V25.0109: General Chemistry I (Honors) **Professor M.E. Tuckerman**
First Midterm Examination **October 19, 2007**

NAME and ID NUMBER:

There should be **19** pages to this exam, counting this cover sheet. Please check this exam NOW!

There are three pages of formulae/data and a periodic table (with molar masses) at the back of this exam. Books, notes, etc. are not permitted, however calculators are. Not all questions are equally difficult. Spending all your time on one question is generally a bad idea. Partial credit will be given but only if your answers can be deciphered. Therefore, make sure that your writing is neat and that your logic is clear, organized, and easy to follow. Unreadable answers will not be given the benefit of the doubt. Good luck.

GRADING

1. (15 points)

2. (15 points)

3. (30 points)

4. (20 points)

5. (20 points)

TOTAL: 100 points

Extra Credit:

1. (**15 points**)
   In the molecule formaldehyde (CH_2O), the carbon is the central atom.

   a. (**5 points**)
      Determine the Lewis structure of the molecule including any nonzero formal charges.

b. (**5 points**)
Use the VSEPR theory to determine is basic geometry.

c. (**5 points**)
High-level calculations predict that the HCO angles are approximately 128°, while the HCH angle is 116°. Explain these angles on the basis of your Lewis structure and the geometry you predict from VSEPR theory.

2. (**15 points**)
In a certain model of the water molecule, the bond lengths are 0.98 Å and the HOH bond angle is 105.1°. The *magnitude* of its dipole moment is 1.88D. What are the partial charges on each of the atoms of the molecule?

3. (**30 points**)
The wave functions $\psi_n(x)$ for a particle in a one-dimensional box of length L that extends from $x = 0$ to $x = L$ satisfy a condition known as *orthogonality*:

$$\int_0^L \psi_n(x)\psi_m(x)dx = 0$$

when $n \neq m$.

Suppose that a particle of mass m in such a box is prepared in a state whose wave function $\Psi(x)$ is a mixture of pure particle-in-a-box wave functions:

$$\Psi(x) = \frac{1}{\sqrt{3}}\psi_1(x) + \sqrt{\frac{2}{3}}\psi_2(x)$$

a. (**5 points**)
Show that $\Psi(x)$ is a properly normalized wave function.

b. (**5 points**)
When the particle is in this state, what is the probability that a measurement of its position will yield a value between $x = L/4$ and $x = L/2$?

c. (**5 points**)
The probability $P(E_n)$ that a measurement of the energy yields one of the allowed energies E_n is

$$P(E_n) = \left| \int_0^L \psi_n(x) \Psi(x) dx \right|^2$$

What is the probability that a measurement of the energy yields the value $\hbar^2 \pi^2 / (2mL^2)$?

d. (**5 points**)
What is the probability that a measurement of the energy yields a value $\hbar^2\pi^2/(3mL^2)$?

e. (**5 points**)
The wave functions $\psi_n(x)$ satisfy the time-independent Schrödinger equation $\hat{H}\psi_n(x) = E_n\psi_n(x)$. The *expectation value* of the energy, which is the average energy over many energy measurements, is given by

$$\bar{E} = \int_0^L \Psi(x)\hat{H}\Psi(x)dx$$

What is the average energy for a particle in the state whose wave function is $\Psi(x)$?

Hint: Although the Hamiltonian $\hat{H}$ is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

for this problem, you can do the whole problem without using this formula or doing any integrals explicitly.

f. (**5 points**)
The potential $V(x) = 0$ inside the box, and therefore, the classical energy in the box is $E = p^2/2m$. Given that the quantum mechanical energy can only take on certain values, E_n, show that the particle's momentum p also has only certain allowed values p_n *and* show, using de Broglie's formula for the particle's wavelength, that these momenta predict the correct wavelengths as they appear in the corresponding wave functions $\psi_n(x)$. Use pictures if these will help your argument.

4. (**20 points**)

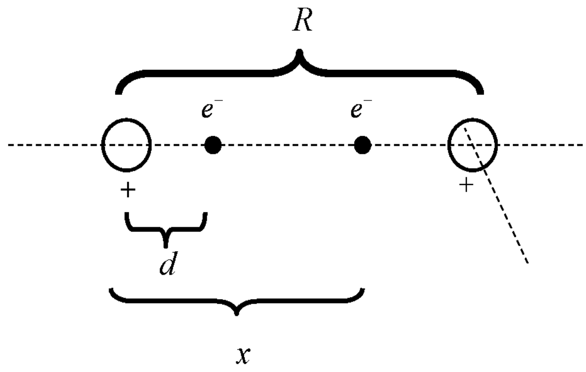
Acetylene (C_2H_2) is produced in the following reaction with an unknown solid substance X:

$$CaCO_3 + aX + bH_2O \longrightarrow cCO_2 + dCO + eCa(OH)_2 + fC_2H_2$$

When 895.78 g of the unknown substance react with 5.0 kg of limestone ($CaCO_3$), 647.30 g of acetylene is produced. After all reactions have ceased, the contents of the reaction vessel are analyzed, and it is found that no X remains, yet there are 2.512 kg of limestone remaining. The only other information we have about the unknown substance is that in its purest form, its molar mass is numerically roughly 4 times its stoichiometric coefficient in the above reaction. Determine the molar mass of X and balance the above reaction. What is the unknown substance?

5. (**20 points**)
Consider a configuration of the two protons and two electrons in the classical H_2 molecule in which all particles lie along the x-axis. Both electrons are assumed to be located between the two protons. Suppose that the two protons are a distance R apart and that the electrons are at distances d and x from one of the protons, respectively (see figure). If x can be varied so as to find the most stable location for the second electron, derive a polynomial equation for x that gives the most stable location for this movable electron. Note, you do not need to find a solution to the equation.

Hint: Does potential energy minimum ring a bell?



Extra Credit (10 points)
The wave function for the *first* excited state of a harmonic oscillator of mass m, frequency ν and spring constant k is

$$\psi_1(x) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} xe^{-\alpha x^2/2}$$

where $\alpha = m\omega/\hbar$ and $\omega = 2\pi\nu = \sqrt{k/m}$. Show that $\psi_1(x)$ satisfies the Schrödinger equation for the harmonic oscillator.

Note: Since this is for extra credit, in order to receive credit, you must show *all* of your steps in a clear an organized fashion (similar to a proof).

POSSIBLY USEFUL INFORMATION

$$N_0 = 6.022 \times 10^{23}\ \mathrm{mol}^{-1}$$

$$k_\mathrm{B} = 1.38066 \times 10^{-23}\ \mathrm{J \cdot mol^{-1} \cdot K^{-1}} = 1.36262 \times 10^{-25}\ \mathrm{L \cdot atm \cdot mol^{-1} \cdot K^{-1}}$$

$$e = 1.60219 \times 10^{-19}\ \mathrm{C} \qquad \epsilon_0 = 8.854 \times 10^{-12}\ \mathrm{C^2 \cdot J^{-1} \cdot m^{-1}}$$

$$h = 6.6208 \times 10^{-34}\ \mathrm{J \cdot s} \qquad \hbar = \frac{h}{2\pi} = 1.105457 \times 10^{-34}\ \mathrm{J \cdot s}$$

$$c = 2.99769 \times 10^{8} \mathrm{m/s}$$

Some conversion factors

$1\ \text{Å} = 10^{-8}\ \mathrm{cm} = 10^{-10}\ \mathrm{m}$
$1\ \mathrm{J} = 1\ \mathrm{kg \cdot m^2 \cdot s^{-2}}$

$1\ \mathrm{D} = 3.336 \times 10^{-30}\ \mathrm{C \cdot m}$
$1\ \mathrm{Ry} = 2.18 \times 10^{-18}\ \mathrm{J}$

Formulas

$$E_\mathrm{Coul} = \frac{q_1 q_2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} = \frac{q_1 q_2}{4\pi\epsilon_0 r} \qquad \mathbf{F} = \frac{q_1 q_2}{4\pi\epsilon_0 r^3}\mathbf{r}$$

$$\boldsymbol{\mu} = \sum_{i=1}^{N} q_i \mathbf{r}_i \qquad \boldsymbol{\mu}(\text{in D}) = \frac{1}{0.2082\text{Å} \cdot \mathrm{D}^{-1}} \sum_{i=1}^{N} \delta_i \mathbf{r}_i (\text{in Å})$$

$$\Delta = \Delta E_\mathrm{AB} - \sqrt{\Delta E_\mathrm{AA} \Delta E_\mathrm{BB}} \qquad \chi_\mathrm{A} - \chi_\mathrm{B} = 0.102\sqrt{\Delta} \qquad \mathrm{EN} \propto \frac{1}{2}(\mathrm{IE}_1 + \mathrm{EA})$$

$$\mathrm{FC} = (\#\ \text{valence electrons}) - (\#\ \text{electrons in lone pairs}) - \frac{1}{2}(\#\ \text{electrons in bonding pairs})$$

$$\mathrm{SN} = (\#\ \text{atoms bonded to central atom}) + (\#\ \text{lone pairs on central atom})$$

$$KE = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad A = \sum_{i=1}^{N} A_i p_i$$

$$V = V_{ee} + V_{en} + V_{nn} \qquad V_\mathrm{eff} = -\frac{Z_\mathrm{eff} e^2}{4\pi\epsilon_0 r}$$

$$\Delta E_{\text{bind}} = -\frac{e^2}{4\pi\epsilon_0 R_e} + \text{IE}_1 - \text{EA} \qquad \Delta E_{\text{d}} = -\Delta E_{\text{bind}}$$

$$\bar{K} = -\frac{1}{2}\bar{V} \qquad F(x) = -\frac{dV}{dx}$$

$$A(x,t) = A_0 \cos\left(\frac{2\pi x}{\lambda} - 2\pi\nu t\right) \qquad v = \lambda\nu \qquad c = \lambda\nu$$

$$V(x) = \frac{1}{2}k\left(x - x_0\right)^2 \qquad F = -k\left(x - x_0\right) \qquad I(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/k_{\text{B}}T} - 1}$$

$$h\nu = \Phi + \frac{p^2}{2m_e} \qquad \lambda = \frac{h}{p} \qquad A(y) = \cos\left(S(y)\right) + i\sin\left(S(y)\right) = e^{iS(y)} \qquad P(y) = \left|\sum_{\text{paths}} A_{\text{path}}(y)\right|^2$$

$$\Delta A \Delta B \geq \frac{1}{2}\hbar \qquad \Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2} \qquad \Delta x \Delta p \geq \frac{1}{2}\hbar$$

$$E_n = -\frac{Z^2 e^4 m_e}{8\epsilon_0^2 h^2}\frac{1}{n^2} = -\frac{Z^2}{n^2} \text{ (in Ry)}$$

$$h\nu = E_{n_i} - E_{n_f} \quad \text{(emission)} \qquad h\nu = E_{n_f} - E_{n_i} \quad \text{(absorption)}$$

$$\hat{H}\psi(x) = E\psi(x) \qquad p(x)dx = |\psi(x)|^2 dx \qquad P(x \in [a,b]) = \int_a^b |\psi(x)|^2 dx$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x) \qquad \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 \qquad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

$$\hat{H}\Psi(x,t) = i\hbar\frac{d}{dt}\Psi(x,t) \qquad E_n = \left(n + \frac{1}{2}\right)h\nu \qquad \nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

Mathematics

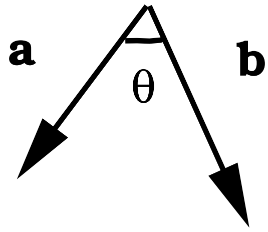


FIG. 1.

$$\mathbf{a} = (a_x, a_y, a_z)$$

$$|\mathbf{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2}$$

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z$$

$$\mathbf{a} + \mathbf{b} = (a_x + b_x, a_y + b_y, a_z + b_z)$$

$$|\mathbf{a} + \mathbf{b}| = \sqrt{|\mathbf{a}|^2 + |\mathbf{b}|^2 + 2\mathbf{a} \cdot \mathbf{b}}$$

$$\theta = \cos^{-1}\left[\frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}|\,|\mathbf{b}|}\right]$$

Trigonometry

$$\cos^2(x) + \sin^2(x) = 1$$

$$\cos^2(x) = \frac{1}{2} + \frac{1}{2}\cos(2x)$$

$$\sin^2(x) = \frac{1}{2} - \frac{1}{2}\cos(2x)$$

$$\sin(x)\cos(x) = \frac{1}{2}\sin(2x)$$

$$e^{ix} = \cos(x) + i\sin(x)$$

$$\frac{d}{dx}\cos(x) = \sin(x)$$

$$\frac{d}{dx}\sin(x) = -\cos(x)$$

Integrals

$$\int \sin(ax)\sin(bx)dx = \frac{\sin[(a-b)x]}{2(a-b)} - \frac{\sin[(a+b)x]}{2(a+b)}$$

$$\int \sin^2(ax)dx = \frac{1}{2}x - \frac{1}{4a}\sin(2ax)$$

$$\int_a^b f(x)dx = F(b) - F(a) \qquad \frac{dF}{dx} = f(x)$$