University of Babylon
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Physical chemistry
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Lectures of Quantum mechanics
The scholar year 2019-2020
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Lecture No. One

General introduction of Quantum mechanics

1- **Introduction.**
2- **Aims of Theoretical chemistry.**
3- **Molecular Structure and chemical activity.**

1-1- Introduction:

A new filed of chemistry has been born depended on different visions of experimental results. Quantization of things that occurs due to interactions between mater and energy. The relation between different components has been used to understand different problems of chemistry since mathematical language been used in physical interpretation for chemical interaction relation of chemical species.

Quantum chemistry is a branch of chemistry whose primary focus is the application of quantum mechanics in physical models and experiments of chemical systems.

It is also called molecular quantum mechanics. Therefore :

<u>Quantum mechanics</u> is a chemical science related to quantization of things through mathematics, physics, and chemist to give up a clear right vision about chemical reaction phenomena.

Quantum mechanics is the mathematical description of matter on the atomic scale.

All substance in our universal consist from essential units they are called atoms that are the smallest building block of matter. Atoms are fabricated by sub small particles (negative electrons) around into oriented orbital about a positive particle (nuclei that have also consisted of another system).

The simplest atom is a hydrogen atom, consisted of one electron and one proton. The diameter of electron equal to 10^{-13} Cm, The diameter of nuclei equal to 10^{-13}-10^{-12} Cm, and The diameter of hydrogen atom equal to 10^{-8} Cm. The density of nuclei is very large that's equal to10^{14} Gm.Cm^{-3} rather than the density of sun and earth 1410 and 5520 kGm.m^{-3} respectively. If you know that the mass of sun equal to $1.99*10^{30}$ k Gm, and the mass of earth equal to $5.98*10^{24}$ kGm.

At the first of Quantum science, it was called classical quantum mechanics due to direct relation about the huge masses bodies. Laws of Newton have been used to describe the movement of plants in our suns group. Small infinite particle likes electrons ($m=9.1083*10^{-31}$ kg) are didn't obey these laws, also they found another phenomena's lead to give up a new science called modern quantum mechanics.

Classical mechanics does not provide an accurate description of matter on the scale of atoms and molecules. Electrons around a nucleus or nuclei do not behave like planets orbiting the sun or like ping-pong balls bouncing around in a container. Experiments show that when observing the properties of very small bits of matter, such as a single electron, the matter exhibits wave-like properties.

1900 (Planck): Max Planck proposed that light with frequency ν is emitted in quantized lumps of energy that come in integral multiples of the quantity,

$$E = h\nu = \hbar\omega \text{ ---------(1) },$$

where $h \approx 6.63 \cdot 10^{-34}$ J · s . h is Planck's constant, and $\hbar \equiv h/2\pi = 1.06 \cdot 10^{-34}$ J · s.

The frequency **ν** of light is generally very large (on the order of 10^{15} s^{-1} for the visible spectrum), but the smallness of h wins out, so the hν unit of energy is very small (at least on an everyday energy scale). The energy is therefore essentially continuous for most purposes. However,

Planck's hypothesis simply adds the information of how many lumps of energy a wave contains. Although strictly speaking, **Planck initially thought that the quantization was only a function of the emission process and not inherent to the light itself**.

1905 (Einstein): Albert Einstein stated that the quantization was, in fact, inherent to the light and that the lumps can be interpreted as particles, which we now call "photons." This proposal was a result of his work on the photoelectric effect, which deals with the absorption of light and the emission of electrons from a material.

1913 (Bohr): Niels Bohr stated that electrons in atoms have wavelike properties. This correctly explained a few things about hydrogen, in particular, the quantized energy levels that were known. 1924 (de Broglie): Louis de Broglie proposed that all particles are associated with waves, where the frequency and wavenumber of the wave are given by the same relations we found above for photons, namely $E = \hbar\omega$ and $p = \hbar k$.

1925 (Heisenberg): Werner Heisenberg formulated a version of quantum mechanics that made use of matrix mechanics. We won't deal with this matrix formulation (it's rather difficult), but instead with the following wave formulation due to Schrodinger.

1926 (Schrodinger): Erwin Schrodinger formulated a version of quantum mechanics that was based on waves. He wrote down a wave equation (the so-called Schrodinger equation) that governs how the waves evolve in space and time. Even though the equation is correct, the correct interpretation of what the wave meant was still missing. Initially, Schrodinger thought (incorrectly) that the wave represented the charge density.

1926 (Born): Max Born correctly interpreted Schrodinger's wave as a probability amplitude. By "amplitude" we mean that the wave must be squared to obtain the desired probability. More precisely, since the wave is in general complex, we need to square its absolute value. This yields the probability of finding a particle at a given location (assuming that the wave is written as a function of x).

1926 (Dirac): Paul Dirac showed that Heisenberg's and Schrodinger's versions of quantum mechanics were equivalent, in that they could both be derived from a more general version of quantum mechanics.

1-2- Aims of theoretical chemistry:

Quantum mechanics or theoretical chemistry is a science tend to find the complementary idea about the matter, system and surrounding through some of the aims:

1. Discussed what is the equilibrium structures and the reactivity of chemical systems (atoms and molecules).
2. Achieved the physical constant calculation without, or with a dependence of chemical experiments.
3. Help us to a deeper understanding of chemical experiments.

Chemical systems have consisted of different proposed structures, usually atoms, or molecules. A stable structure must have consisted from equilibrium structure which energized value depends on the different dimensions between atoms of molecules. Therefore ***equilibrium structure is the lowest energy value structure than other proposed structure or that closer than (geometry optimized structure).***

1-3- Molecular Structure and chemical activity:

Can describe the total energy of molecule A—B as a function of dimension, and distance that separated between two atoms of the molecule.

$$E_{(A\text{-}B)} = f(r_{A\text{-}B}) \quad \text{-----}(2)$$

Investigation of this function gives us a mathematical figure by values of internuclear distance and the potential energy of bonding. As in following the potential figure.

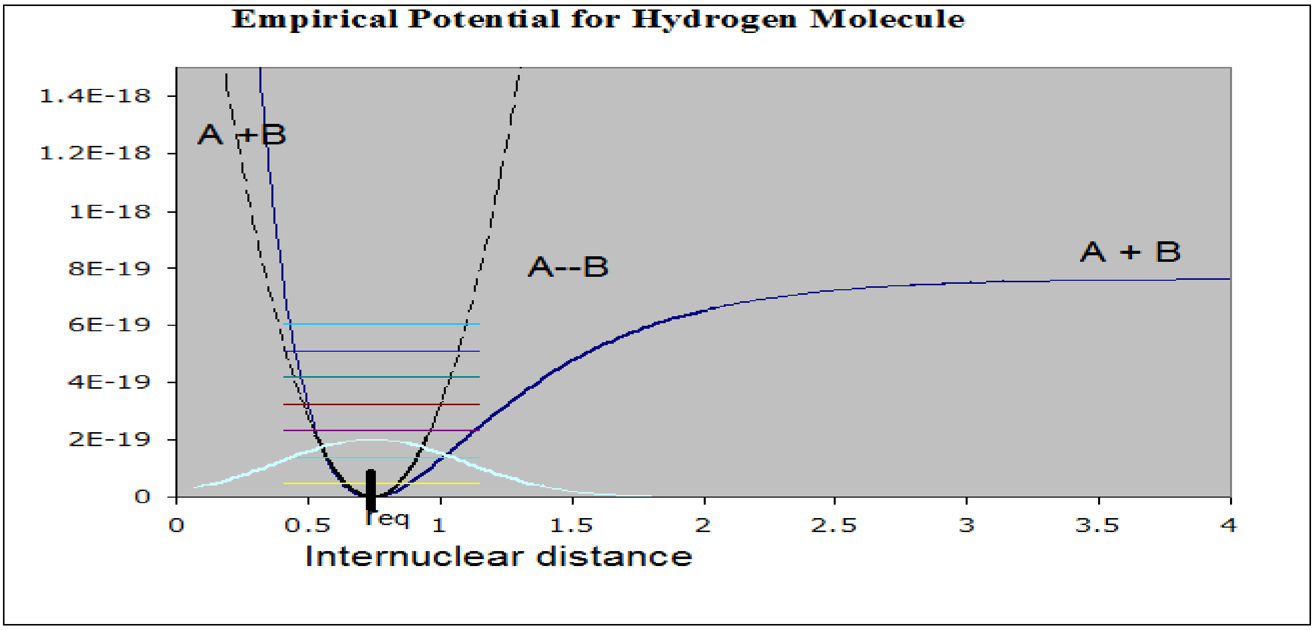

Figure 1-1. Potential energy curve as function to internuclear distance of diatomic molecule.

The total energy of a molecule is E_{A-B} as a function of the distance between these atoms. E_A, and E_B, they are energies of separated atoms. Also, the energy barrier of a chemical bond is referred to as E_b and at last $r_{eq.}$ is the distance between bonding atoms at a stable state of the molecule. The potential energy of molecule at the stable structure is E_{eq}, so can define the bonded state of a molecule by the amount of thermal stability level, that's equal to the difference between the molecular energy at equilibrium distance and the summation of atomic energy of ($E_A + E_B$).

$$E_b = E_{eq} - (E_A + E_B) \text{ -------}(3)$$

Always the value's sign of stable molecular structure is negative, that’s represented the total energy of molecule for multi parameters.

$$E_{A-B} = E_{ele-A} + E_{ele-B} + E_{e1-e2} + E_{AB} \text{ --------}(4)$$

Since:-

E_{ele-A} and E_{ele-B} are attraction energy of electrons in the molecule to the atoms of A, B respectively.

E_{e1-e2} is interaction energy of electrons with each atom.

E_{AB} is repulsion energy of nuclei A with nuclei B.

The molecular energy is described with the geometrical dimensions that are oriented into space to get on the best thermal stability. Several relations are governing or controlling the optimized structure rather than several proposed structures depending on theoretical calculations. The most stable suggested structure with the lowest energy value is the closest structure than real structure. Therefore this relation is one of the important aims of modern theoretical chemistry that gets on by using package programs of quantum mechanics to attend the real and stable structures of chemical compounds.