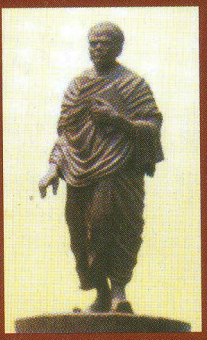
DIRECTORATE OF DISTANCE EDUCATION



SYLLABUS

M.Sc. Course in Chemistry

VIDYASAGAR UNIVERSITY
MIDNAPORE - 721102

VIDYASAGAR UNIVERSITY

Department of Chemistry & Chemical Technology

Syllabus

(M.Sc. Course in Chemistry)

Distribution of Papers and marks

M.Sc. Part-I

Paper	Marks	
	Theoretical	**Practical**
I. (Physical Chemistry)	75	50
II. (Organic Chemistry)	75	50
III (Inorganic Chemistry)	75	50
IV (Industrial Chemistry	75	50*
Total	**300**	**200**

* Industrial = 20, Computer = 20, Industry visit = 10

M.Sc. Part-II (Special #) # Physical/Organic/Inorganic

Theoretical Papers	Marks	Practical Papers	Marks
V	75	Special Practical	150
VI	75		
VII	75	Professional/Project	50
Professional Paper)	♦75		
Total	**300**		**200**

Polymer Science for Physical & Organic Special, Environmental Chemistry for organic Special.

M.Sc. Part-I

Paper-I FM-75

Physical Chemistry (General)

Unit

01. Quantum Mechanics: (15-20 lectures)

The wave-particle duality and the development of Schrödinger equation, interpretation of ψ, postulates of quantum mechanics with necessary explanations, formulation of quantum mechanical operators, angular momentum operators (in cartesian and polar co-ordinates), step-up and step-down operators, commutation relations; the Gedanken experiment to derive an expression for the uncertainty principle; free particle, particle in a box, particle in a ring, particle in a sphere, free electron molecular orbital (FEMO) model; one dimensional harmonic oscillator, rigid rotator (in three dimensions), potential barrier, tunneling, hydrogen atom, concept and shape of orbital, space and spin quantisation; the Aufbau principle and the many electron atom, vector atom model and the spectroscopic states; hydrogen molecular ion and the concept of molecular orbital, hydrogen molecule; homo-and hetero-nuclear diatoms, importance of overlap, hybridization.

Elementary idea of variation and perturbation theorems with some simple applications.

02. Classical and Statistical Thermodynamics, Transport Phenomenon: (15-20 lectures)

Maxwell's relations, thermodynamic equation of state; partial molar quantities, thermodynamics of mixing, activity and fugacity. Nernst Heat theorem, third law of thermodynamics. Thermodynamic probability and entropy. Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Partition functions of diatoms (translational, rotational, vibrational and electronic). Young-Laplace equation, Kelvin equation, surface (interface) thermodynamics. Adsorption, adsorption isotherms (Langmuir and BET

with derivation). Surfactants, micelles, reverse micelles and emulsions and their applications.

Distribution of molecular velocities, principle of equipartition of energy, collision frequency, thermal conductivity, general diffusion expression and Fick's laws general features of transport of matter (diffusion), thermal energy (thermal conductivity) and momentum (viscosity).

03 Electrochemistry (15-20 lectures)

Mean activity co-efficient of electrolytic solutions, Debye-Huckel theory, ion association, precise determination of dissociation constants of weak electrolytes – e.m.f and conductometric methods, the Onsager conductance equation, effect of high electric field and high frequency on ion conductance; polarography, overvoltage, surface tension of electrolytic solutions, polyelectrolytes. Basic principle of cyclic voltametry and coulometry.

04 Chemical Kinetics (15-20 lectures)

Principle of detailed balancing (simple idea only), opposing and consecutive reactions, static, flow and relaxation methods of measurement of reaction rates, flash photolysis. Kinetics of fast reaction, collision theory of reaction rates (detailed), preliminary idea of transition state theory.

Homogeneous and heterogeneous catalysis, autocatalysis, oscillatory reactions (general introductions only), redox reactions, preliminary idea of inner sphere and outer sphere reactions of transition metals.

05 Molecular Structure and Molecular Spectroscopy (15-20 lectures)

Dielectric polarisation, Debye-Langev in equation, dipole moment – determination and applications, intermolecular forces and their contribution to intermolecular potential. General features of molecular spectra, quantum mechanical rigid rotator, pure rotational spectra of linear molecules, non-rigid rotator, expression for centrifugal distortion constant; quantum mechanical harmonic oscillator, vibrational spectra of diatoms,

anharmonicity and molecular dissociation, hot band and overtones, zero point energy and uncertainty; rotational and vibrational Raman spectra – general features and applications, principle of mutual exclusion.

Vibrational structure of electronic spectra. Frank-Condon principle.

Photoionisation of atoms and molecules, electron energy analyzer and photoelectron spectra, molecular orbitals and photoelectron spectra.

Books Recommended :

1. Physical Chemistry : Berry, Rice and Ross.
2. Physical Chemistry : Moore.
3. Physical Chemistry : Atkins
4. Physical Chemistry : Levine
5. Chemical Kinetics : Laidler
6. Kinetics and Mechanism : Frost and Pearson
7. Heat and Thermodynamics : Zemansky and Dittman
8. A Treatise on Heat : Saha and Srivastava
9. Quantum Chemistry : Eyring. Water and Kimbal
10. Quantum Chemistry : Pilar
11. Quantum Chemistry : Levine
12. Electrochemistry : Glasstone
13. Electrochemistry : Bockris and Reddy
14. Molecular Spectroscopy : Banwell
15. Molecular Spectroscopy : Barrow
16. Molecular Spectroscopy : Grabeal
17. Molecular Spectroscopy : Chang.

M.Sc. part-I

(Physical General) Practical

Unit

01 **List of Experiments :**

[1] Determination of the exact concentration of HCI solution of N/10 order by NaOH Conducometorically.

[2] Determination of the exact concentration of oxalic acid solution of N/10 order by NaOH Conducometrically.

[3] Determination of the exact concentration of KCI solution of N/10 order by $AgNO_3$, Conductmetrically.

[4] Determination of exact concentration of KCI solution of N/10 order by $AgNO_3$, Potentiometrically.

[5] Study of the Kinetics of Inversion of Cane sugar by polarimetry.

[6] Study of Kinetics of Iodination of Acetone in presence of Acid. Hence find out the order with respect to iodine or acetone.

[7] Determination of Partition Co-efficient of Benzoic acid between Water & Benzene. Hence show that benzoic acid dimerizes in benzene layer.

[8] Determination of Critical Solution Temperature of Phenol-Water system.

[9] Determination of Solubility Product of PbI_2 and verification of Debye-Huckel limiting law.

[10] Find the absorption maximum of an aqueous $KMnO_4$ solution and verify Beer's Law.

[11] Determination of E of quinhydrone electrode.

[12] Determination of exact concentration of HCI and oxalic acid in their mixture conductometrically.

[13] Determination of composition of copper(II)-ammonia complex analytically.

[14] Determination of dissociation constant of weak acid (acetic acid, benzoic acid) by pH measurement.

At least ten (10) experiments are to be performed by a student of M.Sc. part-I (Physical general) during the laboratory session.

Practical Examination of M.Sc. Part-I Physical general :

Unit 01 :

Physical Chemistry Experiments [Two days (Six hours each day) examination]

Total Marks : 30 (thirty only).

Unit 02 :

Internal Assessment.

Total Marks : 10 (ten only).

Unit 03 :

Viva-voce and Laboratory Note Book (during examination)

Total Marks : 10 (ten only)

M.Sc. Part-I, PAPER – II

ORGANIC CHEMISTRY (GENERAL)

(Every unit consists of 15-20 lectures, Full Marks =75)

Unit

01 **Structure and Reactivity of Organic Molecules :**

Advanced reaction mechanisms, delocalized systems-cyclic and acyclic (M.O.approach). Concept of aromaticity, antiaromaticity and homoaromaticity. Introductory course on pericyclic reactions – electrocyclic reactions, sigmatotropic rearrangements, cycloadditions, Rationalization on the basis of Frontier Orbital Theory, Hammett Equation and applications. Nonclassical carbocations . Advanced treatment of topics of reaction mechanisms included in B.Sc (Hons) syllabus.

02 **Stereochemistry and Conformational Analysis**

Symmetry and molecular chidrality. Stereochemical nomenclature for acyclic and cyclic molecules. Conformation in acyclic and cyclic systems – energy barrier to rotation, potential energy profiles. Conformation and physical properties of 6-membered rings and reactivity in acyclics. Stereochemistry of trivalent carbon.

Prostereoisomerism, Asymmetric synthesis – addition of achiral reagents to chiral ketones and aldehydes. Models for stereochemical control, Cram, Karabatros and Fehlkin models, sterospecific and stereoselective reactions. Molecular rearrangements – generalized treatment of stereochemical features.

03 **Heterocyclic Chemistry and Spectroscopy :**

Monocyclic and bicyclic heterocycles having one or two heteroatoms principles of NMR spectroscopy (elementary ideas). Application of UV IR and NMR in structure elucidation of organic molecules.

04 **Natural Products ; Bioactive Molecules :**

Terpenoids : Isoprene rules, acyclic monoterpenoids such as citral, geraniol, neral, linalool, monocyclic, terpenoids menthol. aterpineol. Alkaloids : phenylethylamine series, coniine, nicotine. Synthesis and reactions of heterocycles : generalized approach.

Isolation, structure elucidation, sydnthesis and biogenesis of representative examples of Proteins and Peptides (elementary ideas), Nucleosides and Nucleotides (elementary ideas).

05 **Synthetic Methodology and Reagents :**

Retrosynthetic analysis, disconnection approach, functional group intercoversions; examples to illustrate disconnection approach to organic synthesis.

Organophosphorous and organosulfer reagents, organoboranes, organosilanes, organostannanes, metal hydrides, Birch reduction, hydroxylation reagents, uses of peracids. Woodward and Prevost hydroxylation. Mitsunobu reaction. Sharpless epoxidation. Bayer-Villiger reaction, Chichibabin reaction and newer methods in organic synthesis. Phase transfer catalysis, reactions on solid supports, Merrifield resin, solid-phase synthesis, template synthesis.

References :

1. Advances in Organic Chemistry, Part A and B, F.A. Carey and R.J. Sundberg.
2. Advances in Organic Chemistry, Jerry March, McGraw Hill.
3. Organic Chemistry. R.T.Morrison and R.W. Boyd. Wiley Eastern.
4. Organic Chemistry. S.H. Pine. McGraw Hill.
5. Fundamentals in Organic Chemistry. T.W.G.Solomons, John Wiley.

M.Sc. Part – I

(Organic Chemistry Practical)

(Two days examination – 6 hours per day, Full Marks = 50)

Unit

01 **(a) Qualitative Analysis of Solid Organic Compounds leading to**

(i) Detection of elements (N.Cl.Br.I.S) : Solubility tests.

(ii) Systematic Analysis to detect the functional groups : alcoholic/ phenolic OII, Carboxylic, alehydes, ketone, ester, nitro, amino, amido, N-substituted amino, imido groups, unsaturation (C=C) aromatic hydrocarbons and halogenated derivatives.

(iii) Preparation of Crystalline derivatives/suitable derivatives to identify the compound.

Students will have to analyse atleast 6 (six) samples including solid compounds during their course work.

Each candidate during the examination shall be assigned one solid sample for analysis during the examination. (20)

(b) Preparation of pure organic compound by single-step or two step procedure. Submission of crystallised produced.

02 **Sessional Work** (15)

To be awarded by the class teacher on the basis performance of the students during the course work. (5)

03 **Viva Voce**

To be jointly conducted by the external and internal examiners during the examination. (10)

M.Sc. Part – I, PAPER – III

INORGANIC CHEMISTRY (GENERAL)

(Every unit consists of 15 – 20 lectures, Full Marks = 75)

Unit

01. Symmetry and Group Theory

Groups and their properties : The concept of groups, Group Multiplication tables and rearrangement theorem, subgroups and classes.

Symmetry elements and operations of molecules and crystal systems. Point groups : molecular and crystallographic, Matrix representation of symmetry operators.

Representation of point groups : Matrix representation of point groups, reducible and irreducible representations, the great Orthogonality theorem (without deriviation) and its corrolaries, construction of character tables in simple cases (C D), reduction of a reducible representation, direct product and its decomposition.

Models of MO and VB theories – application to H H qualitative M.O. theory – energy levels of homo – and hetero – nuclear diatomic molecules of second period elements, equivalence of MO and VB theories, electronic structure of solids – band theory.

02. COORDINATION CHEMISTRY

Crystal Field theory, Adjusted Crystal Field Theory, Distortions (tetragonal and trigonal), crystal field stabilization energy, thermodynamic aspects of crystal field splitting (Variation of ionic radii, lattice-energy, hydration energy), Kinetic aspects of crystal field splitting (labile and inert complexes). Qualitative MO treatment : the electronic structure of the MI (octahedral) and ML_4 (tetrahedral) complexes on the basis of simple symmetry and overlap principles, energy level diagrams. - d transitions in weak field cases, Orgel diagram and electronic spectra of transition metal complexes (d_1 - d_9) effort of substitution, spectro chemical series,

charge transfer spectra. Magnetic properties of free ions and metal complexes – a qualitative approach.

Complex formation in solution : stability constants (overall and stepwise), Irving – Williams order, methods for the determination of complex composition (Job's, mole ratio and slope ratio methods), Bjerrum's half integer method for the decom-position of stability constants, chelate effect and macrocyclic effect.

03. Chemistry of d-block elements

Chemistry of 3d, 4d and 5d transition metals i.e. Ti –Hf, v-Ta, Cr –W, Mn – Re and platinum metals with reference to

(i) Aqueous chemistry, oxidation states, co-ordination number and complexes, redox behaviour.

(ii) Iso-and hetero – polyacids and salts of Mo.W.

(iii) Di nit gen and di oxygen complexes.

(iv) Intramolecular charge transfer : Creutz – Taube ion.

(v) Binary carbonyl complexes : structures and bonding.

(vi) Property, structure and bonding ion, molybdenum blue, tungsten blue, tungsten bronze, ruthenium red, Creiutz – Taube complex, Nb, Ta halide clusters.

Introduction to organometallic chemistry : definition and classification (on basis of ligand type), examples of carbene and carbyne complexes. hapticity, structure and bonding in η^2ethylenic and η^3allylic complexes, fluxional molecules.

Essential elements in Biology (major and trace), beneficial and toxic elements, role of metal ions in biology – metalloproteins and metalloenzymes : transport and storage proteins (Ferritin and Transferrin), dioxygen carrier and storage proteins (haemoglobin and myoglobin), electron transfer proteins : ferredoxin, rubredoxin etc. nitrogen fixation.