TECHNO INDIA UNIVERSITY
WESTBENGAL

EM 4, Sector V, Salt Lake, Kolkata-700091, West Bengal, India
Phone: +91 9836544416/17/18/19, Fax: +91 33 2357 1097

2-Year Master of Science (M.Sc.) Curriculum and Syllabus for Chemistry

Third Semester

Course Code	Course Title	Contact Hrs. / Week			Credit
		L	T	P	
Theory					
TIU-PMA-L201	Career Advancement & Skill Development	2	1	0	3
TIU-PCH-T203	Structure & Spectroscopy-I	3	1	0	3
TIU-PCH-T205	Biological Chemistry	3	1	0	3
TIU-PCH-T207	Specialization Paper-I (P)*	3	1	0	3
TIU-PCH-T211	Specialization Paper-I (O)*				
TIU-PCH-T215	Specialization Paper-I (I)*				
TIU-PCH-T209	Specialization Paper-II (P)*	3	1	0	3
TIU-PCH-T213	Specialization Paper-II (O)*				
TIU-PCH-T217	Specialization Paper-II (I)*				
Practical					
TIU-PCH-L223	Inorganic Chemistry Lab	0	0	3	2
Sessional					
TIU-PES-S299	Entrepreneurship Skill Development	0	0	2	2
	Total	14	5	3	**19**

*P-Physical Chemistry O-Organic Chemistry I-Inorganic Chemistry

Specialization Papers (I and II)

Physical Chemistry

TIU-PCH-T207**:** Quantum Mechanics and Chemical Applications of Group Theory

TIU-PCH-T209**:** Electrochemistry

Organic Chemistry

TIU-PCH-T211**:** Advanced Organic Chemistry-I

TIU-PCH-T213**:** Advanced Organic Chemistry-II

Inorganic Chemistry

TIU-PCH-T215**:** Organometallic Chemistry of Transition Metals

TIU-PCH-T217**:** Advanced Bioinorganic Chemistry

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Semester-III

Structure and Spectroscopy-I
TIU-PCH-T203

L-T-P: 3-1-0 **Credit: 3**

Module 1

Introduction: Interaction of electromagnetic radiation with matter, Einstein coefficient, transition probability, transition dipole moments and selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy.

Rotational and rotation-vibrational spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, eigen values and eigenstates, selection rules, normal coordinates and their symmetry (CO_2), vibration and group frequency, FT-IR instrumentation.

Raman spectroscopy: Raman Effect (basic principles only), rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines.

Module 2

Electronic spectroscopy: Vibronic spectroscopy of diatomic molecules, Franck-Condon factor, dissociation and pre-dissociation, rotational fine structure, solvent effects.

Lasers in spectroscopy: Principles of laser action, laser characteristics, population inversion, Basic elements in laser (resonator, gain medium, pumping technique), pulsed lasers, laser cavity modes, Q-switching, mode locking, harmonic generation, different lasers: He-Ne, Nd-YAG, titanium-sapphire, dye lasers, semiconductor lasers, and applications of lasers.

Photoelectron Spectroscopy and Diffraction Methods: Photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS of molecules; Principle of electron, neutron and X-ray diffraction methods in determining the structure of molecules, synchrotron.

Module 3

Magnetic resonance: A review of spin angular momentum, basic principles and relaxation times, intensity of NMR signals, electronic shielding, NMR in liquids: chemical shifts, spin-spin couplings, NMR spectra of AX, A_3X and AB systems.

FT-NMR: Rotating frame of reference, effect of RF pulses, FID, Multi pulse operation, measurement of T_1 by inversion recovery method, spin echo and measurement of T_2.

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Recommended Books

1. J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd., Chichester.
2. C. N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
3. A Carrington and A. D. Mc Lachlan, Introduction to Magnetic Resonance, (1979) Chapman and Hall, London.
4. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, (1986) Addison Wesley, Longman Ltd, London.
5. G. Herzburg, Infrared and Raman Spectra (1945), Spectra of Diatomic Molecules (1950), Van Nostrand, New York.

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Biological Chemistry
TIU-PCH-T205

L-T-P: 3-1-0 **Credit: 3**

Module 1
Biomolecules

A. Amino acids and Proteins

Amino acids (Structure, titration curve, iso-electric point, reactions involving amino acids) peptide bond, Structure of protein (Primary, secondary, tertiary and quartenery), Ramachandran plot, methods involved in C-/N- amino acid sequencing, Reactions (Ninhydrin reaction, Van Slyke reaction and others), Denaturation of proteins, factors effecting denaturation, structural aspect of protein with respect to haemglobulin and myoglobulin. Methods involved in protein purification, Bruce-Merrifield reaction (artificial peptide synthesis), Oxygen uptake proteins: Hemerythrin and hemocyanin.

B. Enzymes: Classification, nomenclature, Kinetics of enzyme action, Enzyme inhibition, Regulation of enzyme (allosteric enzymes), isozymes, Enzyme active site, Metalloenzymes:Hydrolytic and redox enzymes: Carbonic anhydrase and superoxide dismutase, structure and function of Nickel and Zinc containing enzymes (Urease, Hydrogenase, Carboxy-peptidase etc.).

C. Vitamins and Hormones: Fat soluble and water soluble vitamins, Vitamins as coenzymes and co-factors, NAD, FAD, TPP, Folic acid, Vit.B6, Vit.B2, Lipoic acid, Co ASH, Epinephrine, nor epinephrine.

D. Lipids and Steroids: Structure and function of lipids, steroids, Cholesterol, prostaglandins, and bio membranes.

E. Carbohydrates: Classification, structure, reactions and importance in biology.

Module 2

Nucleic Acids: Structure of nucleic acid-nitrogen base pairing with reference to adenine, guanine, cytosine, thymine and uracil, Structure of DNA (double helical structure), RNA, base pairing, m-RNA structure, t-RNA structure, Reaction (cyclitization reaction) DNA binding protein- Zinc finger protein. Replication, Transcription and translation, Regulation of gene expression.

Module 3

Bioenergetics: Bioenergetics (concept), Glycolysis, citric acid cycle (TCA), electron transport chain, oxidative phosphorylation, Active and passive transport mechanism (pumps)

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Recommended Books

1. L. Stryer, Biochemistry, 5th edition (2002), Freeman & Co., New York.
2. D. L. Nelson and M. M. Cox, Lehninger, Principles of Biochemistry, 3rd edition (2002) McMillan North Publication.
3. M. N. Hughes, Inorganic Chemistry of Biological Processes, (1981) John Wiley.
4. M. B. Smith, Organic Synthesis, (1995) McGraw Hill Inc., New York.
5. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.

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Specialization – I: Physical Chemistry
Quantum Mechanics and Chemical Applications of Group Theory
TIU-PCH-T207

L-T-P: 3-1-0 **Credit: 3**

Module 1
Quantum Mechanics

A. Fundamentals: General formulation of Quantum Mechanics, Postulates of Quantum Mechanics, Review of rigid rotor, harmonic oscillator and Hydrogen atom problems. Angular momentum: commutative relations and ladder operators.

B. Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of Helium atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients.

C. Many Electron Atoms: Hartee SCF method, Electron correlation, Addition of angular momenta – Clabsch-Gordan series, Spin-orbit interaction, Condon Slater rule.

D. Molecular Structure: Born-Oppenheimer approximation. Molecular orbital treatment for homonuclear molecule. Hückel MO treatment of simple polyenes.

Module 2
Chemical Applications of Group theory

A. IR and Raman Spectroscopy: Brief introduction to molecular vibrations; selection rules for fundamental vibrational transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C_{2v}, C_{3v}, C_{4v}, D_{2h}, D_{3h}, D_{4h}, T_d and O_h point groups).

B. Crystal Field Theory: Splitting of levels and terms in chemical environment, construction of energy level diagrams, selection rules and polarizations.

C. Molecular Orbital Theory: Introduction, transformation properties of atomic orbitals; hybridization schemes for σ− and π−bonding, hybrid orbitals as LCAOs; Molecular Orbital Theory for some typical AB_n types (n = 2, 3, 4, 6) of molecules (H_2O, NH_3 and BH_3).

Recommended Books

1. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 3rd edition (1997), Oxford University Press. Oxford.
2. I. N. Levine, Quantum Chemistry, 5th edition (2000), Pearson Educ., Inc., New Delhi.
3. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach, (1998), Viva Books, New Delhi.

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4. A. K. Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata McGraw Hill, New Delhi.
5. L. Pauling and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, (1935), McGraw Hill, New York.
6. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn. (1999), John Wiley & Sons, New York.

Specialization – II: Physical Chemistry

Electrochemistry
TIU-PCH-T209

L-T-P: 3-1-0 **Credit: 3**

Module 1

Ion-Solvent Interaction: Introduction, Born model and Born equation, enthalpy of ion-solvent interaction and its evaluation, Eley-Evan model, solvation number and its determination

Module 2

Electrical Double Layer at Metal/Semiconductor-Electrolyte Interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface, Structure of the double layer**:** Helmholtz-Perrin, Gouy-Chapman, and Stern models. Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot. Thermodynamics of double layer, Electrocapillary equation, Determination of surface excess and other electrical parameters-electrocapillarity, excess charge capacitance, and relative surface excesses.

Module 3

Electrode Kinetics: Polarizable and non-polarizable interfaces. Multistep reactions-a near equilibrium relation between current density and over potential, concept of rate determining step. Determination of reaction order, stochiometric number, and transfer coefficient. Electrocatalysis-comparison of electrocatalytic activity. Importance of oxygen reduction and hydrogen evolution reactions and their mechanisms.

Module 4

Applications of Electrochemistry: Electrochemical cells, Corrosion, Cyclic Voltammetry

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Recommended Books

1. J. O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 1 & 2A and 2B, (1998) Plenum Press, New York.

2. A. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd edition, (2001) John Wiley &Sons, New York.

3. Samuel Glasstone, An Introduction to Electrochemistry: Edition 1st, East-West Press Pvt Ltd New Delhi, India.

Specialization-I: Organic Chemistry
Advanced Organic Chemistry-I
TIU-PCH-T211

L-T-P: 3-1-0 **Credit: 3**

Module 1

Organic Photochemistry-I: Photochemical energy, Jablonski diagram, photosensitisation and quenching, Norrish Type-I and Type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds: rearrangement of unsaturated compounds; photo-induced reactions in aromatic compounds.

Module 2

Organic Photochemistry-II: Photo-induced functionalisation in organic molecules involving Barton reaction, Hofmann-Loffler-Freytag reaction; photochemical rearrangements, photo induced disproportion reaction, photo induced substitution reaction in aromatic systems, chemiluminescence in organic reactions.

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Module 3

Application of Important Organic Reactions in Organic Synthesis: Hydroboration, Witting reaction, Birch reduction and few important reactions in organic synthesis.

Module 4

Organic Synthetic Chemistry: Organic synthetic process and uses of Phosphorus, Silicone and Sulphur compounds in synthetic organic chemistry, Planning a synthetic pathway; molecular characteristics: Retrosynthesis; method of formation of carbon skeleton: carbon to carbon bond formations, logistic and stereochemistry. Phospho ylide and sulphur ylide.

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Recommended Books

1. T. H. Lowry and K. C. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edn, Harper and Row, New York, 1998.
2. H. O. House, Modern Synthetic Reactions, 2nd Edn, Benjamin, 1971.
3. W. Caruthers, Modern Methods of Organic Synthesis, 3rd Edn, Cambridge University Press, Cambridge, 1996.
4. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, Oxford University Press, Oxford, 2001.
5. O. L. Chapman, Some Aspects of Organic Photochemistry, Dekker, 1967.
6. J. M. Coxon and B. Halton, Organic Photochemistry, Cambridge University Press, Cambridge, 1974.
7. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rd Edn, ELBS, 2003.
8. J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, 3rd Edn, New Age International (P) Ltd, India, 2012.
9. A. Griesbeck, M. Oelgemoller and F. Ghetti, Organic Photochemistry and Photobiology, 3rd Edn, Vol I, CRC Press, Boca Raton, FL, 2012.
10. H.O. House, Modern Synthetic Reactions, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.
11. L.F. Fieser and M. Fieser, Reagents for Organic Synthesis, Vol. 1-16 (Vol. 1, 1967), Wiley-Interscience, New York.
12. M.B. Smith and J. March, March's Advanced Organic Chemistry – Reactions, Mechanisms &Structure, 5th ed. (2001), Wiley-Interscience, New York.
13. M. B. Smith, Organic Synthesis, McGraw Hill Inc., New York (1995).
14. J. Clayden, N. Greeves, S. Warren, and E. Wothers, Organic Chemistry, Oxford Univ. Press, Oxford (2001).
15. P. R. Jenkins, Organometallic Reagents in Synthesis, Oxford science Publ., Oxford (1992)

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Specialization-II: Organic Chemistry
Advanced Organic Chemistry-II
TIU-PCH-T213

L-T-P: 3-1-0 **Credit: 3**

Module 1
Alkaloids: Classification, general reactions of alkaloids, typical reaction conversions and rearrangement of morphine, papaverine, cinchona alkaloids.

Module 2
Terpenes: Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of carryophyllene, abietic acid, beta-amyrin, alpha and beta-carotenoids. Camphor, Longifolene*, Abietic acid, and Taxol.(***Synthesis only)**.

Module 3
Natural Pigments: General methods of isolation, structure elucidation and synthesis of anthocyanins, flavones, isoflavones, aurone, chalcone, xanthone and their chemical interconversions.

Recommended Books

1. Nitya Anand, J.S. Bindra and S. Ranganathan, Art in Organic Synthesis, 2nd Edition (1970), Holden Day, San Francisco.
2. S. W. Pelletier, Chemistry of the Alkaloids, Van Nostrand Reinhold Co., New York (1970).
3. K.W. Bentley, The Alkaloids, Vol. I., Interscience Publishers, New York (1957).
4. I. L. Finar, Organic Chemistry, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi.
5. J. W. Apsimon, Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York (Vol. 1, 1973).
6. J. S. Bindra and R. Bindra , Creativity in Organic Synthesis, Academic Press, NY (1975).
8. K. C. Nicolaou, Classics in Total Synthesis of Natural Products, Vol. I (1996) & Vol. II (2003).

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Specialization-I: Inorganic Chemistry
Organometallic Chemistry of Transition Metals
TIU-PCH-T215

L-T-P: 3-1-0 **Credit: 3**

Module 1

Organo-metallics: Application of 18- electron and 16- electron rules to transition metal Organometallics, structure, bonding (pictorial mo-approach) and reactions of η^2-ethylinic , η^3-allylic and η^5-cyclo-pentadineyl compounds: K[Pt (η^2-C_2H_4)Cl_3], [(η^3-C_3H_5) Pd Cl]$_2$, (η^5-C_5H_5)$_2$ Fe]; carbene and carbyne complexes, Stereo-chemical non rigidity and fluxional behavior of organo-metallic compounds with typical examples, Metal-metal single and multiple bonding (pictorial mo –approach), Bond orders, bonding in direhnium compounds, Isolobal and isoelectronic relationships, Organo-metallic catalysts.

Module 2

A. **Inorganic π-Acid Ligands**: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.
B. **Complexes of σ-donor ligands**: Transition metal alkenyls, alkynyls, carbenes and carbines.
C. **π-complexes of unsaturated molecules**: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

Module 3

A. **Transition metal compounds in catalysis**: Hydrogenation, hydroformylation and polymerization; Waker Process.
B. **Transition metal Compounds with M-H bonds**: Metal hydrides (classical and non-classical). Agostic interaction. Application of NMR in studying hydrido complexes.

Recommended Books

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed. (1999) John Wiley & Sons, NY.
2. J. E. Huheey, Keiter and Keiter, Inorganic Chemistry.
3. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, John Wiley.
4. Ch. Elschenbroich and A. Salzer, Organometallics, VCH.

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5. J. P. Collman, L. S. Hegedus, J. R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley. California.

Specialization-II: Inorganic Chemistry
Advanced Bioinorganic Chemistry
TIU-PCH-T217

L-T-P: 3-1-0 **Credit: 3**

Module 1

Metal ions in biology: Essential and trace elements in the biological systems, metal of life, basic reactions in the biological systems and the roles of metal ions in biological process. Ion transport (active) across biological membrane and its significance, mechanism of Na^+ K^+ -ion pump.

Module 2

A. Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes.

B. Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (ferredoxines). cytochrome c oxidase.

C. Redox enzymes: Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems. Molybdo enzymes: nitrate reductases, sulfite oxidase.

Module 3

Toxicity and drugs: Toxic effects of metal ions, detoxification by chelation therapy, metal dependent diseases and metal complexes as drugs, Pt, Ru, Rh and Au drugs.

Recommended Books

1. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed. (1981), John-Wiley & Sons, New York.
2. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York (1995).
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).

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4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).

Inorganic Chemistry Lab
TIU-PCH-L223

L-T-P: 0-0-3 **Credit: 2**

Experiment 1: Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non-aqueous media.

Experiment 2: Quantitative separation and determination of pairs of metal ions using gravimetric and volumetric methods.

Experiment 3: Synthesis of a series of metal complexes (with ligands of varying ligand field strength), electronic spectral interpretation and calculation of various ligand-field parameters.

Experiment 4: Synthesis of a macrocycle and purification by column chromatography

Experiment 5: Acetylation of ferrocene and separation of the acetyl derivative by column chromatography

Experiment 6: Synthesis of inorganic polymer

Experiment 7: Quantitative analysis of major and minor components in ores and alloys by volumetric, complexometric, gravimetric and other instrumental methods after separation of the components by solvent extraction or chromatographic techniques.

Experiment 8: Determination of composition and formation constants of selected systems by *p*H-metric and spectrophotometric methods.

Experiment 9: Preparation of inorganic and coordination compounds and their Characterization: Bi-, tri- and polydentate ligands

a. Complexation and purification
b. Growing of single crystals
c. Elemental analyses (C, H, N, S)
d. Spectral studies