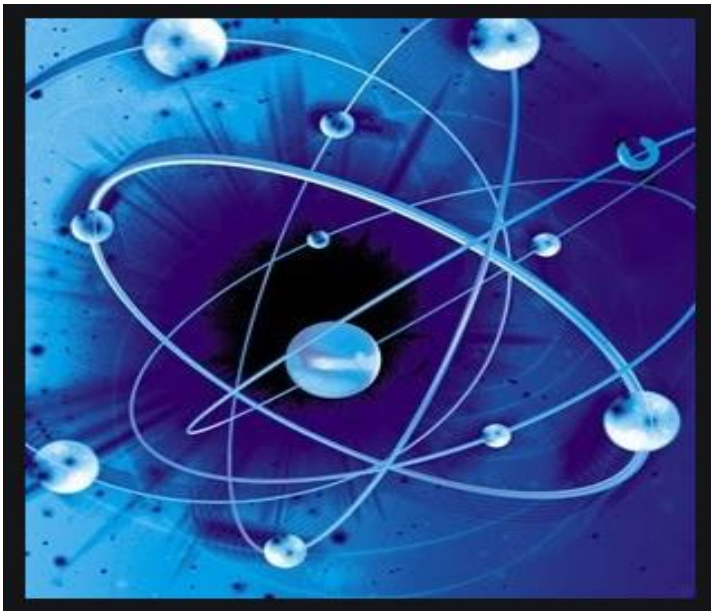
Quantum Mechanics

In the late seventeenth century **Newton** discovered classical mechanics .

The laws of motion of macroscopic objects .

In the late nineteenth century , investigations of electric discharge tubes and natural radioactivity showed that atoms and molecules are composed of charged particles .



Electrons have a negative charge .the proton has a positive charge equal in magnitude but opposite in sign to the electron charge and is 1836 times as heavy as the electron.

The third constituent of atoms, the neutron is uncharged and slightly heavier than the proton.

The chemical properties of atoms and molecules are determined by their electronic structure, and so the question arises as to the nature of the motions and energies of the electrons.

Since the nucleus is much more massive than the electron we expect the motion of the nucleus to be slight compared with the electron motion.

In the earth twentieth century physicists found that classical mechanics does not correctly describe the behavior of very small particles such as the electrons and nuclei of atoms and molecules .

The behavior of such particles is described by a set of laws called quantum mechanics.

Quantum chemistry applies quantum mechanics to problems in chemistry

The influence of quantum chemistry is evident in all branches of chemistry .physical chemists use quantum mechanics to calculate thermodynamic properties (for example , entropy , heat capacity) of gases , to interpret molecular spectra ,thereby allowing experimental determination of molecular properties (for example , bond lengths and bond angles , dipole moments , energy differences) to calculate molecular properties theoretically :to calculate properties of transition states in chemical reactions , thereby allowing estimation of rate constants to understand intermolecular forces, and to deal with bonding in solids .

The development of quantum mechanics began 1900 with **Planck** study of the light emitted by heated solids so we start by discussing the nature of light.

Max Planck developed a theory that gave excellent agreement with the observed black body –radiation curves and assumed that the atoms of the black body could emit light energy only in amounts given by hv. Where v is the radiations frequency :

h is Planck constant	$=6.6 \times 10^{-34}$ J.s
C is speed of light	$=2.99 \times 10^{8}$ m/s
λ	wave length
1 nm	$= 10^{-9}$ m
1^0A	$= 10^{-10}$ m

$$\mathbf{v = c / \lambda}$$

$$\mathbf{\lambda v = c}$$

In 1905 **Einstein** showed that these observations could be explained by regarding light as composed of particle like entities called photons with each photon having an energy .

$E._{photon} = hv.$

Quantum Mechanics: including quantum field theory in a fundamental theory in physics which described nature at the smallest scales of energy levels of atoms and subatomic particles.

Quantum Mechanics cannot predict the exact location of a particle in space only the probability of finding it at different locations.

Quantum Mechanics is a subfield of physics that describes the behavior of particles , atoms , electrons , photons and almost everything in the molecular and sub molecular .

Coordinates Systems

The purpose of a coordinate system is to make it convenient to describe a point , curve ,or a surface in space .

There are many different kinds of coordinate systems, and four will be used in this text :

1-Cartesian Coordinates

2-Spherical polar Coordinates

3-Cylindrical Coordinates

4-Confocal ellipsoidal Coordinates

The coordinate system is always chosen to make the mathematical equations that describe the problem as simple as possible .

1-Cartesian Coordinates

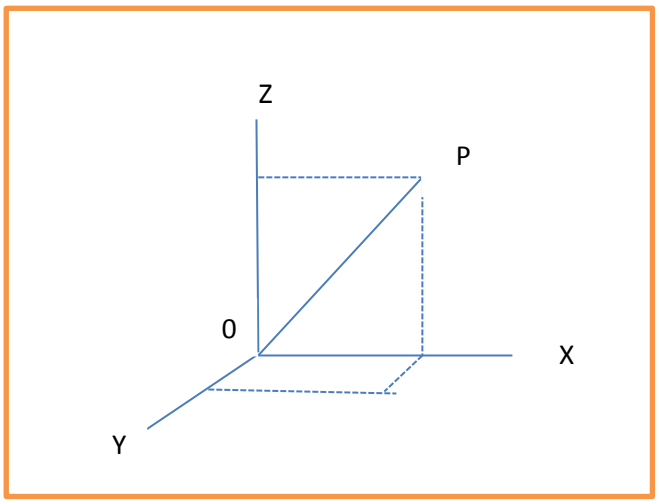
Position any point in space .

$\partial t = \partial x\, \partial y\, \partial z$

$-\infty \leq X \leq +\infty$

$-\infty \leq Y \leq +\infty$

$-\infty \leq Z \leq +\infty$



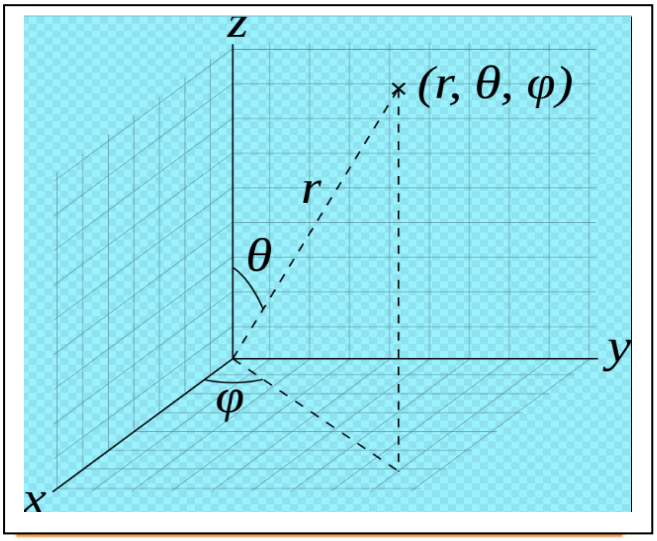
2-Spherical polar Coordinates

Point in space determined (r) the radius , Θ the colatitude , and ϕ the azimuth .

$0 \leq r \leq +\infty$

$0 \leq \Theta \leq \pi$

$0 \leq \phi \leq 2\pi$



$X = r \sin\Theta \cos\phi$

$Y = r \sin\Theta \sin\phi$

$Z = r \cos\Theta$

$\partial t = r^2 \sin\Theta \, \partial r \, \partial\Theta \, \partial\phi$

Example 1: Equation to change from Cartesian to spherical ?

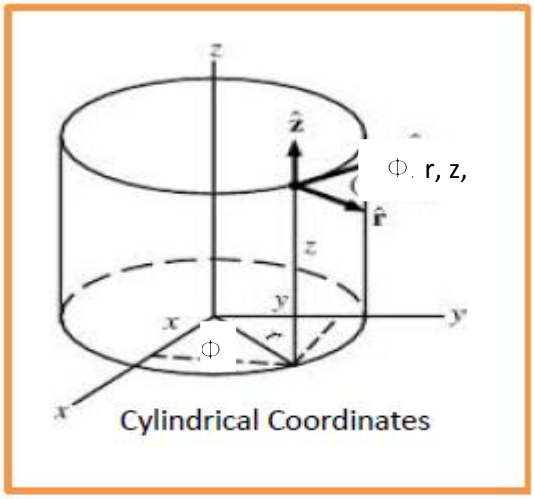
$x = r \sin\theta \cos\phi$

$Y = r \sin\theta \sin\phi$

$z = r \cos\theta$

3- Cylindrical Coordinates

Determinate two distance and angle (r, Z, Φ)



$0 \leq r \leq +\infty$

$0 \leq \Phi \leq 2\pi$

$-\infty \leq Z \leq +\infty$

$X = r \cos \Phi$

$Y = r \sin \Phi$

$Z = Z$

$\partial t = r\, \partial r\, \partial \Phi\, \partial Z$

Example 2: Equation to change from Cartesian to cylindrical ?

$X = r \cos \Phi$

$Y = r \sin \Phi$

$Z = Z$