

Hello and welcome students to today's session. We will start with the program 1st and that is

Bachelor of science for 3rd year. Subject is chemistry, semester 5

paper code : CHC-105 and paper title is Physical Chemistry. We're talking about Unit 2 that is quantum

chemistry and the model name is quantization of energy levels, zero point energy.

The module number is 40.

Myself. Mrs Pooja Gadekar from Dnyanprassarak Mandal's College and Research Centre, Assagao Mapusa Goa.

In the outline, what we're having is

The quantized energy levels.

Energy level diagram for hydrogen Atom and summery

Zero point energy

At the end of session in the learning outcomes the students will be able to apply the concept of Quantization energy levels

Know the importance of quantization of energy levels through energy diagram for Hydrogen atom

Zero point energy

In the introduction quantized energy levels.

From quantum mechanics, we know that the solutions to Schrodinger's equation have quantized energy levels. That is

$$H\psi = E\psi$$

Another way to describe a particle's energy is the specific set of allowed values, and it is given by;

$$E_n = \frac{h^2}{8mL^2} n^2$$

E_n is the energy of the particle

h - Planck's constant

m - Particle mass (kg)

L - Length of box (m)

n - The allowed energies are each labelled by an integer n . The lowest possible energy level has $n = 1$ ($n = 1, 2, 3, \dots$)

Because of the wave nature of matter, a confined particle can only have certain energies.

The quantization of energy is the result that a confined particle can have only discrete values of energy.

The number n is the quantum number, and each value of n specifies one energy level of a particle in a box.

The lowest possible energy a particle in a box can have is equal to

$$E_1 = \frac{h^2}{8mL^2}$$

In terms of the lowest possible energy, all other possible energies are given as

$$E_n = n^2 E_1$$

The allowed energies are inversely proportional to both mass m and L^2 . Both m and L must be exceedingly small before energy quantization has any significance.

An atom is more complicated than a simple one-dimensional box, but an electron is “confined” to an atom.

The electron orbits are, in some sense, standing waves, and the energy of the electrons in an atom must be quantized.

A harmonic oscillator and Electromagnetic radiation are other examples. The energy Eigenvalues are

$$E_n = (n + 1/2) \hbar \omega$$

where $n = 0, 1, 2, 3, \dots$

Thus once again the energy levels are quantized. In this case they are evenly spaced by an amount $\Delta E = \hbar \omega$.

Now coming to real example,

The Hydrogen Atom.

Since the electron is bound to the atom by the attractive force of the nucleus, the total energy of the electron is quantized. The expression for the energy is:

$$E_n = \frac{-me^4}{16n^2\epsilon_0^2\hbar^2n^2} \quad \text{where } n = 1, 2, 3, \dots$$

where m is the mass of the electron, e is the magnitude of the electronic charge, n is a quantum number, \hbar is Planck's constant.

The above formula is applicable to any one-electron atom or ion. We can construct an energy level diagram for the allowed energy values.

ENERGY LEVEL DIAGRAM:

The energy depends only on the quantum number n . Therefore it is also called as principle quantum number.

In this case, $E \propto 1/n^2$, and as n is increased the E becomes less negative with the spacing between the energy levels decreasing in size.

Now coming to this diagram in the figure what we can see on the Y axis is the energy in electronvolts. As such there is no X axis but we can see these rows like horizontal lines, which can be considered as a ladder. Now between $n = 1$ and $n=2$ we can observe that there is a gap. This gap is bigger initially, but as

the value of n goes on, increasing the spacing between the energy levels goes on decreasing up to where n becomes infinity.

And similarly, if we come on the Y axis where energy is seen, what we observe is as n values are increasing, the energy value that is the negative sign goes on decreasing such that once it reaches 0 where n is infinity, the particle becomes free.

As I've told you in the explanation of this diagram, the average distance between the nucleus and the electron increases as the energy or the value of n increases. Thus energy must be supplied to pull the electron away from the nucleus.

The lowest energy associated with $n=1$ is $E_1 = -13.6 \text{ eV}$. If all the constants which appear in the expression for E_n are represented by a constant K then,

$$E_n = -K/n^2$$

$$\text{i.e. } E_n = -13.6 \text{ eV}/n^2$$

The minus sign indicates that the electron is bound to the nucleus.

The electron can 'jump' between any two allowed levels n_1 and n_2 by absorbing/emitting radiation w.r.t. Einstein's frequency relation:

$$E = h \nu$$

$$\nu = \frac{E_{n2} - E_{n1}}{h}$$

When the electron is in a quantum level other than the lowest level (with $n = 1$) the electron is said to be in an excited state.

In the summary.

The energies are quantized.

That means only certain energies are allowed, while all others will be forbidden due to the wave like properties of matter.

The second point is the ground state is the most stable one.

That implies quantum systems seek the lowest possible energy state.

3rd Quantum Systems emit or absorb discrete spectrum of light that is only those photons whose frequencies match with the energy intervals between the allowed energy levels, can be emitted or absorbed, while all others will be rejected.

Moving on to zero point energy.

It is the lowest possible energy that a quantum mechanical system may have. Unlike in classical mechanics, quantum systems constantly fluctuate in their lowest energy. States as described by Heisenberg's Uncertainty principle.

From the energy expression:

$$E = \frac{n^2 h^2}{8mL^2}$$

The lowest value of the quantum number, $n=0$ is not allowed because it makes $\psi=0$. therefore ' n ' should be the minimum one.

$$E_0 = \frac{h^2}{8mL^2}$$

Thus proving that the particle is continuously moving between 0 and L and not resting even at absolute zero temperature.

These are few of my references.

Thank you.