Chemistry 410A **Exam 1** **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. A classical beam of radiation A has an electric field obeying the equation

$$\mathcal{E}_{\mathrm{A}} = \epsilon_{\mathrm{A}} \sin(2\pi\nu_{\mathrm{A}} t),$$

and a second beam B, lined up in the same plane as A, obeys the equation

$$\mathcal{E}_{\mathrm{B}} = \epsilon_{\mathrm{B}} \sin(2\pi\nu_{\mathrm{B}} t).$$

The two beams overlap starting at a **position** $x = 0$, where both fields are exactly zero and about to become positive. Find the first x value (in m) **greater** than zero where the electric field is again exactly zero if $\nu_{\mathrm{A}} = 1.0{\cdot}10^{14}\ \mathrm{s}^{-1}$ and $\nu_{\mathrm{B}} = 1.2{\cdot}10^{14}\ \mathrm{s}^{-1}$.

2. The last electron in a Li^{2+} ion absorbs a photon with energy 6.0 E_{h}. This is enough to ionize the electron and have some energy left over. The remaining energy goes into the kinetic energy of the ionized electron. Calculate the de Broglie wavelength in Å of this ionized electron.

3. Let's assume that the Bohr model is sufficiently accurate to estimate the timescales for motion of the electron in the hydrogen atom. When the electron is excited from the $n = 1$ level to the $n = 2$ level, it has to leave one orbit to enter a new orbit. Calculate the **minimum** time (in seconds) necessary for the electron to change from the $n = 1$ state to the $n = 2$ state in the Bohr model, assuming that the electron travels at the speed $v_{n=1}$ during the transition.

4. We have a wavefunction $\psi(x) = 2xe^{-3x^2}$. Circle the letter below for any operator below where $\psi(x)$ is an eigenfunction of the operator. Write the eigenvalue next to the operator.

   (a) $4x$

   (b) $(1/x)\,\frac{d}{dx}$

   (c) $\frac{d}{dx}\,(1/x)$

   (d) $x^3 e^{-3x^2}\,\frac{d}{dx}\,(e^{3x^2}/x^2)$

5. Begin with a particle of mass m_e and charge $-e$ in the $n = 1$ state of a one-dimensional box of length a. Define ΔE_{12} to be the $n = 1 \rightarrow 2$ transition energy. For each change listed in the table below, indicate the factor by which the new transition energy ΔE changes, compared to this initial value ΔE_{12}.

change initial system by	$\Delta E = \Delta E_{12}$ **times** ...
increasing mass to m_p (the proton mass)	
reducing box length to $a/2$	
turning box to point along z axis instead of x axis	
increasing upper state of transition to $n = 4$	
increasing charge to $-2e$	

$$\text{Balmer:}\quad E_{\text{photon}} = (2.180 \cdot 10^{-18}\ \text{J}) \left(\frac{1}{n''^2} - \frac{1}{n'^2}\right)$$

$$\text{Bohr atom:}\quad r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{Z m_e e^2} = \frac{n^2}{Z} a_0 \qquad v_n = \frac{Ze^2}{4\pi\epsilon_0 n\hbar}$$

$$E_n = -\frac{Z^2 m_e e^4}{(4\pi\epsilon_0)^2 2n^2\hbar^2} = -\frac{Z^2}{2n^2}\ E_{\text{h}} \qquad L_n = m_e r_n v_n = n\hbar$$

$$\text{momentum operator:}\quad \hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$$

$$\text{kinetic energy operator:}\quad \hat{K} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\text{particle in a 1-D box:}\quad \psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Derivatives

dx^c	$= cx^{c-1}dx\ (c \neq 0)$	$d(cx)$	$= c dx$
$d\ln x$	$= \frac{1}{x}dx$	de^x	$= e^x dx$
$d\sin x$	$= \cos x dx$	$d\cos x$	$= -\sin x dx$
$d[f(x)+g(x)]$	$= d[f(x)] + d[g(x)]$	$d[f(x)g(x)]$	$= f(x)d[g(x)] + g(x)d[f(x)]$

Integrals

$\int x^n dx$	$= \frac{1}{n+1}x^{n+1} + C$	$\int a dx$	$= a(x + C)$
$\int \frac{1}{x}dx$	$= \ln x + C$	$\int e^x dx$	$= e^x + C$
$\int \ln x dx$	$= x\ln x - x + C$	$\int \frac{dx}{x(a+bx)}$	$= -\frac{1}{a}\ln\left(\frac{a+bx}{x}\right) + C$
$\int \sin x dx$	$= -\cos x + C$	$\int \cos x dx$	$= \sin x + C$
$\int \sin^2(ax)dx$	$= \frac{x}{2} - \frac{\sin(2ax)}{4a} + C$	$\int \cos^2(ax)dx$	$= \frac{x}{2} + \frac{\sin(2ax)}{4a} + C$
$\int [f(x)+g(x)]dx$	$= \int f(x)dx + \int g(x)dx$	$\int_a^b dx$	$= x\vert_a^b = b - a$
$\int_0^\infty x^n e^{-ax} dx$	$= \frac{n!}{a^{n+1}}$	$\int_0^\infty e^{-ax^2} dx$	$= \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}$
$\int_0^\infty x e^{-ax^2} dx$	$= \frac{1}{2a}$	$\int_0^\infty x^2 e^{-ax^2} dx$	$= \frac{1}{4}\left(\frac{\pi}{a^3}\right)^{1/2}$
$\int_0^\infty x^{2n+1} e^{-ax^2} dx$	$= \frac{n!}{2a^{n+1}}$	$\int_0^\infty x^{2n} e^{-ax^2} dx$	$= \frac{[1\cdot 3\cdot 5 \ldots (2n-1)]\sqrt{\pi}}{2^{n+1}a^{n+(1/2)}}$

Fundamental Constants

Avogadro's number	$\mathcal{N}_A$	$6.0221367 \cdot 10^{23}$ mol^{-1}
Bohr radius	$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$	$5.29177249 \cdot 10^{-11}$ m
Boltzmann constant	k_B	$1.380658 \cdot 10^{-23}$ J K^{-1}
electron rest mass	m_e	$9.1093897 \cdot 10^{-31}$ kg
fundamental charge	e	$1.6021773 \cdot 10^{-19}$ C
permittivity factor	$4\pi\epsilon_0$	$1.113 \cdot 10^{-10}$ C^2 J^{-1} m^{-1}
gas constant	R	8.314510 J K^{-1} mol^{-1}
	R	0.08314510 L bar K^{-1} mol^{-1}
	R	0.08206 L atm K^{-1} mol^{-1}
hartree	$E_\mathrm{h} = \frac{m_e e^4}{(4\pi\epsilon_0)^2\hbar^2}$	$4.35980 \cdot 10^{-18}$ J
Planck's constant	h	$6.6260755 \cdot 10^{-34}$ J s
	$\hbar$	$1.05457266 \cdot 10^{-34}$ J s
proton rest mass	m_p	$1.6726231 \cdot 10^{-27}$ kg
neutron rest mass	m_n	$1.6749286 \cdot 10^{-27}$ kg
speed of light	c	$2.99792458 \cdot 10^{8}$ m s^{-1}

Unit Conversions

	K	cm^{-1}	kJ mol^{-1}	kcal mol^{-1}	erg	kJ
kHz =	$4.799 \cdot 10^{-8}$	$3.336 \cdot 10^{-8}$	$3.990 \cdot 10^{-10}$	$9.537 \cdot 10^{-11}$	$6.626 \cdot 10^{-24}$	$6.626 \cdot 10^{-34}$
MHz =	$4.799 \cdot 10^{-5}$	$3.336 \cdot 10^{-5}$	$3.990 \cdot 10^{-7}$	$9.537 \cdot 10^{-8}$	$6.626 \cdot 10^{-21}$	$6.626 \cdot 10^{-31}$
GHz =	$4.799 \cdot 10^{-2}$	$3.336 \cdot 10^{-2}$	$3.990 \cdot 10^{-4}$	$9.537 \cdot 10^{-5}$	$6.626 \cdot 10^{-18}$	$6.626 \cdot 10^{-28}$
K =	1	0.6950	$8.314 \cdot 10^{-3}$	$1.987 \cdot 10^{-3}$	$1.381 \cdot 10^{-16}$	$1.381 \cdot 10^{-26}$
cm^{-1} =	1.4388	1	$1.196 \cdot 10^{-2}$	$2.859 \cdot 10^{-3}$	$1.986 \cdot 10^{-16}$	$1.986 \cdot 10^{-26}$
kJ mol^{-1} =	$1.203 \cdot 10^{2}$	83.59	1	0.2390	$1.661 \cdot 10^{-14}$	$1.661 \cdot 10^{-24}$
kcal mol^{-1} =	$5.032 \cdot 10^{2}$	$3.498 \cdot 10^{2}$	4.184	1	$6.948 \cdot 10^{-14}$	$6.948 \cdot 10^{-24}$
eV =	$1.160 \cdot 10^{4}$	$8.066 \cdot 10^{3}$	96.49	23.06	$1.602 \cdot 10^{-12}$	$1.602 \cdot 10^{-22}$
hartree =	$3.158 \cdot 10^{5}$	$2.195 \cdot 10^{5}$	$2.625 \cdot 10^{3}$	$6.275 \cdot 10^{2}$	$4.360 \cdot 10^{-11}$	$4.360 \cdot 10^{-21}$
erg =	$7.243 \cdot 10^{15}$	$5.034 \cdot 10^{15}$	$6.022 \cdot 10^{13}$	$1.439 \cdot 10^{13}$	1	10^{-10}
J =	$7.243 \cdot 10^{22}$	$5.034 \cdot 10^{22}$	$6.022 \cdot 10^{20}$	$1.439 \cdot 10^{20}$	10^{7}	10^{-3}
dm^3 bar =	$7.243 \cdot 10^{24}$	$5.034 \cdot 10^{24}$	$6.022 \cdot 10^{22}$	$1.439 \cdot 10^{22}$	$1.000 \cdot 10^{9}$	0.1000
kJ =	$7.243 \cdot 10^{25}$	$5.034 \cdot 10^{25}$	$6.022 \cdot 10^{23}$	$1.439 \cdot 10^{23}$	10^{10}	1

distance	1 Å =	10^{-10} m	
mass	1 amu =	$1.66054 \cdot 10^{-27}$ kg	
energy	1 J =	1 kg m^2 s^{-2}	= 10^7 erg
force	1 N =	1 kg m s^{-2}	= 10^5 dyn
electrostatic charge	1 C =	1 A s	= $2.9979 \cdot 10^9$ esu
	1 D =	$3.3357 \cdot 10^{-30}$ C m	= $1 \cdot 10^{-18}$ esu cm
magnetic field strength	1 T =	1 kg s^{-2} A^{-1}	= 10^4 gauss
pressure	1 Pa =	1 N m^{-2}	= 1 kg m^{-1} s^{-2}
	1 bar =	10^5 Pa	= 0.98692 atm