Chem 4A, Fall 2010
Midterm Exam 1, September 22, 2010.
Prof. Head-Gordon, Prof. Saykally

Name: KEY GSI: ____________

Grade:			
	1.	(5 points)	________
	2.	(5 points)	________
	3.	(4 points)	________
	4.	(7 points)	________
	Total:		________

Closed book exam. There are 6 pages. Calculators are OK. Show all working.
Use back side of pages for scribble paper. Don't spend too much time on any one problem!
Read all parts of each question and include units in all answers.

Some possibly useful facts and figures:

$R = 8.3145$ J mol^{-1} K^{-1}	molar volume at STP = 22.4 L
$h = 6.6261\times 10^{-34}$ J s	1 J = 1 kg m^2 s^{-2}
$c = 2.9979 \times 10^{8}$ m s^{-1}	
$m_e = 9.1094 \times 10^{-31}$ kg	
$N_0 = 6.0221 \times 10^{23}$ mol^{-1}	

Some possibly relevant equations:

Planck relation:	$E = h\nu$	
de Broglie relation:	$p = h/\lambda$	
wave equation:	$c = \nu\lambda$	
uncertainty principle	$\Delta p \Delta x \geq h/4\pi$	
particle-in-a-box	$E_n = \dfrac{n^2h^2}{8mL^2}$	$\Psi_n = \sqrt{\dfrac{2}{L}}\sin\dfrac{n\pi x}{L}$
hydrogen atom	$E_n = -\dfrac{Z^2}{n^2}R_\infty$	$R_\infty = 2.18\times 10^{-18}\,J$
linear momentum	$p = mv$	
kinetic energy	$T = \frac{1}{2}mv^2 = p^2/2m$	

1. Stoichiometry and elementary bonding theory. A compound is being tested as a possible rocket propellant, and elemental analysis reveals that it is 18.54% F, 34.61% Cl, and 46.85% O by mass (relative atomic masses are 18.998 (F), 35.343 (Cl), 15.994 (O)).

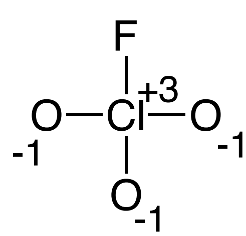
(a) (3 points) Determine the empirical formula of the compound.

F:	18.54 g	÷	18.998 g mol^{-1}	= 0.9759 mol
Cl:	34.61 g	÷	35.343 g mol^{-1}	= 0.9793 mol
O:	46.85 g	÷	15.994 g mol^{-1}	= 2.929 mol

F:Cl:O = 1:1:3

$ClFO_3$

(b) (1 point) If the molecular formula is the same as the empirical formula, write a Lewis diagram for the molecule, assuming that Cl is at the center.



(c) (1 point) Use the VSEPR model to predict the geometry of the molecule.

Tetrahedral

2. Waves behaving like particles and particles behaving like waves…

(a) (2 points) The work function of the metal chromium is 7.2×10^{-19} J. If chromium is exposed to radiation with wave length 2.0×10^{-7} m, can photoelectrons be ejected, and if so, with what kinetic energy release?

$E_{max} = h\nu - \Phi$
$\Phi = 7.2 * 10^{-19}$ J

$E_{radiation} = h * c \div \lambda = h * c \div (2.0 * 10^{-7}\ m) = 9.94 * 10^{-19}$ J

So yes, photons can be ejected, and their energies will be:

$E_{max} = h\nu - \Phi = 9.94 * 10^{-19}\ J - 7.2 * 10^{-19}\ J =$ **$2.7 * 10^{-19}$ J**

(b) (3 points) Calculate the kinetic energy necessary to achieve a de Broglie wavelength of 2 Å for helium atoms and electrons (relative atomic mass of He is 4.003). Use your results to comment on which approach would be likely to cause more surface damage in imaging a surface by diffraction.

$T = p^2 \div [2 * m] = h^2 \div [\lambda^2 * 2 * m]$

Helium atom:

mass $= 4.003\ g\ mol^{-1} \div (6.0221 * 10^{23}\ mol^{-1})$
$= 6.65 * 10^{-27}$ kg

$T = h^2 \div [(2 * 10^{-10}\ m) * 2 * (6.65 * 10^{-27}\ kg)] =$ **$8.3 * 10^{-22}$ J**

Electron:

$T = h^2 \div [(2 * 10^{-10}\ m) * 2 * (9.1094 * 10^{-31}\ kg)] =$ **$6.0 * 10^{-22}$ J**

Therefore an electron is likely to cause more damage.

3. Bohr model for 1-electron atoms, and the Lyman series.

(a) (2 points). The Lyman series involves the emission of radiation from excited H atoms to their ground state. Calculate the Lyman frequency of radiation that is emitted when the initial level is n=3.

For emission, $E_i = E_f + h\nu$

$$\nu = E_I - E_f = [R_\infty * Z^2 * (1/n_f^2 - 1/n_i^2)] \div h$$

$$= [R_\infty * Z^2 * (1/1 - 1/9)] \div h$$

$$= \mathbf{2.92 * 10^{15}\ s^{-1}}$$

(b) (2 points). If He^+ ions are present in the same region as the emitting H atoms, such as in close to stars, explain fully whether they can or cannot absorb the radiation emitted in (a) above.

For He^+ ions to absorb the radiation from part (a), they would have to have an energy transition such that $E_f - E_i = (8/9) * R_\infty$

Therefore, $(8/9) * R_\infty = [R_\infty * 2^2 * (1/n_f^2 - 1/n_i^2)]$

$$(8/9) = 4/n_f^2 - 4/n_i^2$$

By inspection, $\mathbf{n_i = 2}$ and $\mathbf{n_f = 6}$

4. The particle in a box and the zero point energy.

(a) (2 points) Use Heisenberg's uncertainty principle to estimate the minimum uncertainty in momentum (and thus the minimum momentum) for an electron in a box of length 2Å.

$\Delta p * \Delta x \geq h \div [4 * \pi]$

$\Delta p \geq h \div [4 * \pi * \Delta x]$

$\Delta p \geq h \div [4 * \pi * (2 * 10^{-10}\ \mathrm{m})]$

$\Delta p \geq$ **$2.6 * 10^{-25}$ kg m s^{-1}**

(b) (1 point) From your result in (a), estimate the minimum energy associated with a particle in a box of length 2Å.

Option 1:

$E = T + V = T = p^2 \div [2 * m]$
$= (2.6 * 10^{-25}\ \mathrm{kg\ m\ s^{-1}})^2 \div [2 * (9.1094 * 10^{-31}\ \mathrm{kg})]$
$=$ **$3.8 * 10^{-20}$ J**

Option 2:

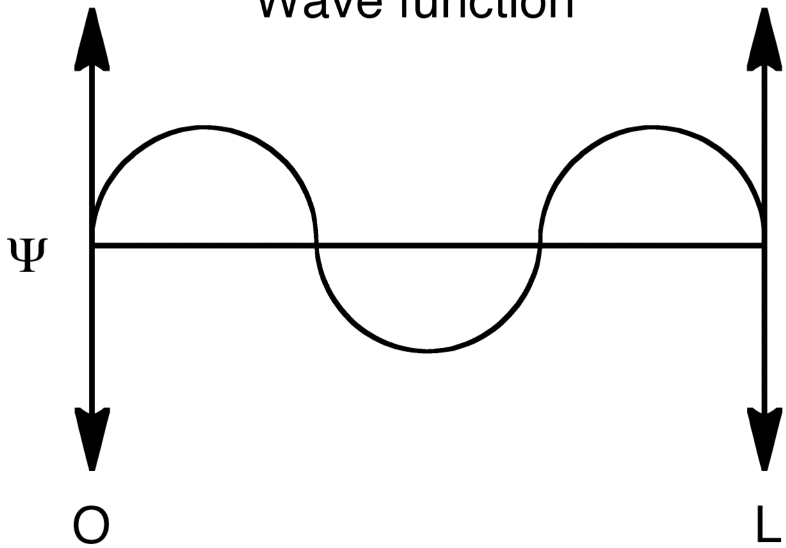
$E = n^2 * h^2 \div [8 * m * L^2]$
$= 1^2 * h^2 \div [8 * (9.1094 * 10^{-31}\ \mathrm{kg}) * (2 * 10^{-10}\ \mathrm{m})^2]$
$=$ **$1.5 * 10^{-18}$ J**

(c) (2 points) Suppose an electron is confined to a box of length 2Å. What photon energy would be required to promote the electron from the n=2 level to the n=3 level?

$E = n^2 * h^2 \div [8 * m * L^2]$
$E_3 - E_2 = (9 - 4) * h^2 \div [8 * (9.1094 * 10^{-31}\ \mathrm{kg}) * (2 * 10^{-10})^2]$
$=$ **$7.5 * 10^{-18}$ J**

(d) (2 points) Make a sketch of the wave function and probability density associated with the n=3 level of the particle in a box.

Wave function



Probability Density