## Part I: Classical Derivation of the Bohr Radius

Throughout this activity, you'll be doing a lot of calculations with fundamental physical constants. I suggest using a Mathematica notebook or Excel spreadsheet to keep track of your variables and let the computer keep track of the calculations for you.

Just as planets are gravitationally attracted to their star, electrons are electrostatically attracted to their nuclei. We can *approximate* this attractive force as the cause of centripetal acceleration. One postulate of Bohr's model is that the negative electron moves around the positive nucleus, but *only* at certain radii. We'll number those radii in increasing order using $n = 1, 2, 3\ldots.$ where $n$ is the **quantum number.** Our goal is to find an expression for radius as a function of the other fundamental properties of the atom. *This will only work for the case of ONE electron orbiting a nucleus – this is known as a* hydrogen-like *atom.*

1. What is the atomic number, $Z$, of carbon? How many electrons would you have to remove from a carbon atom to make a *hydrogen-like* atom?

Recall that centripetal acceleration $a = v^2/r$ and electrostatic force $F^{elec} = \frac{kq_1q_2}{r^2}$ where $k$ is Coulomb's constant.

2. Use Newton's Second Law to write an equation describing the magnitude of net force on and magnitude of acceleration of the electron ($F = ma$, and use the acceleration and force given above). Assume the electron has charge $-e$, mass $m_e$, velocity $v_n$, radius $r_n$. The nucleus has charge $Ze$ (where $Z$ is the number of protons).

(← Call this Eqn A)

The second postulate of Bohr's model is the *first quantization condition*. Recall that Planck found, with blackbody radiation, that energy in any oscillating system is quantized. Bohr's quantization condition is instead expressed in terms of *angular momentum* $L_n$ and states:

$$L_n = \frac{nh}{2\pi} \text{ for } n = 1, 2, 3\ldots \qquad \text{Eqn 1}$$

where $h$ is Planck's constant.

3. If angular momentum is quantized, do you expect energy of the electron to be quantized? Why or why not?

4. Recalling the definition of angular momentum for a point particle (look it up if you have forgotten), substitute this definition in for the left-hand side of Equation 1.

5. Solve your equation for the velocity of the electron.

(← Call this Eqn B)

6. Substitute in the velocity of the electron in for your expression from Newton's 2nd Law (Equation A above). Solve for radius as a function of all other variables, now that we have eliminated velocity.

7. In your equation above, which variables are fundamental physical constants? Which ones depend on the atom and the state of the electron? Rewrite your equation so it looks like $r_n = \left(constants\right) \times \left(others\right) = a_0 \frac{n^2}{Z}$.

8. Using accepted values of the fundamental constants, calculate $a_0$. Don't forget units!

Note that your book uses somewhat different physical constants. They use $\hbar = \frac{h}{2\pi}$, called the "Reduced Planck's Constant" (pronounced "h-bar"). Instead of Coulomb's constant *k* they use $k = \frac{1}{4\pi\varepsilon_0}$, which is the more common way to write the electrostatic force in electrodynamics. You should still find the same result. Additionally, the book focuses on the derivation for the hydrogen atom only. We've found the general result for any *hydrogen-like* atom, that is, one electron orbiting a nucleus of any size and charge.

9. Is there a smallest possible radius for an electron orbiting a hydrogen nucleus? If so, what is it?

10. Is there a largest possible radius for an electron orbiting a hydrogen nucleus? If so, what is it?

**Part II: Energy Levels in the Bohr Atom**

11. As the radius increases, does the velocity of the electron increase, decrease, or stay the same? How about the kinetic energy? Explain how you concluded this.

In order to discuss potential energy, remember that we must define the point at which the potential energy of a system is considered to be zero. By convention, we define the potential energy of the electron-atom system to be zero when the two particles are infinitely far apart.

12. As the radius increases, does the potential energy of the electron-nucleus system increase, decrease, or stay the same? Is it negative, positive, or zero? *Hint: think about the work it would take to bring the particles closer together or farther apart.*

13. The total energy of the electron is a sum of the kinetic and potential energies. We can continue to use classical physics for this part. Write an expression for the kinetic energy of the electron in terms of $r_n$. You'll use previous results from this handout.

14. Write an expression for the potential energy in terms of $r_n$. Reminder: for two point sources, $U = \frac{kq_1q_2}{r}$. Double check: is it positive or negative? Does this match your previous answer to Question 12?

Next, we'll add your two expressions together to find an expression for the total energy as a function of $r_n$.

$$E = K + U \qquad \text{Eqn 2}$$

$$E_n = \frac{1}{2} m_e v_n^2 - \frac{kZe^2}{r_n} \qquad \text{Eqn 3}$$

How can we simplify this expression and get the kinetic and potential energy terms written as functions of the same variables (e.g. just $r_n$ or just $v_n$, since the two are related)? Using your expression for $v_n$ from Equation B is one possibility, but then you'll need to do a ton of simplifying. It will be easier to instead solve Equation A for $v_n^2$, and substitute that into the kinetic energy term, because I can see that Equation A uses many of the same variables as my potential energy term.

15. Solve Equation A for $v_n^2$, then substitute it into Equation 3. Simplify to show that $E_n = -\frac{1}{2}\frac{kZe^2}{r_n}$.

16. Substitute in your expression for $r_n = a_0 \frac{n^2}{Z}$.

17. Substitute in numbers for all physical constants to find an expression for $E_n$ as a function of a constant $E_0$ in eV (to three significant figures), $n$, and $Z$. This expression will work as long as $Z$ is not too large.

**Part III: Creating the Energy Level Diagram for Hydrogen**

We will now focus exclusively on the hydrogen atom, for which $Z = 1$. Let's create an energy level diagram of the hydrogen atom using the provided graph paper. This is a one-dimensional graph, where the vertical axis represents the potential energy of the electron. A horizontal line on the diagram will represent the energy level, $E_n$, of a state of quantum number $n$. First, we must choose an appropriate scale.

1. What is the lowest energy level possible? What is the quantum number of this state? This is called the **ground state energy of the hydrogen atom.**

2. What is the highest energy level possible? What is the quantum number of this state?

3. Now that you have your minimum and maximum values, choose an appropriate scale to fit on the page. 1 grid square = ________ eV.

4. Draw a horizontal line that corresponds to the energy of the ground state, and label this $n = 1$.

5. Calculate the energy level of the $n = 2$ state, and draw and label this as a horizontal line. Repeat this procedure for $n = 3, 4, 5$, and 6.

6. As you move to higher quantum numbers, how does the spacing of the energy levels change?

**Part IV: State Transitions, PhET Simulation**

You've observed emission line spectra in a general chemistry class. What is happening on the atomic level? We'll use the PhET simulation titled "Neon Lights & Other Discharge Lamps" to find out (https://phet.colorado.edu/en/simulation/legacy/discharge-lamps).

1. After you open the simulation, the diagram on the right should look familiar. What is it?

2. What happens when you click "Fire Electron?" Why?

3. What happens when you use the slider to change the voltage of the battery? Why? Be sure that you test what happens when you reverse the battery as well.

4. Return the voltage of the battery to its default value of 23.00 V. Click the "Spectrometer" option. A spectrometer appears. Now change "Electron Production" to continuous. What happens?

5. We know that there are 4 hydrogen emission lines in the visible spectrum, but so far our spectrometer has yet to detect any! What is the special name given to those 4 lines? Why are they given that name?

6. Figure out what TWO things you can change in the simulation to produce those four lines. You may need to be patient and watch the simulation for a minute to confirm that your change worked. Describe each change and WHY it now produces the four visible emission lines.

7. The atom we are studying in the discharge tube has a number on it that keeps changing. What does that number represent?

8. Now click on the top tab that says “Multiple Atoms” and allow the simulation to run with continuous electron production. Turn on your Spectrometer as well. The diagram on the right looks slightly different. What does it represent?

9. What color would you see with your eyes if you looked at this discharge tube in real life?

10. Check your prediction by clicking “View Picture of Actual Discharge Lamps” on the bottom of the screen. Were you correct?

11. Turn the voltage of the battery down to 6.00 V. What would you see with your eyes if you looked at this discharge tube in real life?

**Part V: State Transitions, Mathematical**

Due to conservation of energy, if the electron changes state, it must be accompanied by either the absorption of energy (from an incoming photon of light, or a collision with another particle) or emission of energy (via a photon of light). Remember $h = 4.14 \times 10^{-15} \mathrm{eV} \cdot \mathrm{s}$.

1. Imagine that the electron moves from state $n_i = 2$ to state $n_f = 5$. On your energy diagram, draw an arrow starting at $n = 2$ and ending at $n = 5$ to represent this transition. Is energy absorbed or released for the electron transition – how much? What is the wavelength of the photon absorbed or released?

2. Imagine that the electron moves from state $n_i = 3$ to state $n_f = 1$. Repeat the above questions for this new transition. What is the special name assigned to a transition like this?

3. Write a general equation for the change in energy of a state transition, $\Delta E = E_{final} - E_{initial}$.

4. Use that equation to write a general equation for the $1/\lambda$, where $\lambda$ is the wavelength of light produced by emission lines of hydrogen in meters. Does this match a famous equation? For whom was it named?

5. Imagine an electron bound to a hydrogen nucleus is in the ground state.
   a. What will happen if the electron is struck by a photon with energy of 5.00 eV?

   b. What will happen if the electron is struck by a photon with energy of 12.09 eV?

   c. What will happen if the electron is struck by a photon with energy of 14.0 eV?