Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- The Eighth lecture -

Stage 4

Prof. Dr Hassan sabih

3) Atomic Spectra

In the case of the stirring of atoms emit radiation and this radiation provides information representing the nature of the electronic composition of atoms and scientific experiments have shown that the absorption spectra Absorption and emission emission of atoms are not continuous but consist of a number of spectral lines with specific frequencies.

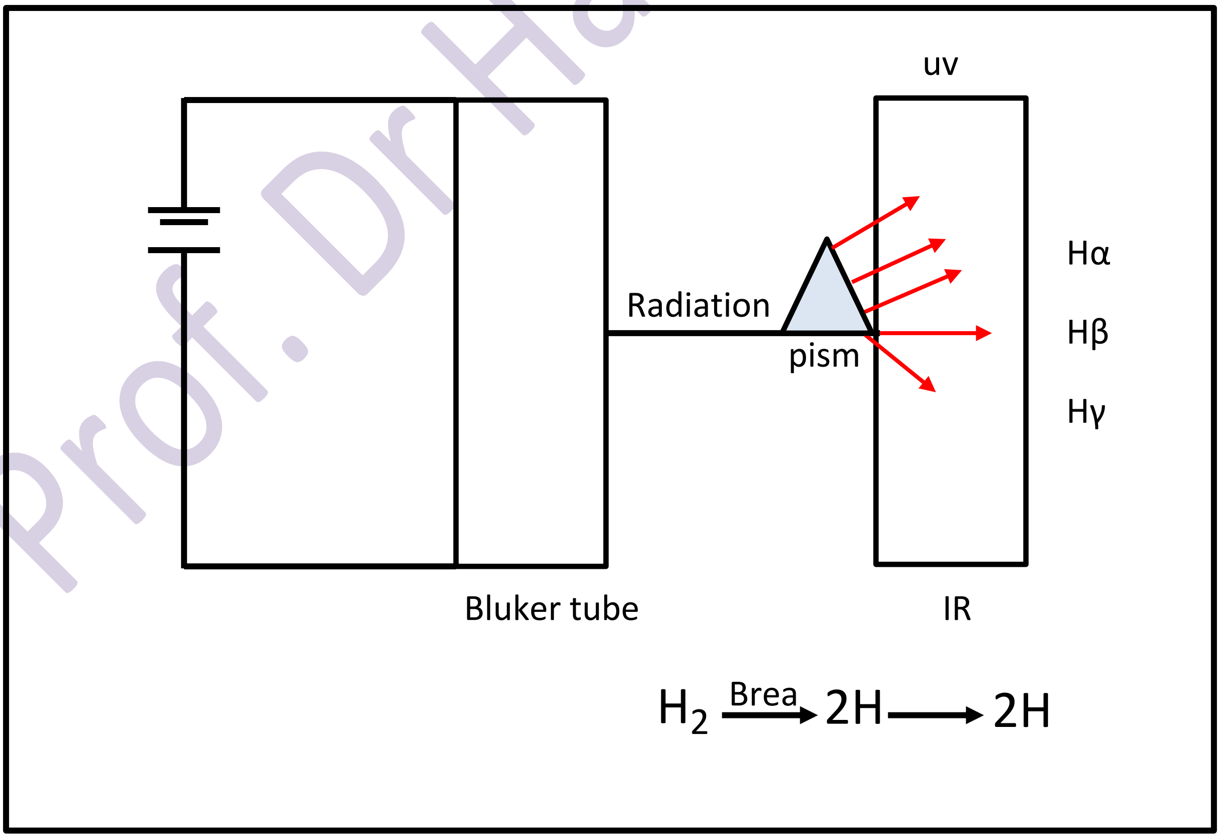
The first scientist to illustrate the atomic spectra is Newton, where sunlight was passed through a glass prism and found to decompose into a group of colors from violet to red and because there are no separate areas between one color and another called this spectrum with continuous spectrum and called the continuous emission spectrum. continuose emission speat

(Is the group of decaying colors of sunlight that start from violet and end in red and are connected to each other))

There's another spectrum called line emission spectrum.

((Is the group of decaying colors of the atoms of a pure element in thegaseous state and the colors are separate i.e. separates each color from the other extended distances and relatively large and each element has a linear spectrum that distinguishes it from other elements))

Another experiment of the atomic spectrum is when hydrogen is placed in a low-pressure, high voltage vacuum tube called bluker Tube, which emits visible light when analyzing a prism where the spectrum consists of regular spectral lines called this spectrum (the atomic hydrogen gas spectrum resulting from the disintegration of gas molecules and these lines are called spectra spectrum lines).



The disintegration of hydrogen atoms into atoms and energy triggers the disintegrating atoms to hydrogen atoms, so that the frequency, wavelength, wavelength, wavelength) can be calculated according to the following relationship:

$$y' = \frac{1}{\lambda} = \left(\frac{R}{n_1^2} - \frac{R}{n_2^2}\right) \_\_\_\_\_\_(1)$$

$$y' = \frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \_\_\_\_\_\_(2)$$

n:- A reference to energy levels and always be

$(n_j < n_i)$ $(n_1 < n_2)$

Therefore, the following relationship can be expressed:

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

Constant Redberg R_H = Rydberg Constant

= $109677.6\ cm^{-1}$

To explain this phenomenon we go back to atomic composition and there are attempts (theories)

a)Ruther ford Ruther Theory

The scientist assumed that the atom is a positive nucleus surrounded by electrons in a state of movement, electrons are a charge in the case of continuous movement according to electrodynamical theory so the movement of any charged object accompanied by the emission of electromagnetic radiation over time and thus energy consumes, decreases and drops the electron within the nucleus.

It is concluded that Rutherford's idea of atomic composition (unstable) where when the electron moves a spiral movement (spril), the emerging spectra are continuous, not linear, which is not true because spectra must be linear.

b) Buhr Theory

The Danish physicist Bor explained that electrons are within energy levels, so he explained a set of hypotheses of atomic composition.

1) atom energy is specific or lying, and there are certain energy conditions called continuous conditions.

2) The atom in its stable state does not radiate electromagnetic radiation when the atom is removed from one state to another that must absorb energy or emit energy.
$\Delta E = E_2 - E_1 = hy$

3) The electron is in a circular motion state.

4) The electron moves in circular orbits around the nucleus and is subject to the laws of traditional mechanics resulting from the $E_T = T + V$ power of electrostatic attraction between the electron and the nucleus, so the energy depends on the radius of the orbit and the energy is a contraction so the orbits must be limited only.

5) The electron in its orbits has angular momentum, so we conclude fromatpour's assumptions:

a. Atoms don't collapse.

B. The emission of light from atoms at a certain frequency (so energy changes are specific and specific)

The angular momentum can thus be calculated .(L)

$$L = n \cdot \frac{h}{2\pi} \text{\_\_\_\_\_\_}(1)$$

$$L = n\hbar \text{\_\_\_\_\_\_}(2)$$

$$\therefore L = mvr \text{\_\_\_\_\_\_}(3)$$

equally

$$mvr = n\frac{h}{2\pi} \text{\_\_\_\_\_\_}(4)$$

From this relationship, the radius and momentum can be calculated, where Burr was able through his hypotheses to calculate the fairness of the permitted countries as well as the energies of stable situations through the following relationship:

$$r = \frac{n^2h^2}{4\pi^2me^2z}$$

Z:- Atomic number

m:- Electron mass 9.11*10-31

E:- Electron charge 1.6*10-19

For a hydrogen atom, z = 1 and if it is stable n = 1 so we can calculate the radius of the hydrogen atom in a stable state (bor radius) α_o

$$r_H = \frac{n^2 h^2}{4\pi^2\, me^2\, z}$$

n, z = 1

$$r_H = \frac{h^2}{4\pi^2\, m\, e^2} = \frac{\hbar^2}{me^2}$$

$$0.529 * 10^{-18}\ cm^{-1} = 0.529\ A^o$$

Thus, the equation of atomic spectrum pressures can be derived as follows:

$$En = \frac{-2\pi^2 me^4}{h^2} \cdot \frac{z^2}{n^2} \text{ \_\_\_\_\_\_ } (1)$$

Negative signal where the electron moves in reverse

$$\left.\begin{aligned} E_1 &= \frac{-2\pi^2 me^4}{h^2} \cdot \frac{z^2}{(1)^2} \\ E_2 &= \frac{-2\pi^2 me^4}{h^2} \cdot \frac{z^2}{(2)^2} \end{aligned}\right\rangle \text{ \_\_\_\_\_\_ } (2)$$

$$\because \Delta E = hy \longrightarrow y = \frac{\Delta E}{h} \_\_\_\_\_(3)$$

Emission $\quad y = \frac{E_2 - E_1}{h}$

Absorption $\quad y = \frac{E^1 - E^2}{h}$

That's why the frequency.

$$y = \frac{E_j - E_i}{h} = \frac{1}{h}(E_j - E_i)\_\_\_\_\_(4)$$

We make up 2 in 4.

$$y = \frac{2\pi^2 me^4 z^2}{h^3} \cdot \left(\frac{1}{n_j} - \frac{1}{ni}\right)\_\_\_\_\_(5)$$

$$\because y' = \frac{1}{\lambda} = \frac{y}{c} = \frac{2\pi^2 me^4 z^2}{ch^3}\left(\frac{1}{n_j} - \frac{1}{n_i}\right)\_\_\_\_\_(6)$$

where $R_H = \frac{z\pi^2 me^4}{ch^3} = 109677.6\ cm^{-1}$

$$\therefore y' = R_H\, z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)\_\_\_\_\_(7)$$

Atomic Spectrum Pressure Equation

It is clear from the last equation that the electron's energy is a (unstable) amount based on the number of quantum (n) $n = 1,2,3,4,\cdots\cdots$

And so the hydrogen atom fits the n-box that the energy

$$E = -\frac{z^2 R}{n^2}$$

$$E \propto -\frac{1}{n^2}$$

Negative signal means electron is attracted to the nucleus so the higher the value of n the energy increases and when $n = \infty$the E=zero, which is the state of ionization of the rh value, considering that the nucleus is fixed and electrons are in motion as well as the electron mass was taken only, but it later became clear that the nucleus is not stable (fixed), i.e. the system consisting of the nucleus and electrons is in motion, so the mass of the nucleus must be taken, so we conclude that the electron mass is replaced by the reduced mass.

$$m = \frac{m_1 * m_2}{m_1 + m_2}$$

The following table shows electronic transmission chains

Series	n_1	n_2	Radiation
1) Lyman	1	2,3,4....	uv
2) Blmer	2	3,4,5....	visbile
3) Baschen	3	4,5,6....	IR
4) prackkt	4	5,6,7....	IR
5) pfond	5	6,7,8....	IR

Ex // what is the wave length for lyman series for atomic H_2?

Ioni zation energy ionization energy

Is the energy needed to remove the electron from the earth's state of the atom to form a positive ion and the electron is free.

Expressed in electron units volt ev or erg

And there's ionization energy, second ionization energy, and so on.

For example, a neutral atom is available.

$$A \longrightarrow A^{+} + e^{-}$$

$$A^{+} \longrightarrow A^{++} + e^{-}$$

Where the energy in the H atom depends on n only and the highest energy so the $(n = \infty)$ionization energy of $n = 1 \longrightarrow n_2 = \infty$

And when compensated in the relationship of the atomic spectrum

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

$$= R_H z^2 \left(\frac{1}{(1)^2} - \underbrace{\frac{1}{\infty}}_{0}\right)$$

$$\therefore = R_H z^2$$

When converting to e.v, we must convert energy fromerg ← e.v.

$$E = y' = R_H z^2 c \; x \; ev$$