

Quadrant II – Transcript and Related Materials

Programme: Third Year Bachelor of Science

Subject: Chemistry

Paper Code: CHC105

Paper Title: Physical Chemistry

Unit: Unit 2 – Quantum Chemistry I

Module Name: Schrodinger equation and its application: Degeneracy

Module No: 39

Name of the Presenter: Dr. Celia Braganza

Glossary of terms/words:

Degenerate: A quantum state is degenerate when there is more than one wave function for a given energy.

Degeneracy: Degeneracy results from particular properties of the potential energy function that describes the system.

Notes

Analysis of the Schrödinger wave equation in 3D introduces three quantum numbers that quantize the energy.

A quantum state is degenerate when there is more than one wave function for a given energy.

The number of independent wave functions associated with the given energy level is called its DEGENERACY

Concept of Degeneracy

When the sides of the 3D box are equal $a=b=c$

Energy of the particle in 3D box is

$$E = \frac{h^2}{8m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

$$a=b=c=1$$

$$E = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

Quantum Number States

n=1 111

**n= 2 211 121 112
 221 122 212
 222**

n= 3 311 131 113

Energy of the states

$$\Psi_{111}$$

n=1 states $n_x, n_y, n_z = (111)$

$$E = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

$$E = \frac{h^2}{8ma^2} (1^2 + 1^2 + 1^2)$$

$$E = \frac{h^2}{8ma^2} (1 + 1 + 1)$$

$$E = \frac{3h^2}{8ma^2}$$

Since there is only one state with this energy value, it is called Non degenerate state.

$$\Psi_{211}$$

$n=2$ state $n_x, n_y, n_z = (211)$

$$E = \frac{h^2}{8ma^2} (2^2 + 1^2 + 1^2)$$

$$E = \frac{6h^2}{8ma^2} \quad [\Psi_{211} \Psi_{121} \Psi_{112}]$$

Similarly other states 121 and 112 will have the same energy. Hence will be called Degenerate

Since there are THREE states with same energy, this state is Triply degenerate.

$$\Psi_{221}$$

$n=2$ state $n_x, n_y, n_z = (221)$

$$E = \frac{h^2}{8ma^2} (2^2 + 2^2 + 1^2)$$

$$E = \frac{9h^2}{8ma^2} \quad [\Psi_{221} \Psi_{122} \Psi_{212}]$$

Similarly other states 122 and 212 will have the same energy. Hence will be called Degenerate

Since there are THREE states with same energy Triply degenerate.

$$\Psi_{222}$$

$n=2$ state $n_x, n_y, n_z = (222)$

$$E = \frac{h^2}{8ma^2} (2^2 + 2^2 + 2^2)$$

$$E = \frac{12h^2}{8ma^2}$$

Since there is only one state with this energy value, it is called Non degenerate state.

$n=3$ state $n_x, n_y, n_z = (311)$

$$E = \frac{h^2}{8ma^2} (3^2 + 1^2 + 1^2)$$

$$E = \frac{11h^2}{8ma^2} \quad [\Psi_{311} \Psi_{131} \Psi_{113}]$$

Similarly other states 113 and 131 will have the same energy. Hence will be called Degenerate

Since there are Three states with same energy, this state is Triply degenerate.

