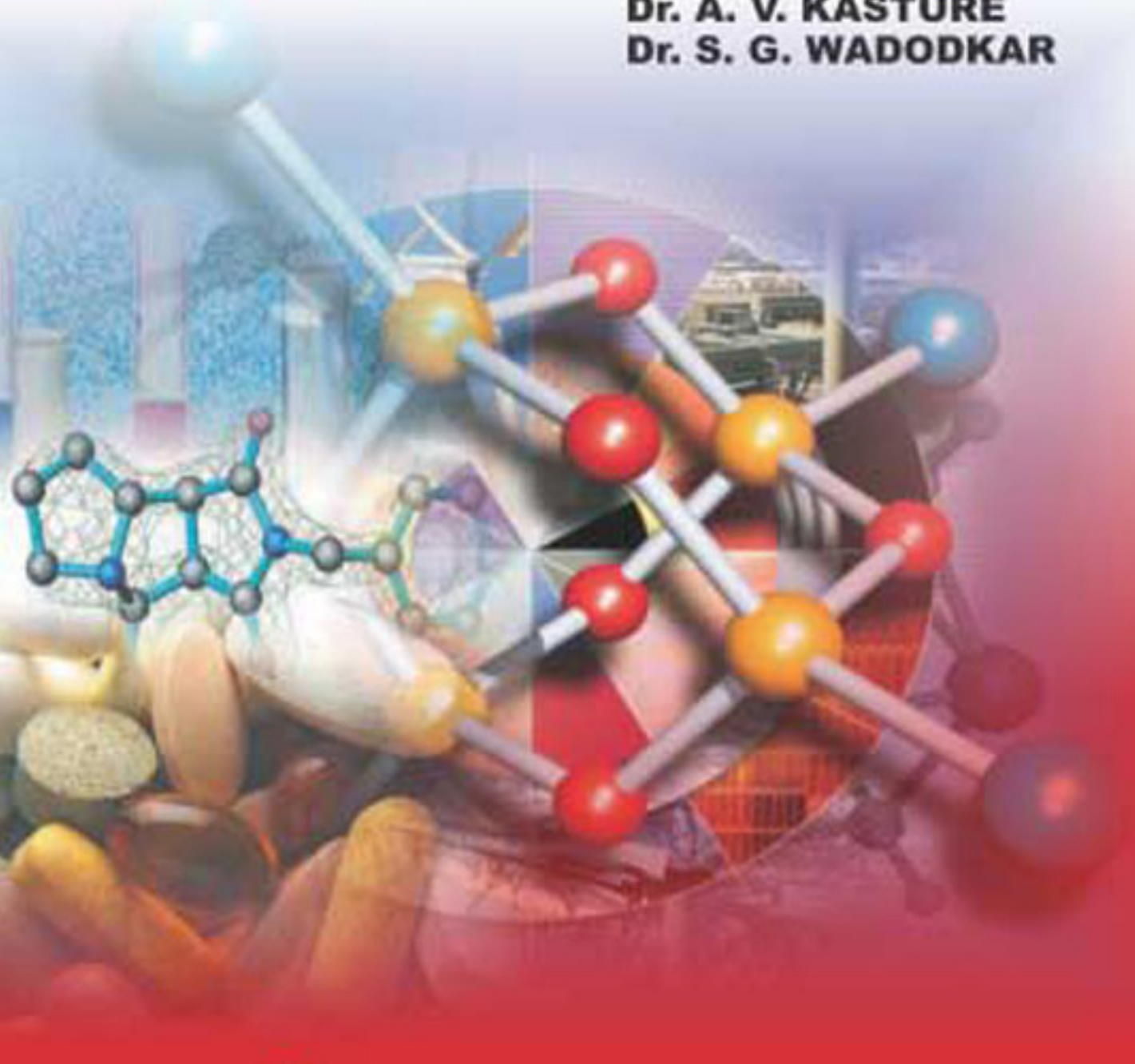


Pharmaceutical Inorganic Chemistry

Dr. A. V. KASTURE
Dr. S. G. WADODKAR



NIRALI PRAKASHAN

A BOOK OF

PHARMACEUTICAL INORGANIC CHEMISTRY

For

First Year B. Pharm. Course

Dr. A. V. Kasture

Former Professor of Pharmaceutical Chemistry
Department of Pharmaceutical Sciences
Nagpur University, NAGPUR - 440 010

Late Dr. S. G. Wadodkar

Former Reader in Pharmaceutical Chemistry
Department of Pharmaceutical Sciences
Nagpur University, NAGPUR - 440 010

Price ₹ 140.00

 **NIRALI**TM
PRAKASHAN
ADVANCEMENT OF KNOWLEDGE

N1622

Thirteenth Edition : January 2018© : **Authors**

The text of this publication, or any part thereof, should not be reproduced or transmitted in any form or stored in any computer storage system or device for distribution including photocopy, recording, taping or information retrieval system or reproduced on any disc, tape, perforated media or other information storage device etc., without the written permission of Authors with whom the rights are reserved. Breach of this condition is liable for legal action.

Every effort has been made to avoid errors or omissions in this publication. In spite of this, errors may have crept in. Any mistake, error or discrepancy so noted and shall be brought to our notice shall be taken care of in the next edition. It is notified that neither the publisher nor the authors or seller shall be responsible for any damage or loss of action to any one, of any kind, in any manner, therefrom.

Published By :**NIRALI PRAKASHAN**

Abhyudaya Pragati, 1312, Shivaji Nagar
Off J.M. Road, PUNE – 411005
Tel - (020) 25512336/37/39, Fax - (020) 25511379
Email : niralipune@pragationline.com

(-Ve)**Printed By :****SHIVANI PRINTERS**

Shop No. 7, 8, 9 Kinara Sahakari Gruh Sanstha
1311, Kasbapeth, Pune – 411011
Phone (020) 24577245

DISTRIBUTION CENTRES**PUNE**

Nirali Prakashan : 119, Budhwar Peth, Jogeshwari Mandir Lane, Pune 411002, Maharashtra
Tel : (020) 2445 2044, 66022708, Fax : (020) 2445 1538

Email : bookorder@pragationline.com, niralilocal@pragationline.com

Nirali Prakashan : S. No. 28/27, Dhyari, Near Pari Company, Pune 411041

Tel : (020) 24690204 Fax : (020) 24690316

Email : dhyari@pragationline.com, bookorder@pragationline.com

MUMBAI

Nirali Prakashan : 385, S.V.P. Road, Rasdhara Co-op. Hsg. Society Ltd.,
Girgaum, Mumbai 400004, Maharashtra
Tel : (022) 2385 6339 / 2386 9976, Fax : (022) 2386 9976

Email : niralimumbai@pragationline.com

DISTRIBUTION BRANCHES**JALGAON**

Nirali Prakashan : 34, V. V. Golani Market, Navi Peth, Jalgaon 425001,
Maharashtra, Tel : (0257) 222 0395, Mob : 94234 91860

KOLHAPUR

Nirali Prakashan : New Mahadvar Road, Kedar Plaza, 1st Floor Opp. IDBI Bank
Kolhapur 416 012, Maharashtra. Mob : 9850046155

NAGPUR

Pratibha Book Distributors : Above Maratha Mandir, Shop No. 3, First Floor,
Rani Jhanshi Square, Sitabuldi, Nagpur 440012, Maharashtra
Tel : (0712) 254 7129

DELHI

Nirali Prakashan : 4593/15, Basement, Aggarwal Lane, Ansari Road, Daryaganj
Near Times of India Building, New Delhi 110002
Mob : 08505972553

BENGALURU

Pragati Book House : House No. 1, Sanjeevappa Lane, Avenue Road Cross,
Opp. Rice Church, Bengaluru – 560002.
Tel : (080) 64513344, 64513355, Mob : 9880582331, 9845021552
Email: bharatsavla@yahoo.com

CHENNAI

Pragati Books : 9/1, Montieth Road, Behind Taas Mahal, Egmore,
Chennai 600008 Tamil Nadu, Tel : (044) 6518 3535,
Mob : 94440 01782 / 98450 21552 / 98805 82331,
Email : bharatsavla@yahoo.com

Note: Every possible effort has been made to avoid errors or omissions in this book. In spite this, errors may have crept in. Any type of error or mistake so noted, and shall be brought to our notice, shall be taken care of in the next edition. It is notified that neither the publisher, nor the author or book seller shall be responsible for any damage or loss of action to any one of any kind, in any manner, therefrom. The reader must cross check all the facts and contents with original Government notification or publications.

niralipune@pragationline.com | www.pragationline.com

Also find us on  www.facebook.com/niralibooks

Preface ...

This book on Pharmaceutical Inorganic Chemistry has been written with a view to cover the syllabus framed by Maharashtra University of Health Sciences, Nasik. The new syllabus underwent changes more than once. This resulted in some delay in presentation of this book.

Though number of standard textbooks are available on inorganic chemistry, there are only few books which deal with the pharmaceutical aspect. The inorganic compounds referred in Pharmacopoeia of India and those which are used in Pharmaceutical industry need more discussion from teaching point of view. These are some of the points that prompted us to write and present this book.

The book has been divided into various chapters as per the syllabus of Maharashtra University of Health Sciences, Nasik. Not only the compounds mentioned therein are covered, but some more related compounds have been discussed to give comprehensive coverage. It is our endeavor to present concise information about the various topics.

We hope this book will prove useful to the B. Pharm and Diploma in Pharmacy students. We will be glad to receive comments and suggestions from readers to improve upon this edition.

We express our sincere thanks to Mr. Dineshbhai Furia, publisher of Nirali Prakashan, Pune for helping us to bring out this book in a short period.

A. V. Kasture

S.G. Wadodkar

Syllabus ...

F. Y. B. PHARM. SCIENCE PHARMACEUTICAL INORGANIC CHEMISTRY (THEORY)

1. Atomic structure - Bohr's model, Wave nature of electron, Shrodinger wave equation, Quantum numbers and geometry of orbital. (6) Hrs.
 2. Theoretical Principles of qualitative analysis, Separation of cations and anions (4) Hrs.
 3. Mole concept, Standard solutions and solubility - Stoichiometry. (4) Hrs.
 4. Sources of contamination in pharmaceuticals and methods of control them, Various limit tests including chloride, Sulfate, Arsenic lead, Iron, Heavy metals.
Limits of insoluble matter, non-volatile matter, residue on ignition and ash values.
Qualitative test for alkali and alkaline earth metals. (8) Hrs.
 5. Introduction to the study or monographs of official compounds in I.P. (2) Hrs.
 6. Water : Detailed study from the view point of water as Universal Pharmaceutical Vehicle. (2) Hrs.
 7. Major extra and intra cellular electrolytes and ions, Chloride, Phosphate, Bicarbonate, Sodium, Potassium, Calcium, Magnesium, their physiological properties and uses, Infusion fluids, Electrolytes use for replacement therapy like sodium chloride, Potassium chloride, Calcium chloride, Compounds to maintain acid-base balance-sodium acetate, Sodium lactate and ammonium chloride. Regulatory mechanisms in body. (6) Hrs.
 8. Essential and trace elements : Iron, Copper, Zinc, Manganese Selenium sulphur and Iodine, Their official compounds and uses and their role in compounds - Ferrous fumarate, Ferrous gluconate, ferrous sulphate, Ferric ammonium citrate, Potassium iodide. (7) Hrs.
 9. Gastrointestinal agents and acids - Sodium bicarbonate, Aluminum hydroxide, Magnesium carbonate, Magnesium hydroxide. Protective and adsorbents - bismuth subcarbonate, Kaolin Cathartics - Magnesium sulphate. (6) Hrs.
 10. Tropical agents, protective - Talc, Zinc oxide, Silicon polymers, Antimicrobials and Astringents - Hydrogen peroxide, Potassium Permanganate, Iodine solutions, Sulphur boric acid, Alum. (8) Hrs.
 11. (a) Dental Products - Sodium fluoride, Sodium phosphate, CaCO_3 , Ca_2HPO_4 Dentifrices (2) Hrs.
(2) Hrs.
(b) Official Gases (1) Hrs.
 12. Expectorants, Emetics and their official compounds - Ammonium chloride, KI, Sodium chloride Copper Sulphate and Antitussives. (1) Hrs.
 13. Antidotes - Sodium nitrite, Sodium thiosulphate (1) Hrs.
 14. Radio - Opaque contrast media - barium sulfate. (1) Hrs.
 15. Buffers - Acids and Bases, Buffer capacity, buffer action and buffer index and buffer used in pharmaceuticals. (2) Hrs.
 16. Radiopharmaceuticals - Uses of radioisotopes in health sciences, general discussion of possible applications, Radiation Dosimetry, Radioisotopes as therapeutic and diagnostic aids, method of placement, Radioisotopes used in medicinal and related applications. Iodine-131, Phosphorus-32, Chromium-51, Cobalt-60, Iron-59.
Quality Control of Radiopharmaceuticals.
-

Contents ...

1. Atomic Structure	1.1 – 1.16
2. Principles of Qualitative Analysis	2.1 – 2.14
3. Solutions and Solubility Pharmaceuticals	3.1 – 3.4
4. Control of Purity and Limit Tests of Pharmaceuticals	4.1 – 4.14
5. Monograph of Official Compounds	5.1 – 5.6
6. Water	6.1 – 6.8
7. Major Intra and Extra - Cellular Electrolytes and Ions	7.1 – 7.18
8. Essential and Trace Elements	8.1 – 8.14
9. Gastrointestinal Agents	9.1 – 9.14
10. Topical Agents	10.1 – 10.28
11. (A) Dental Products	11.A-1 – 11.A-4
11. (B) Official Gases	11.B-1 – 11.B-6
12. Expectorants, Emetics and Respiratory Stimulants	12.1 – 12.6
13. Antidotes in Poisoning	13.1 – 13.4
14. Radio - Opaque Contrast Media	14.1 – 14.2
15. Acids, Bases and Buffers	15.1 – 15.8
16. Radio - Pharmaceuticals	16.1 – 16.8
References	R.1 – R.1

ATOMIC STRUCTURE

INTRODUCTION

Ancient Philosophers considered that matter is made up of extremely small particles which are invisible. Now, we know that the fundamental unit of all matter is the atom. The physical and chemical properties of matter or substance are determined by its elemental composition and elements are composed of atoms and their isotopes. Thus, it would be logical to understand the structure of atoms in order to explain and or predict the properties of matter, molecules or atoms.

STRUCTURE OF ATOM (Development)

In the year 1803, John Dalton put forth the simplest theory regarding the structure of an atom, to explain the laws of chemical combination. The assumptions of his theory for structure of atom are as follows :

- (1) Matter is made of very tiny particles called as *atoms* which can be divided further chemically.
- (2) Atoms of same elements are identical in all respect, but differ from the atoms of another element.
- (3) Atoms cannot be created or destroyed.
- (4) An atom of an element has a fixed mass and atoms of different elements can combine in simple whole numbers to form compound atom which is now known as *molecule*.

In the year 1811, Avogadro suggested some modifications of theory of atomic structure proposed by Dalton. He described atom as the smaller particle of an element, which cannot be divided further, but can take part in all chemical changes.

In the year 1898, J. J. Thomson proposed that atoms consist of a positively charged matter in which negatively charged matter is embedded. So for the first time, it was suggested that atoms consist of positively and negatively charged particles (now known as *electrons*).

Rutherford, in the year 1911, performed some excellent experiments, in which he bombarded a thin gold foil with high speed α -particles from radioactive element and used

movable zinc sulphide screen for detecting them. His observations and interpretations were as follows :

- (1) Most of the α -particles pass through the gold foil, indicating that there is lot of empty space inside the atom.
- (2) Few of the α -particles were deflected from their original path through wide angles, indicating that the centre of the atom must be positively charged and is called as *nucleus*.
- (3) Few particles were deflected through 90° and one α -particle out of twenty thousand was completely deflected through 180° , indicating that the nucleus is rigid and thus α -particle is recoiled.

Based on his experiment, Rutherford suggested the following atomic model :

- (1) The central part of the atom contains protons, which carries a unit positive charge and unit mass.
- (2) An atom contains electrons which carries unit negative charge but has a negligible mass.
- (3) As the atom is electrically neutral, it must have same number of protons and electrons.
- (4) In an atom, all the mass and the positive charge is concentrated in the central part known as nucleus.
- (5) The electrons present in the atom are revolving round the nucleus in a definite path called as *orbital*.

Thus, the Rutherford's model of an atom is similar to our solar system in which the planets are revolving around the sun. Later he observed that only on the basis of protons and electrons, the atomic masses of different elements could not be explained. After further experiments, he proposed that some particles which are neutral and have mass, must be a part of an atom.

In the year 1936, Chadwick discovered another particle which was neutral with a mass and named as '*neutrons*'. Thus, the nucleus of the atoms contains protons and neutrons, exception is only hydrogen in which the nucleus contains only one proton.

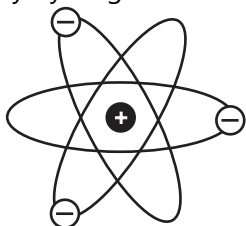


Fig. 1.1 : Rutherford model of atom

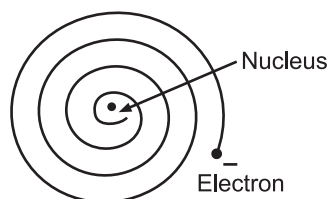


Fig. 1.2 : Orbiting electron radiating energy should be spiral into the nucleus

Rutherford's assumption regarding orbiting electrons around nucleus could not be accepted. Electromagnetic theory states that if a charged particle accelerates around another oppositely charged particle, then the former particle will radiate energy. If electrons radiate energy its speed has to decrease and hence it should go into a spiral motion and ultimately fall into the nucleus. If this happens, then the atom will be unstable. This was the drawback of Rutherford's model of an atom.

Niels Bohr in 1913 proposed another model for atoms which explained not only the drawback of Rutherford's model, but also the emission spectrum of hydrogen. The Bohr model was based on Planck's quantum theory and the model for an atom was thereby proposed. Some of the important assumptions are :

- (1) Centre part of an atom is dense, positively charged and also at rest; it is referred to as nucleus.
- (2) The electrons travel around the nucleus in a specific circular path called *orbit*. There is an electrostatic force of attraction between the nucleus and the electrons, which is balanced by the centrifugal force and thus an electron does not fall into the nucleus and the atom remains stable. The electron in each orbit is associated with definite energy and they are at a fixed distance from the nucleus. They are designated as 1, 2, 3, 4 and K, L, M, N etc.
- (3) In these specific orbitals, the electrons do not radiate energy. The energy of electrons in each orbit remains fixed and are referred as energy levels.
- (4) Electrons in the energy level nearest to nucleus have lower energy, while electrons with higher energy levels are at greater distance from the nucleus.
- (5) An electron can move from one energy level to another level by quantum and not continuously. When the electron is in the orbit of lowest energy level, it is said to be in '*Ground State*', but when the energy is supplied to the electron, it absorbs one quantum or photon of energy and jumps in higher energy level. Such electrons are said to be in '*Excited state*'. The difference between the lower energy level and higher energy level is the amount of quantum or photon of energy absorbed or emitted.

$$E_1 - E_2 = h\nu \quad \dots (i)$$

where, ν is the frequency of energy absorbed or emitted and h is Planck's constant.

- (6) The angular moments of an electron (mvr) moving in the orbit around the nucleus is an integral multiple of Planck's constant divided by 2π .

$$\text{Angular moments} = mvr = n(h/2\pi) \quad \dots (ii)$$

where,

m = Mass of electron

v = Velocity of electron

r = Radius of the orbit

n = 1, 2, 3 etc. and

h = Planck's constant

If the values of n taken as 1, 2, 3, etc., we can get the respective angular moments,

$$\frac{h}{2\pi}, \frac{2h}{2\pi}, \frac{3h}{2\pi} \text{ etc.}$$

As there are no fractional values of $h/2\pi$, the angular moments are said to be quantized. The integer n can be used to designate orbit and corresponding energy levels. 'n' is called the atoms '*Principal quantum number*' .

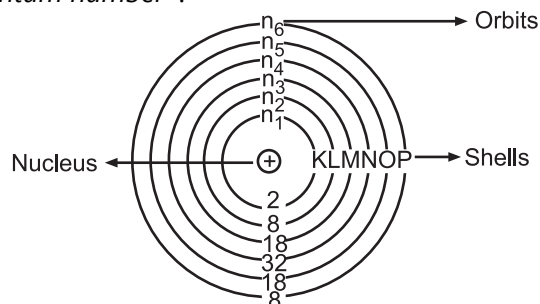


Fig. 1.3 : Diagrammatic Bohr's energy level

Bohr has calculated the radius of each orbit of hydrogen atom, the energy associated with each orbit and the wavelength of radiation associated in transitions between orbits.

Modern concept of Atom :

Now, it is understood that the atom is not the ultimate particle of matter, but it is composed of some fundamental particles known as sub-atomic particles. These sub-atomic particles are electrons, protons and neutrons, thus atom has its own structure.

Electrons :

The atoms are composed of central nucleus surrounded by electrons discovered by J. J. Thomson in the year 1998. The symbol for electron is 'e'. It carries a unit negative charge. Its mass is negligible (0.000555 amu). Its location is extranuclear.

Protons :

The sub-atomic particle proton was discovered by Rutherford in the year 1911. It is within the nucleus of an atom and carries a unit positive charge, its mass is practically equal to the mass of one hydrogen atom, and exact mass is 1.007825 amu. But for all practical purposes, it is taken as 1 amu. It is represented by symbol P or 1H^+ .

As the atom is electrically neutral, the number of electrons and protons must be equal in an atom.

Neutrons :

The presence of this sub-atomic particles was discovered by Chadwick in the year 1932 and is represented by symbol N. It is situated inside the nucleus and is electrically neutral. Its mass is nearly equal to that of proton and exact mass is 1.008665 amu.

Every stable nucleus contains a certain number of protons, which is equal to the number of electrons in a neutral atom, and particular number of neutrons. The atomic mass of the element is the same of the masses of proton and neutron and atomic number related to number of protons.

QUANTUM THEORY OF RADIATION

The wave theory of transmission of radiant energy imply that energy is emitted (or absorbed) in continuous waves. Max Planck studied the spectral line from hot bodies and proposed that these bodies radiate energy not as continuous wave, but small units of waves. The unit wave or pulse of energy is called as '*Quantum*'. Nobel Laureate, Albert Einstein showed that high radiations emitted by excited atoms or molecules, also transmitted as particles or quanta of energy. The light quanta are called as '*Photons*'.

From the quantum theory of electromagnetic radiation, it can be stated that :

(a) When atoms or molecules emit or absorb radiant energy, they do it in units called as 'quanta' or 'photons'. Therefore, the light radiations obtained from excited atoms consist of a stream of photons and not continuous waves.



Fig. 1.4 : Continuous wave



Fig. 1.5 : Quanta of Photons

(b) The energy E of a quantum is given by the relation

$$E = h \nu \quad \dots \text{(iii)}$$

where, ν is the frequency of emitted radiation and h is Planck's constant

$$= 6.62 \times 10^{-27} \text{ erg sec.}$$

$$= 6.62 \times 10^{-34} \text{ J sec.}$$

Velocity of radiation c , is given by the equation

$$c = \lambda \nu \quad \dots \text{(iv)}$$

Substituting the value of ν from (iv) in equation (iii), we can write,

$$E = hc/\lambda$$

Therefore, E is directly proportional to ν (directly proportional to frequency of radiation) and its wavelength.

(c) As only whole number of quanta exist, the atom or molecule can emit or absorb one quantum of energy ($h\nu$) or any whole multiple of this unit.

This quantum theory of electromagnetic radiation helps in explaining atomic structure, atomic spectra and photoelectric effects.

WAVE MECHANICAL THEORY

As per the Bohr's concept of structure of atom, the electrons move in closed orbits around the nucleus. This was later superseded by another theory, suggesting that the electron's motion is of a complex nature and can only be described by its wave properties and probabilities. This theory also applies to radiations and is known as *wave mechanical theory*.

Planck contended that light has dual characteristics i.e. that of wave as well as a particle. Thus, distinction between wave and particle becomes very hazy. Louis deBroglie suggested that the dual characteristics i.e. that of a wave and a particle, is not only confined to

radiations, but can very well be extended to matter. Thus, matter can have dual characteristics of a wave and a particle. The electrons, protons and even atoms when in motion, possess wave properties and are associated with other characteristics of waves such as wavelength, frequency, wave amplitude, etc. The quantum mechanics takes into account the dual characteristics i.e. as particle and wave nature, of the matter.

DeBroglie's Equation :

It states that the *momentum of particle in motion is inversely proportional to the wavelength, where 'h' (Planck's constant) being the constant of proportionality.*

After considering the quantum theory by Planck and Einstein's Theory of Relativity, deBroglie derived relationship between the magnitude of the wavelength associated with mass 'm' of a moving body and its velocity.

According to quantum theory, the photon energy 'E' is expressed as

$$E = hv \quad \dots (i)$$

where, h is Planck's constant and v the frequency of radiation.

The energy associated with photon of mass 'm' can be given by applying Einstein mass - energy relationship and is expressed as

$$E = mc^2 \quad \dots (ii)$$

where, c is the velocity of radiation,

By comparing equations (i) and (ii), we get

$$mc^2 = hv = hc$$

$$\text{or} \quad mc = h/\lambda \quad \dots (iii)$$

Equation (iii) is called de Broglie's equation

Thus, $\text{Mass} \times \text{Velocity} = h/\text{wavelength}$

Momentum (P) $\propto h / \text{wavelength}$

or momentum $\propto 1/\text{wavelength}$

The de Broglie's equation is true for all particles. In small particles like electrons, the wave-like aspect is of significance.

That the moving electrons have momentum of definite wavelength associated with them, was suggested by Broglie, which was later on proved in 1927 by Devisson and Germer by demonstrating that a beam of electron can also be defracted by crystals, e.g. light or X-ray beam.

HEISENBERG'S UNCERTAINTY PRINCIPLE

In the year 1927, Werner Heisenberg developed the uncertainty principle, which is an important aspect of wave mechanics. It discusses the relationship between a pair of conjugate properties of substance. These properties are independent. Considering the uncertainty principle, it is impossible to know simultaneously, the conjugate properties, accurately. For example, position and moments of a particle are interdependent and thus are

conjugate properties. If the momentum of a particle is measured accurately, the position of the particle becomes correspondingly less precise; and if the position is determined precisely, then the momentum becomes less accurately known. Therefore, both the position and momentum of a particle cannot be determined precisely and thus the uncertainty. Heisenberg's principle relates the uncertainty in measurement of position, Δx and uncertainty of determination of momentum, Δp (or Δmv) and is expressed as $\Delta x \Delta p > h/2\pi$ or $\Delta x \Delta mv > h/2\pi$.

The uncertainty product is negligible in case of large bodies, but in case of small bodies, like electrons, the uncertainty values are very large and thus cannot be neglected while considering the structure of atom. As the size of the electron is very small, it is rather impossible to know the position and velocity of any one electron. Therefore, we say the probability, or relative change, of finding an electron with a probable velocity is rare. The Bohr's concept of electrons revolving around the nucleus in the orbit, is now replaced by the probability approach.

SCHRODINGER WAVE EQUATION

Before Schrodinger developed the equation, it was difficult to calculate the probability of finding the electron at various points in the atom. The equation derived by Schrodinger using the concept of electron as standing wave around the nucleus, provided the real meaning to probability approach. The equation is known as Schrodinger wave equation.

$$\psi = A \sin 2\pi x/\lambda$$

where,

ψ (Si) = mathematical function to represent the amplitude of wave (wave function) x , displacement, in a given direction

λ = wavelength and

A = constant

By differentiating above equation twice, with respect to x , we get,

$$\frac{d\psi}{dx} = A \frac{2\pi}{\lambda} \cos 2\pi \frac{x}{\lambda} \quad \dots (i)$$

and

$$\frac{d^2\psi}{dx^2} = \frac{4\pi^2}{\lambda^2} \sin 2\pi \frac{x}{\lambda} \quad \dots (ii)$$

but as we know, $A \sin 2\pi \frac{x}{\lambda} = \psi$

$$\frac{d^2\psi}{dx^2} = \frac{4\pi^2}{\lambda^2} \psi \quad \dots (iii)$$

The kinetic energy (K.E.) of a particle of mass m and velocity v is given by the relation,

$$\text{K.E.} = \frac{1}{2} mv^2 = \frac{1}{2} \frac{m^2 v^2}{m} \quad \dots (iv)$$

and as per Broglie's equation,

$$\lambda = h/mv$$

Therefore

$$\lambda^2 = h^2/m^2v^2$$

or

$$m^2v^2 = h^2/\lambda^2$$

By substituting the values of m^2v^2 , we get

$$\text{K.E.} = \frac{1}{2} \times h^2 / m\lambda^2 \quad \dots \text{(v)}$$

From equation (iii), we have,

$$\lambda^2 = \frac{4\pi^2 \psi}{\frac{d^2\psi}{dx^2}} \quad \dots \text{(vi)}$$

Now, by substituting the value of λ^2 in equation (v)

$$\begin{aligned} \text{K.E.} &= \frac{1}{2m} \cdot \frac{h^2}{4\pi^2\psi} \cdot \frac{d^2\psi}{dx^2} \\ &= \frac{h^2}{8\pi^2m\psi} \cdot \frac{d^2\psi}{dx^2} \end{aligned}$$

where,

E = Total energy of particle

K.E. = Kinetic energy and

P.E. = Potential energy

∴

$$\text{K. E.} = E - \text{P.E.}$$

$$E - \text{P.E.} = \frac{h^2}{8\pi^2m\psi} \cdot \frac{d^2\psi}{dx^2}$$

or

$$\frac{d^2\psi}{dx^2} = -\frac{8\pi^2m}{h^2} (E - \text{P.E.}) \psi$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - \text{P.E.}) \psi = 0$$

This is the Schrodinger equation for one dimension. It is generalised for a particle whose motion is described by the three space co-ordinates x, y and z.

Therefore,

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2m}{h^2} (E - \text{P.E.}) \psi = 0$$

The above equation is known as 'Schrodinger wave equation'. In this equation, the first three terms on the left side are represented by $\Delta^2\psi$ (del square Si)

$$\Delta^2\psi + (E - \text{P.E.}) \psi = 0$$

In the above equation, Δ^2 is known as 'Laplacian operator'.

Using the wave equation, where ψ represents the amplitude of wave, and with modification to meet the requirement of uncertainty principle, one can give a probability of finding an electron within an extremely small volume around a point, which is proportional to the square of the function, ψ^2 at the point.

Wave equation has further given the concept of 'charged cloud' and 'orbitals'. On solving wave equation for an electron, gives a three dimensional arrangement where the electron can probably, i.e., the regions where there is maximum possibility of electron is known as cloud of negative charge. The 'Orbitals' can be described as a three dimensional region where there is maximum possibility of finding an electron with a particular energy.

ELECTRON DISTRIBUTION IN SHELLS OR ORBITS

There are certain rules which govern the distribution of electrons in extra nuclear part of the atom. In the year 1921, Bohr - Bury framed the following rules :

- (1) The maximum number of electrons that can be present in each orbit is $2 \times n^2$, where n is the number of orbit of principal quantum number, starting from the nucleus outward. Thus, the K-shell or orbit n, will contain $2 \times 1^2 = 2$, L shell or next orbit (2) will contain $2 \times 2^2 = 8$, M shell or next higher orbit (3) will contain $2 \times 3^2 = 18$ and N shell or next higher orbit (4) will contain $2 \times 4^2 = 32$ electrons and so on.
- (2) The outermost orbit can contain maximum number of 8 electrons and the earlier to the outermost orbit (penultimate shell) can contain maximum of 18 electrons.
- (3) It is not necessary for an orbit to be completed before another commences to be formed. Actually, when outer orbit contains 8 electrons, the next higher begins.
- (4) The outermost orbit and the inner orbit next to it, cannot have more than 2 and 9 electrons respectively, till all orbits inner to them are completed as per rule (1).

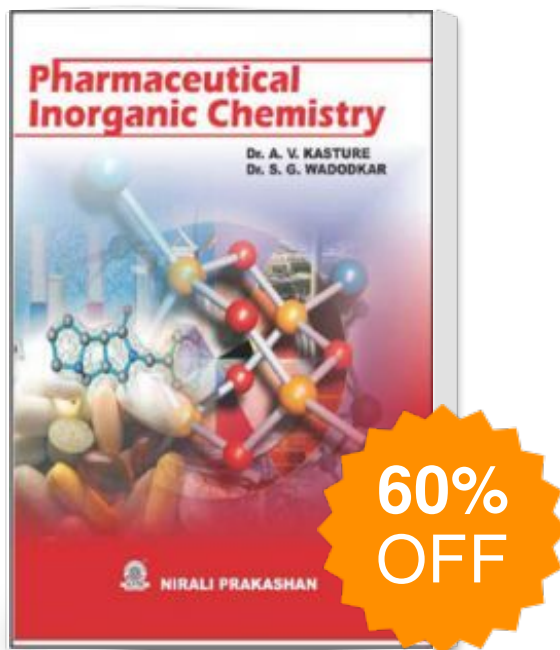
ENERGY LEVELS AND SUB - ENERGY LEVELS

A definite amount of energy is associated with Bohr's stationary orbits or shells. These energy levels are designated by the numbers 1, 2, 3, 4, 5, 6 or denoted by K, L, M, N, O, P etc. The order of increasing energy level is given by 'n' (principal quantum number), that is $K < L < M < N < O < P$ or $1 < 2 < 3 < 4 < 5 < 6$ etc.

With the detailed study of individual spectra, it was observed that there is a presence of close grouping of several spectral lines. Similarly, the electron energy level can be further divided into several levels, or main energy level and sub-energy levels, or sub-shells. The number of sub-energy level is equal to the order of the main energy level from the nucleus. Letters s, p, d, f,...etc. are designated as sub-energy levels or sub-shells and the number can be obtained from its principal quantum number (n). Thus, energy level k (n = 1) will have 1s sub-energy level; L (n = 2) will have 2s, 2p, M (n = 3) will have 3s, 3p and 3d, and N(n = 4) will have 4s, 4p, 4d and 4f sub-energy levels.

The maximum number of electrons in the sub-energy levels are as follows : s = 2, p = 6, d = 10 and f = 14 and these sub-energy levels are in the following order : s < p < d < f.

Pharmaceutical Inorganic Chemistry



Publisher : Nirali Prakashan

ISBN : 9788185790169

Author : Dr. A. V. Kasture,
Late Dr. S. G. Wadodkar

Type the URL : <http://www.kopykitab.com/product/20061>



Get this eBook