Please write your name here: [redacted]

Please write your student number here: [redacted]

Please read this page before starting the exam.

CHM 2330 - **Midterm Exam #2** – March 17, 2017

Professor Pell

Total time available: 1 hour and 20 minutes (80 minutes)

Instructions: Make sure you have all 8 pages. If you write in pencil, you cannot have any part of the exam considered for re-marking. Programmable calculators are not allowed. Include units where appropriate. If you need extra space, you may write on the backs of the pages, but indicate that you are doing so. Show all work for full marks.

Formula sheets: This is a **closed-book exam**. You are not allowed to bring in any of your own formula sheets, notes, books etc. You may rip off the formula sheet (page 7 and 8) from this exam

Cellular phones, unauthorized electronic devices or course notes (unless an open-book exam) are not allowed during this exam. Phones and devices must be turned off and put away in your bag. Do not keep them in your possession, such as in your pockets. If caught with such a device or document, the following may occur: you will be asked to leave immediately the exam and academic fraud allegations will be filed which may result in you obtaining a 0 (zero) for the exam.

By signing below, you acknowledge that you have ensured that you are complying with the above statement.

Please sign your name here: [redacted]

28
32

6.5

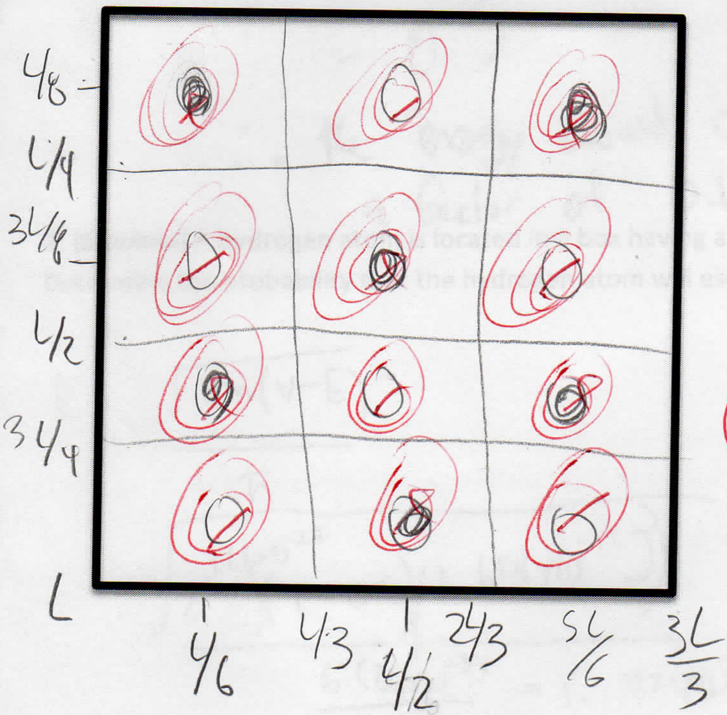
1. Consider an argon atom confined to in a 2-D square box of edge length L.

a) **(1 point)** What is the complete wavefunction describing the state for which the quantum numbers are $n_1 = 3$ and $n_2 = 4$.

$$\boxed{\psi_{n_1 n_2} = \sqrt{\frac{2}{L}} \sin\frac{3\pi x}{L} \sqrt{\frac{2}{L}} \sin\frac{4\pi x}{L}}$$

1

b) **(2 points)** Sketch contour plots of the 2D wavefunction for an argon atom (mass 39.96 u) when it is in a state having quantum numbers for $n_1 = 3$ and $n_2 = 4$.



1.5

c) **(3 points)** Determine the most probable locations (give x and y coordinates) for an argon atom (mass 39.96 u) when it is in a state having quantum numbers for $n_1 = 3$ and $n_2 = 4$.

$$\boxed{X = \frac{L}{6}, \frac{L}{2}, \frac{5L}{6} \qquad Y = \frac{L}{8}, \frac{3L}{8}, \frac{5L}{8}, \frac{7L}{8}}$$

3

d) **(1 point)** If the box were expanded in size would you expect the energy associated with the ($n_1 = 3$, $n_2 = 4$) state to increase, decrease, or remain the same, justify your answer?

$E = \frac{n^2h^2}{\ldots}$ ... $\frac{n^2h^2}{\ldots}$ ... $f\ l = 4 = \frac{n^2h^2}{\ldots}$

[redacted]

7

BONUS: Determine the factor by which the energy associated with the ($n_1 = 3$, $n_2 = 4$) state would change if edge length in the x direction increased from L_1 to $2L_1$ and the edge length in y, increased from L_1 to $3\ L_1$.

$$En = \frac{(3^2)h^2}{8m(2L_1)^2} + \frac{(4^2)h^2}{8m(3L_1)^2} - \left(\frac{3^2 h^2}{8mL_1^2} + \frac{(4^2h^2)}{8mL_2^2}\right)$$

$$= \frac{9h^2}{32mL_1^2} + \frac{16h^2}{72mL_1^2} - \left(\frac{9h^2}{8mL_1^2} + \frac{16h^2}{8mL_2^2}\right)$$

$$\rightarrow 0.5 \quad - \quad 3.125 \qquad \frac{0.5}{3.125}$$

$$= \underline{\underline{0.1611}}$$

∴ the energy would decrease by a factor of 0.1611.

1

2. **(5 points)** A hydrogen atom is located in a box having a barrier of 1.0 eV and thickness 100 pm. Determine the probability that the hydrogen atom will escape the box if it has energy of 0.8 eV.?

$$k = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$= \frac{\sqrt{2(1.66\times10^{-27})(1-0.8)(1.602\times10^{-19}\ J)}}{\frac{6.626\times10^{-34}}{2\pi} \rightarrow 1.054\times10^{-34}}$$

$$= k = 9.91\times10^{9}$$

$$kl = 9.91\times10^{9} \cdot 100\times10^{-12}$$

$$= 0.991$$

$$\varepsilon = \frac{}{}$$

$$T = \left(1 + \frac{(e^{kL} - e^{-kL})^2}{16\varepsilon(1-\varepsilon)}\right)^{-1}$$

$$T = \underline{6.322}$$

4

∴ there is a ~~32~~ 32.2% of tunneling throug

b) **(2 points)** How does this compare to the probability predicted by classical physics?

Classical physics predicts that there is no chance that ~~that~~ ~~the~~ the hydrogen atom escapes

5.5

3. a) **(4 points)** Determine the zero point vibrational energy of an HCl molecule assuming that it is well described by a harmonic oscillator and the force constant for the H – Cl bond is 481 N m^{-1}.

$$E_V = \left(v + \tfrac{1}{2}\right)\hbar\omega \qquad \omega = \left(\frac{k_f}{m}\right)^{1/2} \quad m =$$

$$\omega = \left(\frac{481 \frac{N}{m}}{1.673\times10^{-27}}\right)^{1/2}$$

$$E_V = \frac{1}{2}\cdot\frac{6.626\times10^{-34}}{2\pi}\cdot 5.36\times10^{14} \qquad \omega = 5.36\times10^{14}$$

$$= 2.83\times10^{-20}\,J$$

∴ The zero point vibrational energy is 2.83

4

b) **(2 points)** Calculate the wavelength of a photon needed to excite a transition between the n= 5 and n=6 vibrational state for an HCl molecule described as a harmonic oscillator.

$$E = \frac{hc}{\lambda} \qquad E = (6^2 - 5^2)\cdot\tfrac{1}{2}\hbar\omega$$

$$= 11\cdot\frac{1}{2}\cdot\frac{6.626\times10^{-34}}{2\pi}\cdot 5.36\times10^{14}$$

$$\frac{hc}{\lambda} = 3.1088\times10^{-19}\,J$$

$$\lambda = \frac{6.626\times10^{-34}\cdot 2.988\times10^{8}\,m/s}{3.1088\times10^{-19}\,J}$$

$$= 6.38^{-7}\,m \qquad 638\,nm$$

1.5

638 nm

4

4. a) **(1 point)** The "particle on a sphere" is a reasonable model to describe rotational motion of a diatomic molecule such as HI in which a hydrogen atom can be thought to orbit a stationary iodine atom. What is the E_o based on this model ?

$$E_o = \frac{\hbar^2}{2I}$$

b) **(3 points)** Use the equilibrium bond distance for HI of 160 pm to determine the moment of inertia for the hydrogen atom rotating around the stationary iodine atom and estimate energy associated with the state described by l = 1.

$$E = l(l+1)\frac{\hbar^2}{2I} \qquad I = mr^2$$

$$= 1(1+1)\frac{\left(\frac{6.626\times10^{-34}}{2\pi}\right)^2}{2(4.28\times10^{-47}\,kg\,m^2)} \qquad = 1.673\times10^{-27}\,kg\cdot(160\times10^{-12}\,m)^2$$

$$= 4.28\times10^{-47}\,kg\,m^2$$

$$= \underline{\underline{2.60\times10^{-22}\,J}}$$

$\therefore$ the energy associated with $l=1$ is 2.60×10^{-22} J.

3

c) **(1 point)** What is the degeneracy of a body rotating with l = 1 ?

The degeneracy would be 3 1

$m_l = \underline{-1,0,1}$

5

5. **(3 points)** Light of wavelength 400 nm passes through 2.50 mm of a 0.717 mM solution; the transmission was measured to be 61.5 %. What is the molar absorption coefficient of the solute at this wavelength (express your answer in $cm^2\ mol^{-1}$).

$A = -\log(T) = \varepsilon c l$

$c = 0.717 \frac{mMol}{L} \cdot \frac{1 mol}{1000 mmol} \cdot \frac{100}{1}$

$\rightarrow 0.717 \frac{mol}{m^3} \cdot \frac{1 m^3}{100^3 cm^3} \rightarrow 0.$

$l = 2.5 mm \times \frac{1 cm}{10 mm} = 0.$

$\varepsilon = \frac{-\log(T)}{c\,l}$

$\varepsilon = \frac{-\log(0.615)}{7.17 \times 10^{-7} \frac{mol}{cm^3} \cdot 0.25 cm}$

$= 1.18 \times 10^{6} \frac{cm^2}{mol}$

∴ the molar absorption coefficient would be 1.18×10

or $117.78 \frac{m^2}{mol}$

3

6. **(3 points)** Calculate the ratio spontaneous to stimulated emission for a transition resulting from the interaction with visible light at 500 nm.

$\frac{NB\rho}{N(A + B\rho)} \rightarrow \frac{1}{e^{h\nu/kT} - 1}$

$A = \left(\frac{8\pi h\nu^3}{c^3}\right) B \qquad B = \frac{A}{(8}$

$\rho = \frac{8\pi h\nu^3/c^3}{e^{h\nu/kT} - 1}$

$B\rho = \frac{1}{e^{h\nu/kT} - 1}$

1/

b) **(1 point)** Will the ratio be greater for transitions associated with IR radiation ($3000\ cm^{-1}$)??

$\nu = \tilde{\nu} \cdot c \rightarrow 3000\ cm^{-1} \cdot 2.998 \times 10^{10} cm/s$

$= 8.994 \times 10^{13} Hz$

ok?. what does t

m

Bonus: What is your favourite kind of spectroscopy? Why?

IR Spectroscopy because it exhibits the

1