

Exam 3/Final Exam, (5/9/20, Sturgeon)
Chem 322: Quantum Mechanics (100 pts total)
Material Covered: Chapter 9, 10, and 15.

Name _____

Exam instructions: You may use your textbook, lab notebook, class notes, and/or any other prepared documents for this exam. All parts of this exam are due on Monday, May 11th at 9 pm. Please feel free to email questions regarding the exam.

I agree to follow the guidelines listed above and state that I have neither given nor received any unauthorized aid on this exam.

_____ (signature)

1) ***Wavefunction questions for the hydrogen atom...***

a) (5 pts) Write below the 3s radial wavefunction for the H atom (***no partial credit***).

b) (5 pts) Write below the square of the 3s radial wavefunction for the H atom; ***simplify your answer algebraically and numerically...you can leave constant (a_0) in the wavefunction...leave $(a + b + \dots)^2$ as is.***

c) (5 pts) As discussed in section 9.5, the square of the radial wavefunction is of limited value since the locational probability is also dependent on the available area. For this reason we define the “radial distribution function” $P(r)$. Write below the radial distribution function for the 3s orbital for the H atom, it is okay to ***use your answer in part b as a starting point.***

2) Hamiltonian questions for the hydrogen atom...

The understanding of quantum mechanics as applied to chemistry comes from the application to the simplest of element, the hydrogen atom. Like all introductory model systems (particle in a box, harmonic oscillator, particle on a ring, particle on a sphere) the Hamiltonian involves two parts, the kinetic energy part and potential energy part. For the hydrogen atom, the potential energy part comes from the electrostatic attraction due to the coulombic potential. The coulombic potential is given in eq 9.1 in your text.

a) (2 pt) Write out the coulombic potential term eq. 9.1. (**no partial credit**)

b) (4 pts) Numerically simplify this coulombic potential by inputting the known constants, show all units (**no partial credit**).

c) (1 pt) Unique to the hydrogen atom Schrodinger equation, this equation is partially solved leading to an “effective potential” (V_{eff}) show in eq. 9.6. Write this equation below:

d) (6 pts) Figure 9.1 shows the V_{eff} along with the $V_{centripetal}$ and $V_{coulombic}$ for an electron in the $l=1$ (p-orbital). Based on this plot, what is the approximate values for each term (*read from the axis*) at $r = 1 \text{e-}10 \text{ m}$?

$$- V_{eff} (l=1) = \underline{\hspace{2cm}} \quad - V_{centripetal} (l=1) = \underline{\hspace{2cm}} \quad - V_{coulombic} (estimate) (l=1) = \underline{\hspace{2cm}}$$

e) (9 pts) Based on the equation in answer “c”, calculate the exact values (3 decimal places) for the following:
(**show your work**)

$$V_{centripetal} (l=1) = \underline{\hspace{2cm}}$$

$$V_{coulombic} (estimate) (l=1) = \underline{\hspace{2cm}}$$

$$V_{eff} (l=1) = \underline{\hspace{2cm}}$$

f) (12 pts) Redo the calculations for ($l=2$) and ($l=3$) and then complete the table below:

	$l = 1$	$l = 2$	$l = 3$
$V_{centripital}$			
$V_{coulombic}$			
$V_{effective}$			

Energy questions for the hydrogen atom...

(1 pts) The energy for the hydrogen atom energy levels (orbitals) is given in eq. 9.7; write this equation here.

(4 pts) Eq. 9.8 shows a simplified version of the eq. 9.7 energy level expression. Confirm that this simplified expression is correct by entering the numerical values for all constants (with units) into eq. 9.7, making sure to include all units (ie. dimensional analysis):

(4 pts) It was noted in class that experimentally we **cannot** determine the energy (E_n) of a particular energy level (orbital) but instead the ΔE between two energy levels (orbitals). Use the simplified version of the energy (eq. 9.8 with units of J) to generate an expression for the ΔE between **any** two hydrogen energy levels (n_1 and n_2 , where $n_1 < n_2$).

(4 pts) Use the equation above to calculate the ΔE between $n_1 = n_f = 2$ and $n_2 = n_i = 6$.
Show all work!

(3 pts) Starting with the Rydberg equation (eq. 1.13), calculate the ΔE between $n_1 = 2$ and $n_2 = 6$.
Show all work!