

CHEM 110: CHAPTER 6 ELECTRONIC STRUCTURE OF ATOMS

ELECTROMAGNETIC RADIATION

This is energy in the form of radio waves, microwaves, infrared radiation, visible light, ultraviolet light (UV), x-rays, and gamma rays.

Our eyes are capable of seeing only in the visible light region (400 -700 nm) of the electromagnetic spectrum. SEE pg. 208 in text.

Wavelength and Energy

As the wavelength (symbol λ) decreases, the energy for that wave increases. This is an indirect relationship. So, as you go from gamma rays (the shortest λ) to radio waves (the longest λ) the electromagnetic radiation has lessening energy.

For example, being exposed to x-rays is much more damaging than being exposed to visible light. X-rays are known to trigger cancerous tumor growth and cause deep tissue damage.

Electromagnetic energy has dual properties of both a particle (termed a photon) and that of a wave. Different situations use either property to explain physical phenomenon such as some metals giving off electrons when exposed to light (termed the photoelectric effect). This is explained by seeing light as a particle.

SEE TABLE 6.1 PG. 208 OF TEXT FOR ADDITIONAL INFORMATION.

Section 6.2

Viewing light (electromagnetic radiation) only as a wave cannot explain several of its aspects. For these, we need to consider light as a particle rather than a wave.

THESE ASPECTS ARE:

1. **Blackbody radiation**: the emission of light from black color appearing objects when hot.
2. **Photoelectric effect**: electrons being emitted by metals when light of a particular wavelength shines on them.
3. **Emission Spectra**: a display of light given off from electronically excited atoms of an element

These can be understood by considering energy release as being **quantized**.

Quantization: process in which energy (light) is released in small, discrete packets termed “quanta.”

This aspect of energy release was described by German physicist *Max Planck* in his work on the “quantum theory.” The energy released or absorbed can be determined using $E = hv$, where $h = 6.626 \times 10^{-34}$ J-s and $v =$ the frequency of the wave.

This energy was found to be released in multiples of hv (hv , $2hv$, $3hv$, etc.) proving his theory to be correct.

Please note that this is most noticeable on the atomic rather than macro level.

The Photoelectric Effect

Albert Einstein used Planck's quantum theory to explain why light of a particular frequency (has to be at a minimum value) results in the emission of electrons from metal surfaces. Some metals need higher frequencies than others. ***The minimum energy equal to this frequency is $h\nu$.***

Hence, electromagnetic radiation is quantized. Each quantum of this radiation is termed a photon, i.e., a particle of light.

Thus, light (electromagnetic radiation) exhibits properties of both a particle and a wave depending upon the circumstances.

Line Spectra

A spectrum is a display of light and other forms of electromagnetic radiation. Electromagnetic radiation emitted from objects such as light bulbs and stars are composed of a variety of wavelengths and frequencies.

This type of spectrum in which a variety of wavelengths are displayed is termed a *continuous spectrum*. Examples include such

things as using a prism to produce a visible light spectrum or seeing rain drops do so by producing a rainbow.

Another type of spectrum is produced when only certain wavelengths (colors of light) are seen while the rest of the spectrum is black due to no emission. This results in lines of color due to the particular λ of light being emitted. Hence, it is termed a “bright-line” spectrum.

These spectra are very useful as each particular element has its own unique bright-line spectrum so this aids in identification.

For Hydrogen, the Rydberg equation is used to determine these spectral line wavelengths:

$$\frac{1}{\lambda} = (R_H) \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Where R_H is the Rydberg constant = $1.096776 \times 10^7 \text{ m}^{-1}$

And n_1 and n_2 are positive integers ($n_2 > n_1$).

The Bohr Model

Danish physicist Niels Bohr, *using Ernest Rutherford's atomic model of the electrons orbiting the nucleus of the atom like planets revolving around the sun*, knew that this model could not explain how the electrons maintained their orbit without being pulled into

the positively charged nucleus. He based his new model using Planck's quantum theory to explain that electrons are able to move from one energy level (orbit) to another only if they absorb electromagnetic radiation of a certain energy (as photons) to jump up to a higher energy level and release energy equal to the energy they absorbed in order to fall back down. This amount of energy is emitted and absorbed as a photon using $E = hv$.

Hence the energy states (E) of the hydrogen atom were determined by Bohr to be:

$$E = (-hcR_H)\left(\frac{1}{n^2}\right) = (-2.18 \times 10^{-18} \text{ J})\left(\frac{1}{n^2}\right)$$

Where h = Planck's constant, c = speed of light, and R_H is the Rydberg constant.

The integer n is termed the *principal quantum number* and can have whole number values starting at $n = 1$ which is the lowest energy level termed the *ground state*. The more negative (lower the value of n) the value of E , the more stable the atom is.

If $n \geq 2$, the atom is said to be in an *excited state*.

The change in energy (ΔE) resulting from an electron jumping from a lower to a higher energy level (value of n) in this excitation is given by:

$$\Delta E = (-2.18 \times 10^{-18} \text{ J}) \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Where n_f is the final energy level, and n_i is the initial energy level.

Hence, if an electron goes from $n = 2$ to $n = 7$ it will need to absorb energy of a particular wavelength or frequency (ΔE will be positive); if it goes from $n = 7$ to $n = 2$, it will need to emit that energy it originally absorbed (ΔE will be negative).

The wavelength (λ) can be determined using $\frac{hc}{\Delta E}$

The Wave Behavior of Matter

French physicist, Louis DeBroglie developed the idea that if energy could behave as a wave, why not matter? This idea included not only very small particles such as electrons, protons, and neutrons, but also atoms, molecules, and even living things including human beings.

His formula for determining matter waves is:

$$\lambda = h/mv$$

where h is Planck's constant, and the product mv is the momentum.

Some observations: If the velocity of the object is 0, its matter wave would be undefined; as the mass (m) of the object decreases, its wavelength increases and hence is more easily observable.

Heisenberg's Uncertainty Principle

Can we know the position of small particles, which have wave properties, such as an electron at the same time we know its velocity (momentum)? The answer is NO according to this principle.

$$\Delta x \geq \frac{h}{4\pi m \Delta v}$$

Where $m\Delta v$ is the uncertainty in the momentum

Using this inequality, it would be found that the uncertainty of the hydrogen atom's location is greater than its size. Hence, we don't know for certain where it is located in the atom!

Atomic Orbitals

One way of describing the position of an electron in the atom is through the use of atomic orbitals. These are regions around the nucleus of the atom where there is a high probability of finding the electron. These are given different letters to represent them.

SEE PG. 221 of TEXT: TABLE 6.2 FOR MORE INFORMATION.

The letters n , l , m_l , and m_s are used to designate specifics of these atomic orbitals. These letters have numerical values associated with them and hence are termed “quantum numbers”.

n = the electron shell; its value is the same as the period (row) number of the Periodic Table of Elements

l = the electron subshell; its value can range from 0 to 3 where 0 represents the s orbital, 1 the p orbital, 2 the d orbital, and 3 the f orbital.

m_l is used to designate which orbital of the particular electron subshell; these are also whole numbers that can range from -3 to 3.

s orbital = 0 (There is only one s orbital per electron subshell.)

p orbital = -1, 0, 1 depending upon which of the three p orbitals is being specified.

d orbital = -2, -1, 0, 1, 2 depending upon which of the five d orbitals is being specified.

f orbital = -3, -2, -1, 0, 1, 2, 3 depending upon which of the seven f orbitals is being specified.

Orbitals can be represented by 3-D drawings.

See pgs. 223 - 226 of text.

ENERGY LEVELS OF ELECTRONS AND THE PAULI EXCLUSION
PRINCIPLE

The Bohr model aided in developing the wave-mechanical model in which electrons have a principal energy level n . n is a whole number integer ranging from 1, 2, 3, and on. $n=1$ is termed the ground state, the lowest possible energy level an electron can occupy.

The principal energy level is further divided into sublevels. These sublevels (represented by the letter l) range from 1, 2, 3, and on as the principal levels did and contain spaces for the electrons to occupy termed ORBITALS.

*EACH ORBITAL CAN HOLD A MAXIMUM OF 2 ELECTRONS EACH, AND THESE ELECTRONS MUST HAVE OPPOSITE SPINS. ELECTRONS SPIN ON THEIR AXES AND CAN EITHER SPIN UP (+1/2) OR SPIN DOWN (-1/2). POSITIVE SPIN IS ALSO INDICATED WITH AN \uparrow ARROW, WHILE NEGATIVE SPIN A \downarrow . THIS RULE IS TERMED THE *PAULI EXCLUSION PRINCIPLE*.*

Principal Energy Levels and the Number and Name of Possible Orbitals

For $n = 1$, there is 1 orbital. It is termed an “s” orbital and is written 1s. It can hold a maximum of 2 electrons.

For $n=2$, there are 4 orbitals, one 2s orbital and three 2p orbitals. Each p orbital can also hold only 2, so the 2 from the 2s plus the 6 from the three 2p orbitals gives a maximum of 8 electrons in the 2nd principal energy level.

For $n = 3$, there are 9 orbitals. One 3s, three 3p, and five 3d. This gives a total of 2 e-s for 3s, 6 e- for 3p, and 10 e- (5×2) for 3d. Hence, a maximum of 18 e- are possible for the 3rd principal energy level.

For $n = 4$, there are 16 orbitals. One 4s, three 4p, five 4d, and seven 4f orbitals. This gives a total of $2 + 6 + 10 + 14 = 32$ e- max possible.

For $n = 5$, we only are concerned with the 16 orbitals as for $n = 4$.

ELECTRON CONFIGURATIONS

An electron configuration represents a short-hand way of displaying the energy levels, orbitals, and positions of the electrons in an atom.

In writing e- configurations, the following guidelines are used.

- a. No more than 2 e- can be placed in each orbital, and they must have their spins be opposite.
- b. Electrons fill in the lowest principal energy levels first. If an electron goes into a p sublevel with 3 orbitals, the electrons will go unpaired into each of the 3 first before filling up the remaining vacant space to give a total of 6 e-. All five d orbitals must contain 1 electron each before the 6th electron can be added. This is to obey the PAULI EXCLUSION PRINCIPAL.
- c. Coefficients are used to indicate the energy level followed by the symbol for the orbital and a superscript with it to indicate the number of electrons total it contains. (A p orbital could have a maximum of a superscripted ⁶, while a d orbital a maximum of ¹⁰.)

Starting with H, the simplest atom, the e- configuration would be written $1s^1$.

He: $1s^2$ (It is atomic number 2 so it has 2 e- with it and each of these go into a 1s orbital as it can hold a max of 2.)

Li: $1s^2 2s^1$; Be: $1s^2 2s^2$; B: $1s^2 2s^2 2p^1$; C: $1s^2 2s^2 2p^2$; N: $1s^2 2s^2 2p^3$

O: $1s^2 2s^2 2p^4$; F: $1s^2 2s^2 2p^5$; Ne: $1s^2 2s^2 2p^6$

BE FAMILIAR WITH ORBITAL BLOCK DIAGRAM PGS. 230+ 231 FOR TEST!

SEE PG. 236 OF TEXT FIGURE 6.31 FOR OTHER CONFIGURATIONS.

