Chemistry

Electrons in Atoms
Lesson 12
Lesson Plan
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Models of the Atom

Objectives: Summarize the development of atomic theory; Explain the significance of quantized energies of electrons as they relate to the quantum mechanical model of the atom.

- The Evolution of Atomic Models
    - So far we have described the atom as a nucleus of protons and neutrons surrounded by electrons – this works well for a simple explanation, but does not explain certain properties of elements, such as why metals give off a characteristic color when heated in a flame – or why lasers give off a particular wavelength(s).
    - Remember Dalton? He gave us is atomic theory:
        - All elements are composed of tiny indivisible particles called atoms
        - Atoms of the same element are identical. The atoms of one element are different from atoms of a different element
        - Atoms of different elements can physically mix together, or chemically combine in simple whole-number ratios to form compounds
        - Chemical reactions occur when atoms are separated, joined or rearranged. Atoms of one element are never changed into atoms of another element as a result of a chemical reaction
        - This worked well for about 50 years after Dalton
    - JJ Thompson (who discovered the electron) realized that Dalton's model did not take into account electrons – so he proposed a revised model often called the plum-pudding model
        - This had a central positively charged mass onto which electrons were just stuck to the outside.
        - It did not describe the number of protons and electrons or how they were arranged
    - After discovering the nucleus, Ernest Rutherford proposed the nuclear atom, in which electrons surrounded a dense nucleus – leaving lots of empty space
        - Later experiments showed a nucleus of + charged protons and neutrally charged neutrons, surrounded by – charged electrons.
        - So why did not the – charged electrons fall into the + charged protons of the nucleus?
    - In the early 1900's, Niels Bohr, who was a student of Rutherford, came up with a new atomic theory
        - Bohr proposed that electrons were in circular orbits around the nucleus, much like planets orbit the sun (thus it was called the planetary model)

- As to why the electrons did not fall into the nucleus, Bohr suggested that electrons in a particular orbit have a fixed energy, and that electrons do not lose energy and cannot fall into the nucleus.
- The **energy level** of an electron is the region around the nucleus where the electron is likely to be moving.
- These energy levels are like the rungs on a ladder – just like you can not stand between rungs on a ladder, electrons cannot be between energy levels.
- A **quantum** of energy is the amount of energy needed to move an electron from its present energy level to the next high level.
    - Electrons that have been moved to a higher level are said to be quantized.
    - The term quantum leap comes from describing this sudden change from one level to the next.
    - The higher the energy level, the farther the electron typically is from the nucleus.
    - The energy levels are not the same distance apart – the farther from the nucleus an energy level is the less energy is required to move it to a higher level

- The Quantum Mechanical Model
    - Finally in 1926 Erwin Schrödinger took the atom to its current shape
    - The modern description of the electrons in an atom is called the **quantum mechanical model** and is based on the mathematical equations from Schrödinger.
    - His mathematical equations described the location and energy of an electron in a hydrogen atom.
    - As Bohr, the quantum mechanical model restricts the energy of electrons to certain values – unlike Bohr it does not describe an exact path that the electron follows, rather it estimates the probability of finding an electron in a certain position.
        - The probability of finding an electron within a certain volume of space surrounding the nucleus is represented as fuzzy cloud, which represents where an electron would be found 90% of the time.
- Atomic Orbitals
    - Both Bohr and the quantum mechanical model designates energy levels of electrons by means of a principle quantum number (n)
        - Each principle quantum number refers to a major, or principle, energy level in an atom.
        - They are assigned in order of increasing energy levels – n = 1,2,3,4,5,. . .
        - The average distance from the nucleus increases with each increasing value of n.
    - Within each principle energy level there are sublevels
        - The number of sublevels is the same as the value of n
    - Where are the electrons located?

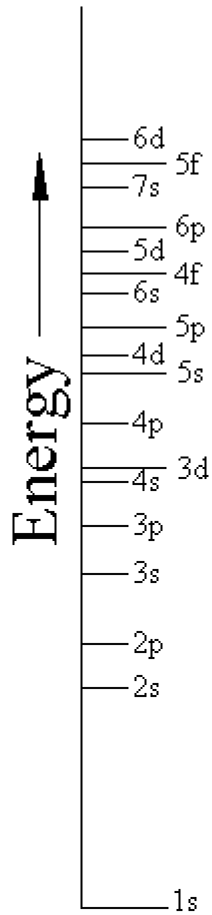
- In the Bohr model we had orbits, but since the quantum mechanical model does not have orbits, but rather regions of probability, the regions are called **atomic orbitals**.
    - Letter designate the atomic orbitals
        - s orbitals are spherical
        - p orbitals are shaped like dumbbells
            - There are 3 kinds of p orbitals, which have different orientations in space (x, y &z)
        - d orbitals are more like two sets of dumbbells at right angles to each other
        - f orbitals are too complex to visualize
- The p and d orbitals taper as they approach the nucleus, indicating areas where electrons have a low probability of existing. Where these regions meet are called **nodes.**
- As noted, principle energy levels have sublevels – the same number of sublevels as the principle energy level number n
    - For n =1, there is one sublevel called 1s.
        - In the s atomic orbital, there is an equal probability of finding an electron in any direction from the nucleus
    - For n =2, there are two sublevels, 2s and 2p
        - The 2s orbital is spherical
        - The 2p orbital is dumbbell shape
            - The 2p orbital is of higher energy level than the 2s orbital
            - The 2p orbital consists of three p orbitals, each aligned on the x, y & z axis
                - These are often referred to as the 2x,
                - 2y, and 2z
        - Thus the second energy level has four orbitals 2s, 2z, 2y, 2z
    - For n=3, there are 3 sublevels, 3s, 3p and 3d
        - As before, there is one 3s orbital and three 3p orbitals – but 3d has 5 orbitals, for a total of 9 orbitals
    - For n=4, there are 4 sublevels, 4s, 4p, 4d and 4f
        - The 4th principle energy level has 16 orbitals
            - One 4s, three4 p, five 4d and seven 4f orbitals
- The maximum number of electrons in a principle energy level is given by $2n^2$, where n is the principle quantum number

	Increasing Energy			
Energy Level n	1	2	3	4
Max # electrons	2	8	18	32

Electron Arrangements in Atoms

Objectives: Apply the aufbau principle, Pauli exclusion principle and Hund's rule in writing the electron configurations of elements; Explain why the configurations for some elements differ from those assigned using the aufbau principle.

- Electron Configurations
    - In all natural phenomena, change proceeds toward the lowest possible energy. High-energy systems are unstable and tend to loose energy to become stable. The same holds true for electrons surrounding a nucleus in an atom.
    - The way that electrons are placed around a nucleus of an atom is called **electron configuration**.
    - There are 3 rules we must follow for correct electron configuration
        - Aufbau principle – electrons enter orbitals of lowest energy first
            - The lowest energy orbital is the 1s, followed by 2s and 2p
            - Starting with the n=3 you may start to get overlap of the levels that you must be aware of:



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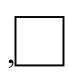
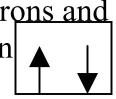
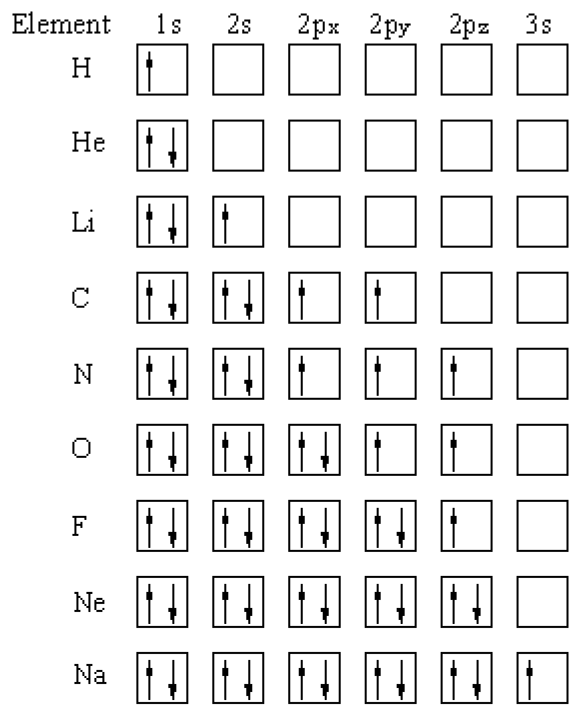
- In an Aufbau diagram, each orbital is represented by a box ,  in which an arrow is placed for each electron in that orbital.
    - Each box can contain 2 electrons and is indicated by an arrow pointing up or down 

    - Pauli exclusion principle – An atomic orbital may describe at most two electrons
        - For example, either one or two electrons can occupy a s orbital – if one then it is designated with a single up arrow. If two then use an up arrow and a down arrow, indicating opposite spin.
            - Electrons spin either clockwise or counterclockwise and must be paired as such.
    - Hund's Rule – when electrons occupy orbitals of equal energy, one electron enters each orbital (starting with s) until all the orbitals contain one electron, then a second electron is added to each orbital
        - For example, for oxygen, which has 8 electrons, we first fill the 1s orbital with 2 electrons, then the 2s with 2 electrons, and then each of the 2p orbitals with 1 electron each, and finally we start back over with the 2p orbitals adding a second electron to the $2p_x$ orbital.

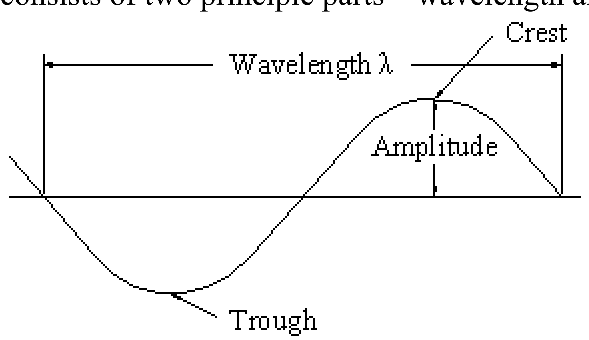


- There is a convenient shorthand method of writing the electron configuration of an atom. It involves writing the energy level and the symbol for each sublevel occupied by an electron. A superscript indicates the number of electrons occupying that sublevel.
    - For hydrogen with one electron in the 1s orbital it would be $1s^1$
    - For helium, it would be $1s^2$
    - For sodium, it would be $1s^2 2s^2 2p^6 3s^1$
    - The sum of the superscripts equals the number of electrons in the atom

- Always the exception!
  - If you were to follow the aufbau diagram for orbital filling, it would work correctly until you got to vanadium (atomic number 23) – then you hit exceptions
  - For chromium you would expect the configuration to be $1s^22s^22p^63s^23p^63d^44s^2$. Remember that the d orbital can have up to 10 electrons, but we only could give it 4, while the 4s orbital got its 2 electrons (since it overlaps the 3d). What really happens is that a half filled orbital is more stable that a partially filled orbital, so the 4s gives up one of its electrons to the 3d orbital, making them both half filled - $1s^22s^22p^63s^23p^63d^54s^1$
  - A similar arrangement happens with copper - $1s^22s^22p^63s^23p^63d^94s^2$ – here the 3d orbital is one shy from being complete, so an electron moves from the completed 4s orbital, making the 3d complete and the 4s half filled – a more stable arrangement.
  - While a totally filled orbital is the most stable configuration, a half filled is next and a partially filled is the least stable configuration.

Physics and the Quantum Mechanical Model

Objectives: Calculate the wavelength, frequency, or energy of light, given two of these values; Explain the origin of the atomic emission spectrum of an element.

- Light and Atomic Spectrum
  - Light was originally thought of as made of small fast moving particles; it was not until later that light as a wave was accepted. Today physicists view light as a wave and a particle (photon)
  - According to the wave model, light consists of a small portion of the **electromagnetic spectrum**.
    - The electromagnetic spectrum starts with very long radio waves(10^2m-300kHz), goes to radio waves, microwaves, infrared, visible light, ultraviolet, x-rays, gamma rays and finally cosmic rays(10^{-14}m – $3x10^{22}$Hz).
    - All electromagnetic radiation travels at 3.0 x 10^8m/s, in a vacuum – slightly slower through air, glass, water, etc.
  - A wave consists of two principle parts – wavelength and amplitude
    - 

    - Amplitude is the height of the wave from where it crosses a zero point, mid way between the crest and the trough

      - The wavelength (λ) of a wave is the distance between two identical points of a wave
      - The frequency (ν) of a wave is the number of wave cycles to pass a given point per unit of time (typically per second) – The SI unit for frequency is the Hertz (Hz) and is cycles/second. Frequency can also be thought of as a reciprocal second (s^{-1}), and is typically used this way in problems
      - The product of frequency and wavelength equals a constant – the speed of light (c) $c = \lambda \nu$
      - Wavelength is inversely proportional to the frequency (shorter wavelengths have higher frequency – longer wavelengths have lower frequency)
   - Sunlight is the most common light source we have. It covers the visible wavelengths in a continuous spectrum (ROYGBIV) (400 nm – 700 nm). Newton discovered that white light could be broken down into the spectrum – yet mankind had been seeing it for thousands of years with the rainbow – sunlight is refracted by rain drops acting as a prism..
      - The longer wavelengths are bent the least by a prism.
      - This is what causes red sunsets and sunrises
   - Every element emits light when heated by the passage of electricity through its gas or vapor.
      - The atoms first absorb energy and then release it the form of light – but the light emitted is of a specific wave length(s), unlike the continuous spectrum of white light. Thus each wavelength corresponds to a specific amount of energy being emitted.
      - The spectrum of such a light is called an **emission spectrum** of the element and is unique to each element
      - Wavelengths of light can also be absorbed by a hot gas when it is cooler than the light source – such as the sun or other stars.
         - Much we know about the composition of the universe comes from observing stars which are billions of miles away.

Sample Problem

Calculate the wavelength of the yellow light emitted by a sodium lamp if the frequency of the radiation is 5.10 x 10^{14}Hz

$$c = \lambda \nu \quad \lambda = \frac{c}{\nu} = \frac{3.0x10^{8}\, m/s}{5.10x10^{14}\, s^{-1}} = 5.88x10^{-7}\, m$$

- The Quantum Concept and the Photoelectric Effect
   - In the early 1900's German physicist Max Planck was trying to describe why a piece of metal that was being heated would change colors while being heated (from black to red to yellow to blue to white).
   - Planck's explanation involved energy of a body changed in small discrete units

- Planck described this mathematically by stating that the amount of radiant energy (E) absorbed or emitted by a body is proportional to the frequency of the radiation
  - $E \propto v$ or $E = h \bullet v$
  - h is another fudge factor called **Planck's constant** and has a value of $6.6262x10^{-34}$J·s, where J is joule, the SI unit for energy.
  - The energy of a quantum then is $h \bullet v$, and any attempt to increase the energy of a system by less than $h \bullet v$ will fail,
  - The size of emitted or absorbed quantum depends on the size of the energy change
    - A small energy change involves the emission or absorption of low frequency radiation
    - A large energy change involves the emission or absorption of high frequency radiation
- Prior to Plank's discovery, people thought that you add any small amount of energy to a system
  - For example, heating water – by the thermometer the temperature rose continuously – not it small jumps. The problem is that the thermometer is unable to detect such small changes – thus we have no experience with energy that is quantized.

- In 1905 Albert Einstein was studying Newton's idea that light was made of particles. From this Einstein stated that light could be described as quanta of energy that behaved as particles. These particles he called **photons**.
  - As described by Plank, the energy of photons is quantized according to $E = h \bullet v$
  - Most classical trained scientists (Newton's theories) found the duality of light to be a bit much to handle – but when it solved several problems they had been facing, the duality of light was easier to accept.
    - Case in point – it was known that when light struck certain metals that electrons (called photoelectrons) were released
    - But the reaction was not present for all wavelengths of light – potassium would not react to red light no matter how strong, but a weak yellow light would work.
    - Classical physics and it's "light is a wave" thought that any wavelength of light should work – even if it was weak , it should build up enough to eventually knock an electron loose.
    - Einstein recognized that there was a threshold below which the photoelectric effect would not take place – if the frequency, and therefore the energy, of the photons is too low then no photoelectrons will be ejected.
    - This photoelectric effect is the basis for solar cells today
    - An example of a similar situation would be a ping pong ball hitting a billiard ball – it is not likely to have much effect. But a golf ball (same size as a ping pong ball with more mass) were to strike a

billiard ball, traveling at the same speed as the ping pong ball, the billiard ball would move – the golf ball has more energy – enough to move the billiard ball.

- An Explanation of Atomic Spectra
    - Bohr's model of the atom (planetary model) is often used to explain the atomic spectra of atoms. Recall that Bohr stated that electrons exist on energy levels.
    - When enough energy is added to an atom to cause a quantum leap, an electron jumps to a higher energy level.
        - This is an unstable situation that is remedied by the electron dropping back to its former energy level. The energy that was absorbed is now released in the form of light
        - The light emitted depends on what energy level an electron is dropping to.
    - There are three principle groups of lines observed in the emission spectrum for hydrogen atoms
        - If the electron is dropping from the 2-7 energy levels to n=1 (ground level), then emission spectra is produced in the ultraviolet wavelengths – these are the Lyman series
        - If the electron is dropping from the 3-7 energy levels to n=2, then emission spectra is produced in the visible wavelengths – these are the Balmer series
        - If the electron is dropping from the 4-7 energy levels to n=3, then emission spectra is produced in the infrared wavelengths – these are the Paschen series
- Quantum Mechanics
    - Bohr's explanation for the model of an atom was good for some things (such as atomic spectra) but it was lacking in helping to understand how atoms bond to form molecules – quantum mechanics to the rescue!
    - In 1924, a French graduate student Louis de Broglie wondered if light could behave as a wave and a particle, could matter (which we think of as particles) behave as a wave?
    - De Broglie derived an equation that described the wavelength of a moving particle - $\lambda = \frac{h}{mv}$, where h is Planck's constant, m is the mass of the particle and v is the velocity of the particle.
        - So an electron with a mass of 9.11×10^{-28}g, moving near the speed of light would have a wavelength of 2×10^{-8}m, which is about the size of an atom
        - De Broglie's equation predicts that all particles exhibit wavelike motion – so why don't we see it?
            - Depends on the mass and the speed of the object
                - A basketball (200g) moving at 30m/s would have a wavelength of 10^{-30}m. This is twice a short as a cosmic wave and we do not have anyway to measure or detect it.

- An electron moving at the same speed would have a wavelength of $2x10^{-1}$m, which is measurable
- De Broglie's prediction of the duality of matter (particle and wave) opened the door to a new branch of science called quantum mechanics.
  - The major difference between classical and quantum mechanics are-
    - Classical mechanics the motions of bodies much larger than the atoms that make it up – energy seems to be absorbed and emitted in any amount
    - Quantum mechanics describes the motions of subatomic particles and atoms as waves – energy is absorbed or emitted in packages called quanta.
- A last taste of quantum mechanics is the uncertainty principle
  - German Werner Heisenberg speculated in 1927 that it was impossible to know both the position and the velocity of a particle at the same time
  - This idea works better with very small objects (subatomic) than with large objects (baseballs)
  - When you try to determine the position of an object, you add energy to the object thus changing it's speed
  - When you try to determine the speed of an object then you cannot determine it's speed
  - For a baseball traveling at 30m/s, the uncertainty is only 10^{-19}m, which is too small to be measured. Where as for an electron with a mass of $9.11x10^{-28}$g, the uncertainty is almost 10 million meters.

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