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Lectures of

Quantum Mechanics of Chemistry

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Lecture No. 1 ((General introduction))

1-1- Introduction:

At first what is chemistry?

Chemistry is the branch of science that deals with the properties, composition, and structure of elements and compounds, how they can change, and the energy that is released, or absorbed when they change.

Second, what is physical chemistry?

Its **branch of chemistry concerned with interactions and transformations of materials**. Unlike other branches, it deals with the principles of physics underlying all chemical interactions, seeking to measure, correlate, and explain the quantitative aspects of reactions.

According to new visions of experimental and theoretical results, quantization of things action has occurred between mater and energy. The relation between different components has been used to understand different problems of chemistry, since mathematical equations depending on physical interpretation for chemical interaction between chemical species, therefore can define the meaning of Quantum mechanics**. So that:**

Quantum mechanics is a chemical science related to the quantization of things through mathematics, physics, and chemist to give us a clear right vision about chemical reaction phenomena.

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

The system of an atom is neutral by the number of electrons equal to the number of protons which is found in nuclei, also nuclei have consisted from another species oriented into energetic orbital are called nucleons(very smallest infinite particles).

Each atom of elements differs from other atoms by this number. The simplest atom is a hydrogen atom, consisting of one electron and one proton. The diameter of an electron is equal to 10^{-13} Cm, The diameter of nuclei is equal to 10^{-13}-10^{-12} Cm, and The diameter of a hydrogen atom is 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 the sun is equal to $1.99*10^{30}$ kg, and the mass of the earth is equal to $5.98*10^{24}$ kg.

At the beginning of Quantum science, it was called classical quantum mechanics due to the direct relation of 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 borne a new science called modern quantum mechanics.

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, $E = h\nu$ ---------(1)

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

Planck’s hypothesis of quantized radiation is not only got rid of the problem of infinity but also correctly predicted the shape of the power curve as a function of temperature.

Planck’s hypothesis simply adds the information of how many lumps of energy a wave contains.

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 of energy.

1925 (Heisenberg): Werner Heisenberg formulated a version of quantum mechanics that made use of matrix mechanics.

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.

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.

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.

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 on chemical experiments.
3. Help us to a deeper understanding of chemical experiments.

3 Molecular Structure and chemical activity:

Chemical systems have consisted of different proposed structures, usually atoms, or molecules. A stable structure must have consisted of an equilibrium structure whose energized value depends on the different dimensions between atoms of molecules. Therefore <u>Equilibrium structure is the lowest energy value structure than other proposed structures or that closer than (geometry optimized structure).</u>

Can describe the total energy of molecule A—B as a function of dimension, and distance that separated between two atoms of a molecule. $E_{(A-B)} = f(r_{A-B})$ -----(2)

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

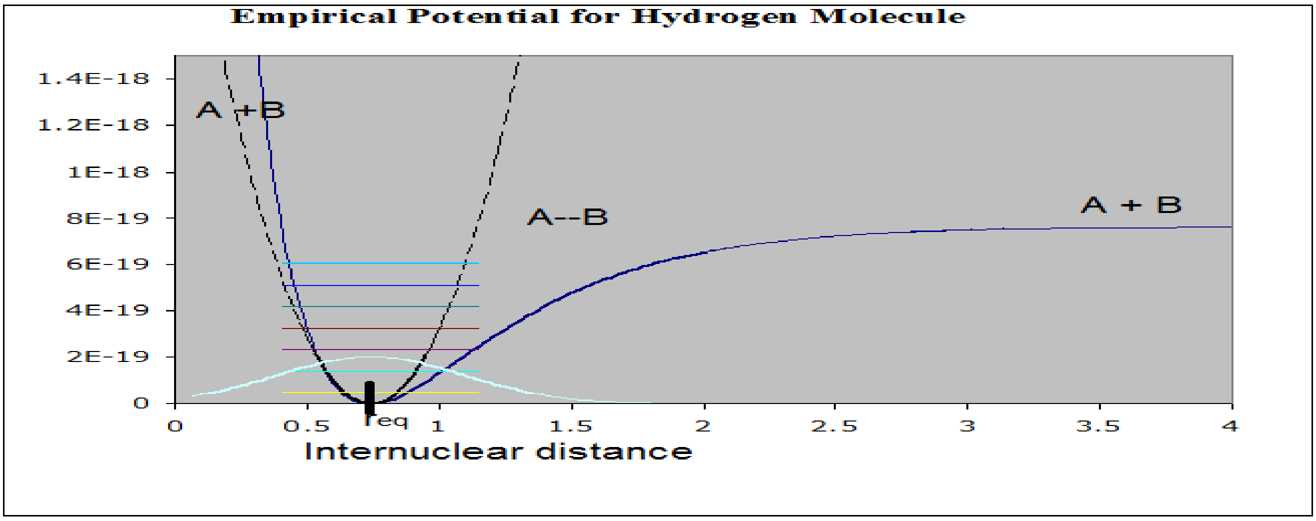

Figure 1-1. Potential energy curve as a function to the internuclear distance of diatomic molecule.

The total energy of the molecule is $E_{\mathbf{A\text{-}B}}$ as a function of the distance between these atoms. $E_{\mathbf{A}}$, and $E_{\mathbf{B}}$, are energies of separated atoms. In addition, the energy barrier of the chemical bond is referred to as $E_{\mathbf{b}}$ and at last, $r_{\mathbf{eq.}}$ is the distance between bonding atoms at the stable state of the molecule. The potential energy of a molecule at a 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).

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

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

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

Since:-

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

$E_{e1\text{-}e2}$ is the interaction energy of electrons with each atom.

$E_{\mathbf{AB}}$ is the 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 <u>the lowest energy value is the closest structure to the real structure</u>. 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 to the real and stable structures of chemical compounds.