Guided Practice Activities

**Module:** Atomic Theory

**Section:** The Hydrogen Atom - Key
Line Emission Spectra and Electrons

Activity 1

The purpose of this activity is to use light (electromagnetic radiation) as a tool to understand the substructure of atoms.

1. Early experiments revealed that when energy was added to different elements different characteristic colors were emitted. Describe the difference between a continuous spectrum, an emission spectrum and an absorption spectrum.

   A continuous spectrum shows all the visible colors. An emission spectrum shows only particular bands of visible light. A corresponding absorption spectrum looks like the continuous spectrum with those particular bands missing.

2. Light is emitted from a hot gas. The following is an example of the emission spectra of hydrogen gas.

   ![Hydrogen Emission Spectra](http://astro.u-strasbg.fr/~koppen/discharge)

   The following is an example of the emission spectra of sodium gas.

   ![Sodium Emission Spectra]

   Observe the two spectra. State the similarities and differences between the two spectra. Speculate to the source of the emission lines.

   Both spectra only show a few lines of visible light. However, the colors that they each express are different. Hydrogen gas seems to have some dim bands in the violet region, a bright band in the blue-green region and a bright red band. Sodium however, has a dim band in the blue-green and yellow-green regions but one very bright band in the yellow region.

   The differences in the emission spectra are a result of differences in their electron configurations. The excited electrons in each of these atoms jump across energy levels, but because sodium and hydrogen have different electron configurations the electrons exhibit distinct energy patterns.
1. Please sketch and explain Bohr’s model of the atom based on the observation of the line emission spectra of elements.

Bohr recognized that the line spectra for elements had sharp, distinct lines of emission and absorption. Furthermore, the emission lines aligned with the absorption lines for the same element. His “shell model” of an atom explains how absorbed or emitted light occurs between set energy levels of electron density. Rather than having electrons and protons mixed together in a random pattern, Bohr’s model showed quantized concentric shells of electron orbits.

2. Please explain Rydberg’s interpretation of the line emission spectra, and write down the Rydberg equation that was derived from his empirical interpretation of the line emission spectra data.

Rydberg cleverly analyzed the line spectra with mathematics. He derived a relationship between distinct energy levels and the energy of light either absorbed or emitted. This was a critical analysis because the relationship he found only worked when the energy levels were integers! When he included distinct, quantized energy levels into his formula, it modeled the observed line spectra beautifully.

There are two forms of the Rydberg equation:
Ryderberg plotted, \( \lambda \), “wavenumber” (the number of waves that can fit a “unit length” of 1) versus the difference of squared integer values (n). The equation relates the amount of energy absorbed or released (\( \Delta E \)) when an electron moves from one energy level (\( n_i \)) to a different one (\( n_f \)). The slope of both linear relationships is \( R \), the Rydberg constant.

\[
\frac{1}{\lambda} = R \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)
\]

\[
\Delta E = R \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)
\]

Activity 3

1. The Rydberg constant can be expressed in energy units (J), Hz (1/s) or wavenumber (1/m). Look up and write down the values for each form of the Rydberg constant. You will not have to memorize these values for an exam in this course, but it is important to be able to recognize which constant to use based on the question asked.

   Values of \( R \):
   - \( 2.178 \times 10^{-18} \) J
   - \( 1.097 \times 10^{-7} \) m\(^{-1}\)
   - \( 3.290 \times 10^{15} \) s\(^{-1}\)

2. Use the Rydberg equation to answer the question: What is the wavelength of light emitted when an electron in a hydrogen atom moves from the \( n = 2 \) level to the \( n = 1 \) level?

   Because we are looking for wavelength, we could use the Rydberg formula that solves for “wavenumber” (the reciprocal of wavelength). We could also solve for the energy emitted and convert energy to wavelength.
A wavelength should be a positive number, because there are no negative lengths!

3. Use the Rydberg equation to answer the following: For the hydrogen atom, an electron moving between which two energy levels in the Balmer series would have to absorb light with a frequency of $4.58 \times 10^{14}$ Hz? (Hint: First determine from which energy level all Balmer series transitions originate.)

The Balmer series is the set of transitions to or from the second energy level ($n = 2$), excluding the transition from $n = 1$ to $n = 2$. Knowing this we only have to determine the final energy level that an electron would jump to if it absorbed this frequency of light.

Additionally, please carefully note that an absorption of light means that $n_f > n_i$ and therefore the difference of inverse squares between $n_f$ and $n_i$ would lead to a negative value. However, we know that absorption should correlate with a positive energy change and a positive value for wavelength (always positive).

To correct for this foreseen issue, we can either take the absolute value of the difference of inverse squares or simply place a negative sign in front of the Rydberg constant. It is always helpful to think through problems using the Rydberg formula so that you solve for the answer correctly!
\[c = v \lambda.\]
\[\lambda = \frac{c}{v}\]
\[\lambda = \frac{(3 \times 10^8 \text{ m/s})}{(4.58 \times 10^{14} \text{ s})}\]
\[\lambda = 6.55 \times 10^{-7} \text{ m}\]
\[\frac{1}{\lambda} = R \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)\]
\[\frac{1}{\lambda} R + \frac{1}{n_i^2} = \frac{1}{n_f^2}\]
\[n_f = \left( \frac{1}{\lambda} R + \frac{1}{n_i^2} \right)^{\frac{1}{2}}\]
\[n_f = \left( \frac{1}{(6.55 \times 10^{-7} \text{ m})(-1.097 \times 10^7 \text{ m}^{-1})} + \frac{1}{(2)^2} \right)^{\frac{1}{2}}\]
\[n_f = \left( -\frac{1}{6.79} + \frac{1}{4} \right)^{\frac{1}{2}}\]
\[n_f = (0.103)^{\frac{1}{2}}\]
\[n_f = 0.333\]
\[n_f = 3\]

OR:
\[\frac{1}{6.55 \times 10^{-7} \text{ m}} = (-1.097 \times 10^7 \text{ m}^{-1}) \left( \frac{1}{n_f^2} - \frac{1}{(2)^2} \right) \]
\[(1.527 \times 10^6 \text{ m}) + (-1.097 \times 10^7 \text{ m}^{-1}) = \left( \frac{1}{n_f^2} - \frac{1}{4} \right) \]
\[-0.139 = \left( \frac{1}{n_f^2} - \frac{1}{4} \right)\]
\[\frac{1}{n_f^2} = -0.139 + \frac{1}{4} = 0.111\]
\[\frac{1}{n_f} = 0.333\]
\[n_f = 3\]
Quantum Mechanical Theory of the Hydrogen Atom

Activity 1

The purpose of this activity is to understand the basics of the quantum mechanical theory of the atom.

1. Once scientists realized that matter had wave-particle duality, it became necessary to develop a new mathematical model to describe the behavior of very small objects. One of the first people to formulate a successful theory was Erwin Schrödinger. Rather than a trajectory, what did Schrödinger use to model the “path” of a small object? He used his equation to solve for particular wavefunctions in order model the path of a small object.

2. What is the simplest example of a wave function in one dimension? The particle in a box model is very helpful here. If we set up an imaginary “box” with infinitely high walls (infinity potential) and plot the location of a tiny particle, it would look like some sinusoidal function. The shape associated with the lowest possible energy is half a sine wave with the values of zero at either end (where the function meets the wall).

3. What does this function tell us about where a tiny object can be in one dimension? The particle does not spend an even amount of time at every location in one dimension. When we observe peaks of the wave function, we can conclude that it is more likely to find the particle at that location.

4. What is meant by the boundary conditions? The boundary conditions of a problem such a particle in box are known values relating to the set-up of the problem. These conditions allow us to determine the particular wave function that would fit within the given boundary conditions. If you change the starting “knowns” of the problem you might change the solution of the problem. In the case of a one dimensional box, we define the value of the potential at the walls as infinite but as zero between the walls. In this way we already know something about the value of the wave function at the walls (zero!).

5. Write the equation for the energy of a particle in a one dimensional box. State what each term in the equation represents.

\[ E = \frac{n^2 \hbar^2}{8mL^2} \]
$E$ is energy. $n$ is an integer value (corresponds with energy levels). $h$ is Planck’s constant. $m$ is the mass of the particle. $L$ is the length of the box.

**Activity 2**

1. **Why did the Bohr model break down?**
   
   Bohr’s model has fixed radii and momentum values for electrons. This violates the Heisenberg’s uncertainty principle. The uncertainties are very large for such small objects.

2. **A new physics was needed to mathematically model very small objects such as electrons, atoms and molecules. The new physics was called quantum mechanics.**

3. **One of the famous physicists who was working on the problem of modeling the electronic configuration of atoms was a man named Schrödinger. He derived a famous equation called the Schrödinger equation that was able to correctly predict the energies of the electrons of the hydrogen atom. His equation had multiple solutions predicting both the possible energies and probabilities of locations of electrons having different energies in the hydrogen atom. These solutions were called the energies and the wave functions.**

4. **The Schrödinger equation yields an infinite number of solutions for the position of an electron in a hydrogen atom. We are interested in the lowest energy solutions. The lowest energy solutions are called the ground state.**

**Activity 3**

1. **Use an energy level diagram to show the relationship between the energies calculated from quantum mechanics and the energy differences calculated by the Rydberg formula and the interpretation based on the Bohr atom.**
   
   Some energy level transitions are shown and tabulated below for hydrogen:
2. Schrödinger replaced the concept of a precise electron trajectory proposed by Bohr with notion of the wave function which when squared is a many solution probability function that describes the probability of where one might find the electron in a region in space called an orbital.

3. If this all seems rather confusing it should! At this point you don’t have the math skills (nor should you) to fully understand the quantum mechanical physical model and as such this is out of the scope of this course. What you can, however, take away is that the electrons are neither particles nor waves, but rather are quantum mechanical things that are difficult to conceive. The idea that the electrons have both particle and wavelike nature is called the wave-particle duality. Additionally, you can take away a physical understanding of the
solutions to the Schrödinger equation and that is: when we apply the wave function to electrons in 3-D space bound by the nucleus an infinite set of solutions are produced. The square of those solutions yield the allowed energies of the probabilities of finding the electrons of given allowed energies in defined regions in space. The defined regions in space are called the orbitals. The solutions to the wave equations are each labeled by an energy, a shape and an orientation.

Quantum Mechanical Solutions – Quantum Numbers for the H Atom

Activity 1

These labels of the wave equation solutions are given characteristic letters: n, ℓ and m. The values of the letters are referred to as the “quantum numbers” for a given electron.

1. The principle quantum number is abbreviated with the letter, __n__, and can range in integer value from __1__ to __∞__. It labels the energy level of the electron.

2. The angular momentum quantum number is abbreviated with the letter, __ℓ__, and can range in integer value from __0__ to __n−1__. It labels the angular momentum of the electron. This quantum number is also labeled by the letters s, p, d, and f, which correspond to the shapes spheres, “dumbbells”, “clover leaves”, and too complex to describe.

3. The magnetic quantum number is abbreviated with the letter, __m ℓ__, and can range in integer value from __−ℓ__ to __ℓ__. It labels the orientation of the shape, and as such is dependent on the value of the angular momentum quantum number.

Quantum Mechanical Solutions - Orbitals

Activity 1

1. Define the radial function and what it tells us about the location of the electron.

The radial function is the relationship between probability of the presence of an electron and distance from the nucleus of the atom. As we can observe on the example below, it is highly improbable to find the electron extremely close to the nucleus. It is probable to find
the electron closer to the nucleus when the electron is in lower energy levels than when it is in higher energy levels.

2. Draw the shapes and state the associated letter designation associated with the quantum number, \( \ell \).

\[ \ell = 0 \rightarrow s \text{ orbital} \]

\[ \ell = 1 \rightarrow p \text{ orbitals} \]

\[ \ell = 2 \rightarrow d \text{ orbitals} \]

To explore the shapes of the more complicated orbitals look at this website:
http://winter.group.shef.ac.uk/orbitron/
Activity 2

1. Fill in the following orbital notation diagrams for the ground state of hydrogen and an excited state of hydrogen.

Notice: In the ground state the one electron of a hydrogen atom is in the lowest energy orbital. In an excited state, that one electron is in a higher energy orbital (in this example, the electron is in one of the 2p orbitals).

2. Write out the ground state electron configuration using orbital notation.
   
   For hydrogen the ground state electron configuration is: 1s

3. Write the associated quantum numbers describing the ground state electron in hydrogen.
   
   \((1, 0, 0)\)
   
   \(n = 1\) (first energy level)
   
   \(\ell = 0\) (in the s orbital)
   
   \(m_\ell = 0\) (\(m_\ell\) can range from \(-\ell\) to \(+\ell\), but in this case there is only one possible answer)

Activity 3

1. What are all the possible allowed quantum numbers for a hydrogen electron in a 3d orbital?
   
   \(n = 3\) (second energy level)
   
   \(\ell = 2\) (in the d orbital)
   
   \(m_\ell = -2, -1, 0, 1, 2\) (\(m_\ell\) can range from \(-\ell\) to \(+\ell\), so there are five possibilities)
   
   There are five unique sets of quantum numbers available to describe a hydrogen electron found in a 2d orbital:
   
   \((3, 2, -2)\); \((3, 2, -1)\); \((3, 2, 0)\); \((3, 2, 1)\); \((3, 2, 2)\)
2. Given the following quantum numbers \((5, 3, -2)\) in what orbital will that electron be found?

When \(\ell\) is 3, then the orbital type is \(f\). We can look at the principle quantum number to tell us that this electron would be in one of the seven available \(5f\) orbitals.

3. The “location” of an electron in a hydrogen atom is described by a wave function known as an atomic orbital.

Each orbital is designated by a set of three quantum numbers and falls into a shell and subshell.

\(n\) is the principle quantum number or “shell”, \(\ell\) is the orbital type or “subshell.”

On the H atom energy level orbital diagram to the right, label the quantum number \((n, \ell \text{ or } m\ell)\) associated with each symbol on the diagram.