Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- The third lecture -

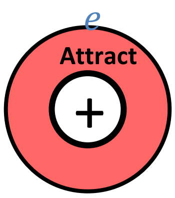
Stage 4

Dr. Hassan Sobeih Jabr

Chapter 2: Mechanic

This is science that studies the movement of bodies and the power that influences between them, so the relationship of chemistry to mechanics (e.g. we take the hydrogen atom)

So we notice



1) Electron movement
2) The electron has a negative charge and the nucleus is a positive charge. So it's a gravitational force in the atomic system, movement and power, which is studied by the mechanical system, so there are two types of mechanics:

1) Classical mechanic
2) Quantum mechanic

Type 1: Classical Mechanics

a) Content energy content: is the sum of the energy of the system (kinetic energy and potential energy) whether the system is made up of atoms, balls or large objects so

$Et = E_{kin} + E_{pot}$

In order to calculate these energies you need the so-called motor issue which is the subject of accurate treatment of motor traits so functions are obtained for all variables

b) Dynamic raviable dynamic variables: There are a number of variables:

1) Coordinate: Each part of the system has coordinates (Xi, Yi, Φi) in mechanics symbolizes these coordinates (qi t)

2) Velocity Speed: In any body of the system and in one direction of the three coordinates has speed and is variable with the function of time symbolized in the science of mechanics and is the first derivative of coordinates with time $\dot{q}\,(t)$

That is, the speed: $\dot{q}_{(t)} = \frac{dq}{dt}$

Can denote q (X, Y, Z) or (ϕ, r, Ø)

3)Accelaration : Is the second derivative of coordinates and is a variable and function of time as well and symbolizes it and $\ddot{q}(t)$calculates from the relationship

$$\ddot{q} = \frac{d^2q}{dt^2} = \frac{dq}{dt}$$

4)Momentum: A certain movement represents the output of mass ingestion in speed and in coordinate

$$Pxi = m * \dot{x}\imath$$
$$Pyi = m * \dot{y}\imath$$
$$Pzi = m * \dot{z}\imath$$

We conclude the momentum as follows:

$$\dot{P}\, qi = m * \mathrm{q}i$$

And in general, the momentum for any coordinate.

* Kinetic energy

We deduce kinetic energy from the solution, which is also a function of the variable over time.

$$KE = \frac{1}{2} m * \dot{x}i^2$$

$$KE = \frac{1}{2} m * \dot{y}i^2$$

$$KE = \frac{1}{2} m * \dot{Z}i^2$$

So kinetic energy is a function of speed and time.

$$KE = f\,(\dot{\mathrm{q}}i * t)$$

KE_T = KEx + KEy + KEz)

* **Potential Energy**

A unified law of latent energy cannot be written, so it is described according to the physical nature of the system and the quality of the voltage (V) affecting the body, so we can describe the potential energy.

1) attraction or revising energy in systems of an electrical nature (-eFx)

e: Electron charge 1.6*10$^{(-19)}$

F: Force Fource

X: Displacement

For large objects, the potential energy represents $\frac{Ze^2}{r}$

Z: Atomic number

e: Electron charge

R: Radius

2) Mechanical attraction energy: Systems that have central attraction such as harmonic vibrator so the underlying energy is calculated by relationship

$$E_{pot} = \frac{1}{2} C X^2$$

C: Constant strength

X: Displacement

Thus, the potential energy is a function of Coordinate and time, i.e. it is

$$E_{pof} = f\,(\,q\,,t\,)$$

So E_{pot} T = V (t) + V (t) + V (t)

X y z

That is, total energy is the sum of kinetic energy and potential energy.

ET = E_{kin} + E_{pof}

$$(\dot{q},t) + (q,t)$$

Type of System

1) Conserative system
2) Non-Conserative system
3) Open System
4) Mechanic System

1) Conserative system (isolated):

is a system whose total capacity does not change over time where total energy is equal to

ET = T_{kin} + V_{pot}

Where the regulations include Conserative that at certain specific conditions,

A specific amount of energy does not change over time. And the conservative system is the system whose total capacity (kinetic potential_+ latent) does not change with time and the forces in it are equal to the negative gradient of the voltage function and the work done must equal the effect of a certain force around a closed road, so it is said that the force is conservative (i.e. lack of friction or dispersion of force)and thus does not fall under external effects

2)Non- Conserative system: it is a system based on time because the system changes its energy over time and thus falls under external effects

3)Open system: Is a system in which particle movement is freely unchanged and moves on three coordinates of degrees of freedom and a particle movement can be determined on three axes

4)Mechanical system: Systems that fall under the effects of external forces such as (electrical, thermal, mechanical, chemical) which all change over time.

Degrees of freedom:

The degree of freedom of the system is defined as: the number of variables needed to locate the system and equal to 3N (N = X, Y, Z).

Through this, it is possible to know the basic legal equations applicable to any system according to the classical mechanics:

1) Newton Dynamic equation: Only cartesian coordinates (so they are application-specific)
2) Laqrang equation: for general coordinates
3) Hamilton equation equation: for general coordinates but in the allowance of momenbum

First: Newton Dynamic Motion Equations

In addition to the law of mass attraction, which has proved useful in describing the movement of celestial bodies as well as the cannon shell of large objects and the most important properties of mechanics that occur is the inevitability i.e. when the location and speed of an object is known in a particular moment, its behavior at all moments is predictable. If the force affecting him is known, then momentum and energy can be known.

That is, any system contains a number of particles, these particles are associated with the strength and forces associated with physical movement, so through Newton's law, which changes the force affecting the body and towards one of the coordinates of the engineering field (X) and equals the product of multiplying the acceleration resulting from this force in the body mass

That is,

F = m a

But in the mechanical system. $F\ (x)\ =\ Xi\ =\ mi\ \bullet\ \ddot{x}$

mi: Body mass (i)

$\ddot{x}$ Ground acceleration

It can be in the direction of engineering coordinates:

$$yi\ =\ mi\ *\ \ddot{y}$$

$$Zi\ =\ mi\ *\ \ddot{Z}$$

The kinetic energy of the particle is defined by the relationship

$$T\ = \frac{1}{2}\, mi\ (\ \dot{x}^2\ , \dot{y}^2\ , \dot{z}^2\ )$$

$$\dot{X}i\ = \frac{dx}{dt}$$

The potential energy of the same body is described according to the nature of the physical system and the quality of the voltage affecting this body, it is described as a gravitational card or dissonance in systems of an electrical nature or mechanical attraction energy in systems with mechanical attraction force such as harmonic oscillator and when the system is considered conservative i.e. isolated from external effects then the forces affecting the mass and causing its movement can be identified as a first differentiation on the geometric coordinates of this movement and thus the forces can be described according to the underlying energy

$$\dot{X}i = -\frac{dV}{dx} \quad , V = \frac{1}{2} C X^2$$

$$\dot{y}i = -\frac{dV}{dy} \quad , \dot{Z}i = -\frac{dV}{dZ}$$

The same forces can also be described as the body's motor energy alternative to coordinate (x)

$$Xi = \frac{d}{dt} \bullet \frac{dT}{d\dot{x}}$$

And when you put the two different middlemen to the same forces with the order you get the relationships that come

$$Xi - xi = \frac{d}{dt} \bullet \frac{dT}{d\dot{x}} + \frac{dV}{dx}$$

$$yi - yi = \frac{d}{dt} \bullet \frac{dT}{d\dot{y}} + \frac{dV}{dy}$$

$$Ƶi - Ƶi = \frac{d}{dt} \bullet \frac{dT}{d\dot{Ƶ}} + \frac{dV}{dƵ}$$

(Newton's equations of movement)

Or cartesin dynamic equation

(Very important)