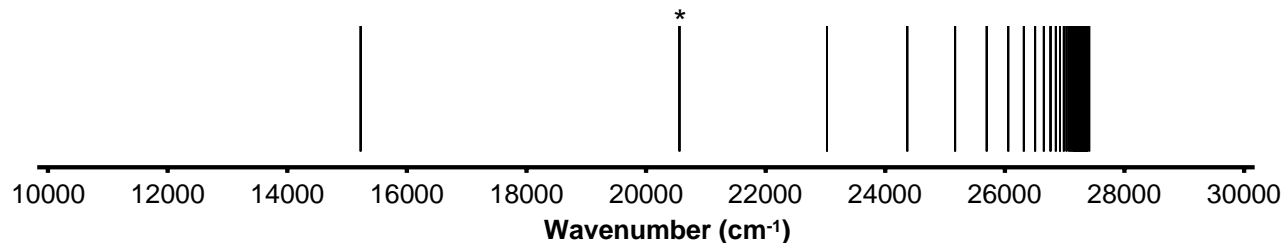
a. What is the value of  $J$  for the  $1D$  term?

b. The next highest energy term (not shown in the above diagram) arises from the electronic configuration  $[\text{He}] 2s^2 2p^3 3s^1$ . Use the shortcut method to determine the term for the three electrons in the  $2p$  orbital and then couple this term with the one arising from a  $3s^1$  electronic configuration to determine the term symbol for lowest energy term arising from the electronic configuration  $[\text{He}] 2s^2 2p^3 3s^1$ .

c. In the space provided draw a qualitative picture showing what happens to each of the  $3P$  levels with increasing magnetic field strength.

d. From the information given calculate the relative population of the  $3P_1$  state at  $100.0 \text{ K}$ .

3. A portion of the emission spectrum of atomic hydrogen is shown below. This particular series starts at  $15228.18 \text{ cm}^{-1}$  and terminates at  $27410.72 \text{ cm}^{-1}$ . There are many more series at lower energy (lower wavenumbers), but only one series at higher energy (higher wavenumbers), neither of which are shown. What is the wavenumber of the peak marked with an asterisk?



4a. For  $^{14}\text{N}_2$  the fundamental occurs at  $2345.15 \text{ cm}^{-1}$ , the first overtone occurs at  $4661.40 \text{ cm}^{-1}$  and the second overtone occurs at  $6983.73 \text{ cm}^{-1}$ . Calculate  $\tilde{\nu}$  and  $x_e\tilde{\nu}$ .

b. What is the force constant for the N–N bond? The atomic mass of  $^{14}\text{N}$  is 14.00307 amu.

c. What is  $D_e$ , the depth of the Morse potential, well for  $\text{N}_2$  (in  $\text{cm}^{-1}$ )?

d. What is the spectroscopic dissociation energy,  $D_o$ , for  $\text{N}_2$  (in  $\text{cm}^{-1}$ )?

5. The complex ion  $[\text{CuCl}_4]^{2-}$  adopts different structures in the solid state depending on the counter ion. In one particular compound the  $[\text{CuCl}_4]^{2-}$  has  $D_{2d}$  symmetry. The ground state is  $^2B_2$  and the possible electronic excited states are  $^2A_1$ ,  $^2B_1$  and  $^2E$ . The absorption spectrum of the single crystal shows peaks at  $5000 \text{ cm}^{-1}$  (x, y polarized) and at  $9000 \text{ cm}^{-1}$  (z polarized). Assign the spectrum (state which electronic transition goes with which peak).