

Atoms and electrons: Atomic Structure: Student Review Notes

Understand that this presentation of atomic structure presented is very brief. As will be the case with all of the student notes, the focus is on hitting the most important points not on an all encompassing explanation.

Atomic Structure:

There are basically two parts to this picture that you have to understand.

1. The nucleus which is comprised of positively charge protons and neutral neutrons.
2. The electrons which are negatively charged and surround the nucleus.

You need to know some history:

The Nucleus

In terms of the nucleus, **Rutherford's gold foil experiment identified the characteristic that atoms have hard positive centers** and are mostly made of empty space. In this experiment, a piece of gold foil was bombarded with alpha-particles (helium nuclei) and a detector was moved around behind the foil to register the angles at which the alpha particles were deflected. Most of the alpha particles went straight through the gold foil—that's the part of the experiment that indicated atoms are made of mostly empty space. As the story goes, by accident, the detector was positioned behind the alpha particle emitter and it was observed that some alpha particles were bounced straight back from the foil. Since alpha particles have a +2 positive charge (2 protons and 2 neutrons) this observation indicated that there was a small hard positive center or nucleus of individual atoms.

Electrons

Electrons and energy in the form of radiation is the other part of the story. Rutherford's experiment broke a contemporary belief that the atom was something like a positively charge pudding that contained negative plums (plum pudding model). The positive pudding was "out" and a hard positive center was "in" but that still left the issue of electrons unresolved.

For most of the nineteenth century, light or electromagnetic radiation was thought to be a wave. This was thought to be the case because when you shine light through two slits, you observe an interference pattern just like if you sent a wave of water at the slits. This diffraction pattern experiment was used to substantiate that light was a wave. Like all waves, in this model, light is assigned a wavelength and frequency.

Around the turn of the century, there were a couple of experimental observations that led to the idea of quantized energy levels for electrons in atoms and that light had particle as well as wave properties.

Atomic Emission Spectra

- 1 When certain gases such as hydrogen were subjected to an electric field, they emitted a discrete pattern of light or **atomic emission spectrum**. This pattern was indicative of the element and what's really important is this idea that it's discrete and reproducible for a particular element. For example in hydrogen, lines with wavelengths of 656 nm (red), 486 nm (blue), 434 nm (indigo) and 410 nm (violet) are visible. The paradox was that this discrete emission was very different from what was observed when you simply heat up a metal. The heated metal emits light at all visible wavelength. The question was, why do these gases only emit light at characteristic discrete wavelengths? You'll need to understand how **Bohr builds on this experimental observation for his model of the hydrogen atom**. And just to reinforce this, **atomic emission spectra indicate a discrete or quantized behavior of the electrons that emit radiation from an element**.

Photoelectric Effect

- 2 The other experiment was the **photoelectric effect**. In this experiment it was observed that shining light on a metal caused the emission of electrons from the metal surface. The paradox here was that below a certain threshold frequency, no electrons were emitted regardless of the intensity of the light. Think of a beach ball floating near a beach. If it's hit by a single wave it moves closer to the beach. If we increase the intensity of the waves (i.e. the number of waves that hit the ball) each wave will move the ball closer to shore until it ends up on the sand. This is wave behavior. In the photoelectric effect, no matter how intense the beam of light if you didn't reach a certain wavelength, the electrons weren't emitted. From the analogy, light was not behaving like a wave because no matter how many little waves hit the beach ball, it would never make it to the shore--the advance of one wave can not be built upon by a successive wave. You'll need to understand how **Einstein used this observation to propose the idea of particles of light**.

Atoms and electrons: Atomic Structure: Student Review Notes

Before moving on to Einstein and Bohr, some credit needs to go to **Max Planck** who, although he did not explain the photoelectric effect or propose a model for the hydrogen atom, did set the stage by proposing a **quantum theory** (again, understand that quantized means discrete).

Postulates of Planck's Quantum Theory

1. **Energy states of an atom/molecule are "quantized."** When transitions occur between energy states, the atom/molecule absorbs or emits energy just sufficient to bring it to another state.

"**ground state**" is the lowest energy state

"**excited state**" is any higher energy state

2. For atoms/molecules absorbing or emitting energy (light), the **change in energy** can be calculated in the following way:

$$\Delta E = E_{\text{final state}} - E_{\text{initial state}} = h\nu = hc/\lambda$$

h = Planck's Constant = 6.626×10^{-34} Js
 c = the speed of light = 2.998×10^8 m/s
 ν = frequency of light
 λ = wavelength of light

3. **Quantum numbers** can be used to describe the allowable energy states of electrons within an atom/molecule.

Planck proposed 4 quantum numbers:

The principle quantum number, n

The angular momentum quantum number, l

The magnetic quantum number, m_l

The electron spin quantum number, m_s

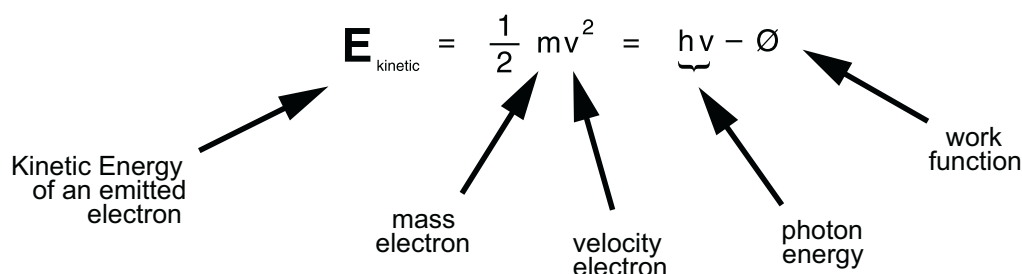
Photoelectric effect

Planck proposed his quantum theory in 1900 and Einstein used it 5 years later in his explanation of the photoelectric effect. The photoelectric effect could not be explained in terms of a wave theory of light. Einstein proposed that light was a **packet of energy or photon** with energy given by Planck's equation for the difference of energy states in an atom/molecule.

$$E = \text{energy of a photon} = h\nu = hc/\lambda$$

$$h = \text{Planck's Constant} = 6.626 \times 10^{-34} \text{ Js}$$

This idea of light as an energy packet is consistent with the observations of the photoelectric effect. If an electron absorbs a photon that doesn't have enough energy to emit it from the metal, the electron just falls back down. The threshold frequency observed in the photoelectric effect marked the energy of a photon that could pop an electron all the way out of the metal. Each metal has a different energy that must be overcome and this property is called the **work function of the metal**. Know how to solve little photoelectric effect problems



Bohr Model for the hydrogen atom

Bohr developed a simple planetary model to describe the hydrogen atom—a **1 electron system**. Bohr put together the following postulates for his model:

- (I) The electron can exist only in discrete states each with a definite energy.
- (II) The electron can exist only in certain circular orbits.
- (III) The angular momentum of the electron is $nh/2\pi$ where n is any positive integer.
- (IV) Radiation is emitted by the atom only when an electron makes a transition from a state of higher energy to one of lower energy.

* Of these, for many electron systems, it was found that (II) was incorrect and (III) was partially correct (the angular momentum is fixed but not in the way Bohr described). For the a 1 electron system though, Bohrs model fits very well.

Bohr defined zero energy when the proton and electron are completely separated ($E = 0$ when $n = \text{infinity}$).

The energy of all other states (values of n) is given by the equation below:

$$n = 1,2,3,\dots \quad E_n = \frac{-2.179 \times 10^{-18} \text{J/particle}}{n^2} \quad \text{or} \quad E_n = \frac{-1312 \text{ kJ/mol}}{n^2}$$

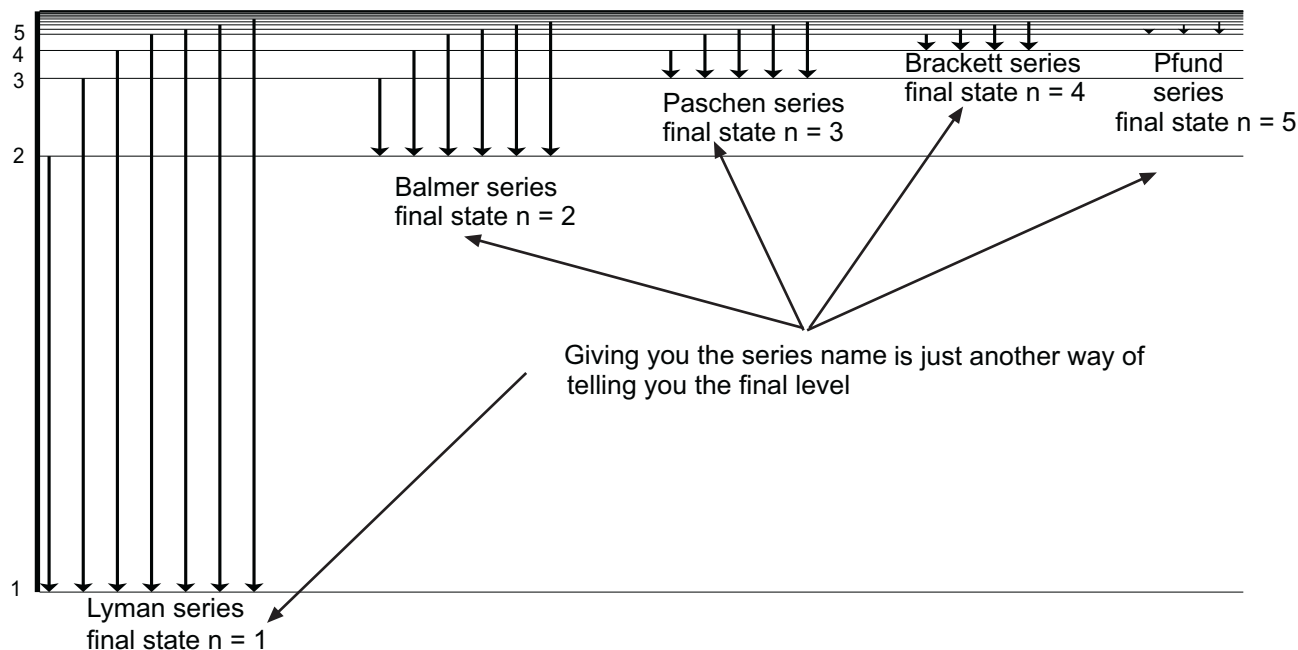
The energy associated with the transition of an electron from one allowable state to another is given by:

$$\Delta E = E_2 - E_1 \quad \Delta E = \underbrace{hv = \frac{hc}{\lambda}}_{\text{energy of emitted/absorbed photon}} = R_h \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$R_h = \text{Rydberg constant} = 2.179 \times 10^{-18} \text{ J}$
 $n_2 = \text{the final state}$
 $n_1 = \text{the initial state}$

For Hydrogen, know that names of each of the emission series:

$n = \text{infinity} = \text{energy of free electron}$. The ionization energy of hydrogen is



Moving on from the Bohr Model to a Little Quantum Mechanics

Bohr and Einstein developed models that showed quantized energy levels for electrons on atoms and the quantum or particle nature of light, respectively. We'll round out the evolution of quantum mechanics with the work of de Broglie, Heisenberg and Schrodinger.

De Broglie: Wave-Particle Duality of Matter

Einstein used the photoelectric effect to theorize the wave-particle duality of light. In a similar way, de Broglie postulated that matter, which we know has particle properties, also must exhibit wave behavior. De Broglie formalized this in an equation by setting energy according to Einstein's $e = mc^2$ equation equal energy according to Planck's $e = hc/\lambda$ equation. He then used particle velocity instead of the speed of light to end up with an equation for the wavelength of a particle. It was then experimentally shown that the wavelength associated with a particle as small as an electron could be measured.

$$\lambda = h/mv$$

Heisenberg's Uncertainty Principle

Heisenberg basically said that there is a limit to which the position and momentum (mass times velocity) of a particle may be simultaneously determined. The equation is this for the x-dimension (in 3D you also have y and z dimensions):

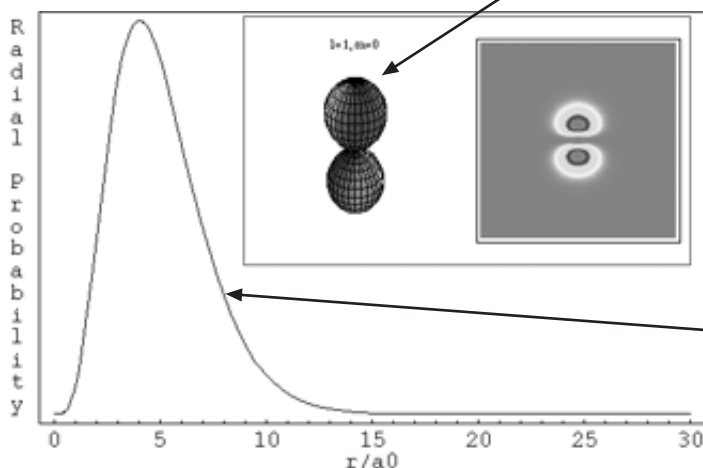
$$\Delta x \Delta mv \geq h/4\pi$$

What this equation says is that the error (delta) in measuring the location times the error (delta) in measuring the momentum has to be greater than or equal to Planck's constant divided by 4π . A crude explanation of this is that any attempt to locate (determine the position) something as small as an electron will disturb momentum of the electron. Think about how we typically locate things—with some form of electromagnetic radiation (light). Light is composed of photons. So you send a photon in to determine the position of an electron and during the collision, energy is exchanged and the momentum is changed.

The Schrodinger Equation

You don't need to know anything about using the Schrodinger equation. It's a big partial differential equation and that is beyond general chemistry. What you do need to understand however is what the solutions to this equation represent. Basically, the solutions to Schrodinger's equation show the probability distribution for finding an electron that is associated with a certain energy level, sublevel and orbital (Planck's quantum numbers n , l and m_l). This is where atomic orbital shapes come from. In three dimensions, these shapes represent a distribution in space of the most probable area in which to find an electron with certain energy level, sublevel and orbital. Take a look, here is the solution to the Schrodinger equation for an electron on the second energy level and the p-sublevel (quantum numbers $n = 2$, $l = 1$, $m_l = 0$)

The dumbbell shape is the shape of a p-orbital



The radial distribution is normalized as a number of Bohr radii. It's just a look at the distance from the nucleus and how the probability density for finding an electron changes.