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

Fourth Semester

Course Code	Course Title	Contact Hrs./ Week			Credit
		L	T	P	
Theory					
TIU-PCH-S200	Career Advancement Skill Development	2	1	0	3
TIU-PCH-T202	Structure & Spectroscopy-II	3	1	0	3
TIU-PCH-T204	Polymer & Material Science	3	1	0	3
TIU-PCH-T206	Specialization Paper-III (P)*	3	1	0	3
TIU-PCH-T208	Specialization Paper-III (O)*				
TIU-PCH-T210	Specialization Paper-III (I)*				
TIU-PCH-T212	Specialization Paper-IV (P)*	3	1	0	3
TIU-PCH-T214	Specialization Paper-IV (O)*				
TIU-PCH-T216	Specialization Paper-IV (I)*				
TIU-PCH-P298	**Project**	0	0	12	7
Sessional					
TIU-PES-S298	Entrepreneurship Skill Development-IV	0	0	2	2
	Total	14	5	12	**24**

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

Specialization Papers (III and IV)

Physical Chemistry
TIU-PCH-T206: Statistical Mechanics
TIU-PCH-T212: Advanced Solid State Chemistry and Spectroscopy

Organic Chemistry
TIU-PCH-T208: Heterocycles
TIU-PCH-T214: Reagents and Organic Synthesis

Inorganic Chemistry
TIU-PCH-T210: Inorganic Rings, Chains, and Clusters
TIU-PCH-T216: Special Topics in Inorganic Chemistry

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Semester-IV

Structure and Spectroscopy-II
TIU-PCH-T202

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

Module 1

PMR Spectroscopy: Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects, chemical exchange and chemical shifts in chiral molecules. Spin-spin, spin-lattice relaxations, Spin-spin interactions, naming spin systems, magnitude of coupling constant: Germinal, vicinal and long range couplings. Simplification of complicated spectra: Aromatic induced shifts spin decoupling, deuterium exchange, spectra at higher fields. Hindered rotation and rate processes. Nuclear Overhauser effect.

CMR Spectroscopy: General considerations, chemical shift, calculation of approximate chemical shift values, coupling constants. Interpretation of simple CMR spectra. DEPT spectrum.

Advanced NMR Techniques in Structure Elucidation of Organic Compounds: Application of DEPT, ^{1}H-^{1}H COSY, HMBC, HMQC, TOCSY, NOESY.

NMR Spectroscopy of Inorganic Molecules: NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, ^{11}B, ^{19}F, ^{27}Al, ^{31}P – NMR spectroscopy with typical examples.

Nuclear Quadruple Resonance (NQR) Spectroscopy: Qudrupole nuclei, qudrupole moments, electric field gradient, coupling constant, splitting and simple applications.

Module 2

Mass Spectrometry: Introduction, ion production, fragmentation, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra.

Structure elucidation based on spectroscopic data (IR, UV, NMR and Mass).

Module 3

EPR: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions, Application.

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Mössbauer: Gamma ray emission and absorption by nuclei, Mössbauer effect, Isomer shift, quadrupole splitting, Application to the elucidation of structure and bonding of Fe(III) and Fe(II), Sn(IV) and Sn(II) compounds, detection of oxidation states and in equivalent MB atoms.

Optical Rotatory Dispersion and Circular Dichroism : Basic Principles of ORD and CD techniques. ORD and Cotton effect, Faraday and Kerr effects; Applications in determining absolute configuration of metal complexes.

Recommended Books

1. R. M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6th Edition (2003) John Wiley, New York.
2. D. H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Edition (1988), Tata-McGraw Hill, New Delhi.
3. P. Y Bruice, Organic Chemistry, 2nd Edition (1998) Prentice-Hall, New Delhi.
4. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edition (1987), Blackwell Scientific Publications, Oxford, London.
5. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
6. R. S. Drago, Physical Methods in Inorganic Chemistry, 1st Edition (1971), Affiliated East-West Press, New Delhi.

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Polymer and Material Science
TIU-PCH-T204

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

Module 1

Polymers: Classification of polymers, chemistry of polymerisation, molecular weight and size, kinetics of addition and condensation polymerization, stereochemistry, flexibility of polymer chain, statistics of polymer dimensions and configurations, glass transition temperature, crystallinity in polymers and copolymerisation. Polymer solutions: criteria for polymer solubility, Flory-Huggins model. Polymer modification and manufacturing of commodity polymers: grafting, cross-linking, blending, compounding.

Specialty polymers: Liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymer, nanocomposites of polymers, biomedical polymers.

Module 2

Material Science:

A. Crystal Structure and X-ray Diffraction: Definitions related to crystal structure, reciprocal lattice, Brillouin Zones, structure factor and intensity diffraction of X-rays by crystals: The Laue equations and Bragg's law, X-ray diffraction experiments: the powder method and the single crystal method, Band theory, insulators, semiconductors and conductors and their applications.

B. Theoretical aspect of nanomaterials, preparation, characterization, and applications of nanomaterials, optical properties of semiconducting nanomaterials, electronic properties of low dimensional materials.

C. Different Instrumental Techniques for characterization: Basic principles and applications of electron microscopies (SEM, TEM), scanning probe microscopies (STM), atomic force microscopy (AFM), optical microscopies [confocal microscopy, scanning near field optical microscopy, particle size analysis (DLS)], thermal (DSC, DTA) and optical (IR, FTIR, Raman) methods.

Recommended Books

1. F. W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Willey-Interscience, New York.
2. P. W. Atkins, Physical Chemistry, 8th Edition, Oxford University Press, New York.
3. G. Odian, Principles of Polymerization, 3rd Edition (1991), John Wiley, Singapore.

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4. P. Bahadur, N.V. Sastry, Principle of Polymer Sciences, Narosa Publishing House, New Delhi (2002)
5. V.R. Gowarikar, N.V. Vishwanathan, J. Shreedhar, Polymer Sciences, Wiley Eastern, New Delhi (1986)
6. L.V. Azaroff, Introduction to Solids, (1977) Tata McGraw-Hill, New Delhi.
7. A. J. Dekker, Solid State Physics, Prentice Hall
8. C. Kittel, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York.

Specialization – III: Physical Chemistry
Statistical Mechanics
TIU-PCH-T206

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

A. Introduction to Statistical Mechanics: Ensemble. Micro/Macro/Grand-canonical ensemble. Entropy. Gibbs paradox. Entropy of a two level system. Equipartition of energy. Ideal gas in canonical and grand canonical ensembles. Phase space. Equal a priori probability. Quantization of phase space. Liouville theorem.

B. Partition Function: Review of rotational, vibrational and translational partition functions. Applications of partition function to specific heat of solids, chemical equilibrium and real gases.

C. Bose-Einstein Distribution: Einstein condensation. Thermodynamic properties of ideal BE gas.

D. Fermi-Dirac Distribution: Degenerate Fermi Gas. Electron in metals. Magnetic susceptibility.

E. Fluctuations: Mean square deviation and fluctuation in ensembles. Concentration fluctuation in quantum statistics.

F. Non-equilibrium States: Boltzmann transport equation. Particle diffusion. Electrical conductivity.

Recommended Books

1. B. K. Agarwal and M. Eisner, Statistical Mechanics, (1988) Wiley Eastern, New Delhi.
2. D. A. McQuarrie, Statistical mechanics, (1976) Harper and Row Publishers, New York.

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Specialization –IV: Physical Chemistry
Advanced Solid State Chemistry and Spectroscopy
TIU-PCH-T212

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

Module 1

Advanced Solid State Chemistry

A. Solid State Reactions: General principles and experimental procedure of solid state reactions, growth of single crystals: Czochralski method, Bridgman and Stockbarger methods.

B. Phase Transitions: Thermodynamic and Burger's classification of phase transition, kinetics of phase transition, nucleation and growth.

C. Thermal Properties of Solids: Specific heat- lattice heat capacity, Einstein theory, Debye theory, Born's modification of the Debye theory.

D. Free electron theory of metals: Free electron gas model of metals, free electron gas in a one-dimensional and three dimensional box, filling up of the energy levels.

E. Band theory of solids: Wave functions in a periodic lattice and the Bloch theorem, The Kronig-Penny model, the tight binding approximation, Band theory of insulators and semiconductors, intrinsic semiconductors, extrinsic semiconductors, doped semiconductors, p-n junctions.

F. Magnetic Properties: Behaviour of substances in a magnetic field, effect of temperature: Curie and Cuire-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagentic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

Module 2

Advanced Spectroscopy

Nonradiative transition, polarised light emission and absorption: anisotropy, solvation dynamics, resonance energy transfer, fluorescence quenching, and introduction of nonlinear spectroscopy.
Application of lasers as excitation source, time resolved fluorimetry, transient absorption spectroscopy, surface plasmon spectroscopy, multiphoton spectroscopy, single molecule spectroscopy, fluorescence correlation spectroscopy, upconversion, microscopy (optical, phase contrast, confocal, FLIM), SERS,CARS.

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Recommended Books

1. A. R. West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore.
2. L.V. Azaroff, Introduction to Solids, (1977) Tata McGraw-Hill, New Delhi.
3. A. J. Dekker, Solid State Physics, Prentice Hall
4. C. Kittel, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, Chichester.
5. J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd., Chichester.
6. J.R. Lakowicz, Principles of Fluorescence Spectroscopy
7. W. Demtroder, Laser Spectroscopy.

Specialization – III: Organic Chemistry
Heterocycles
TIU-PCH-T208

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

Module 1

A. General Considerations: Structure, synthesis and reactivity

B. Synthesis and reactions of the following ring systems

(a) Three-membered rings: Aziridines.

(b) Four-membered rings: Azetidines and their 2-oxo derivatives.

(c) Five-membered rings containing two heteroatoms: Oxzoles, Imidazoles, Thiazoles, Isoxazoles, Pyrazoles.

(d) Pyrimidines.

(e) Purines: Uric acid and Caffeine.

(f) Five-membered ring heterocycles with three or four heteroatoms

Module 2

Steroids and Prostanoids: Diels' hydrocarbon, Cholesterols, Chemistry, elucidation of structure and synthesis; Bile acids, Androsteron, Estrone

Recommended Books

1. T. L. Gilchrist, Heterocyclic Chemistry, 3rd Edition (1997) Addison-Wesley Longman Ltd., England

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2. R. K. Bansal, Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms, 3rd Edition (1999), New Age International, Publisher, New Delhi.
3. A. R. Katritzky, C. A. Ramsden, J.A. Joule and V. V. Zhdankin, Handbook of Heterocyclic Chemistry, 3rd Edition (2010), Elsevier, Oxford, UK.
4. Heterocyclic Chemistry, 4th edition, J. A. Joule and K. Mills, Blackwell Publishing, Indian Reprint 2004.
5. Heterocyclic Chemistry Vol-III,III, 1st edition. R.R. Gupta, M. Kumar, V. Gupta Springer-Verlag, Berlin Heidelberg Publication (2005)
6. Aromatic Heterocyclic Chemistry: David T. Davies, (1992), Oxford University Press.

Specialization – IV: Organic Chemistry
Reagents and Organic Synthesis
TIU-PCH-T214

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

Module 1

Oxidation: (i) Oxidation with peracids: Oxidation of carbon-carbon double bonds carbonyl compounds, allylic carbon-hydrogen bonds, (ii) Oxidation with selenium dioxide and Osmium tetraoxide, (iii) Oxidation with lead tetraacetate, mercuric acetate (iv) hypervalent iodine

Module 2

Reagents and Reactions : (i) Gilman's reagent – Lithium dimethylcuprate, (ii) Lithium diisopropylamide (LDA), (iii) Dicyclohexyl carbodiimide (DDC), (iv) 1,3-Dithiane (Umpolung reagent), (v) Peterson's synthesis, (vi) Bakers yeast, (vii) DDQ, (viii) Palladium catalysed reactions, (ix) Woodward and Prevost hydroxylation, (x) Iodotrimethyl silane and (xi) Ionic liquids

Module 3

A. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups

B. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction –substrate, reagent and catalyst controlled reactions

Recommended Books

1. H. O. House, Modern Synthetic Reactions, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.
2. L. F. Fieser and M. Fieser, Reagents for Organic Synthesis, Vol. 1-16 (Vol. 1, 1967), Wiley-Interscience, New York.
3. M. B. Smith and J. March, March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure, 5th ed. (2001), Wiley-Interscience, New York.
4. M. B. Smith, Organic Synthesis, McGraw Hill Inc., New York (1995).
5. J. Clayden, N. Greeves, S. Warren, and E. Wothers, Organic Chemistry, Oxford Univ. Press, Oxford (2001).
6. P. R. Jenkins, Organometallic Reagents in Synthesis, Oxford science Publ., Oxford (1992).

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Specialization – III: Inorganic chemistry
Inorganic Rings, Chains, and Clusters
TIU-PCH-T210

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

Module-1

A. Clusters and element-element bonds: Polyhedral boranes: Electron deficiency *vs* sufficiency. Types and IUPAC nomenclature. Wade's polyhedral skeleton electron pair theory (PSEPT). W. N. Lipscomb's styx rules and semi-topological structures of boranes. Equivalent and resonance structures. Wade's vs Lipscomb's methods of studying higher boranes.

B. Heteroboranes: Types of heteroboranes with special reference to carboranes, structure, bonding and IUPAC nomenclature. Metallaboranes, Metallacarboranes, metal σ and μ bonded borane/carborane clusters. Resemblance of Metallaboranes/Metallacarboranes with ferrocene and related compounds. Applications of Metallaboranes/Metallacarboranes as drug delivery system. Applications of PSEPT over heteroboranes.

C. Principle of Isolobility: Development and formulation of the concept of isolobility and its applications in the understanding of structure and bonding of heteroboranes.

Module-2

Metal Clusters: Metal-metal bonds. Concept of quadrupolar bond and its comparison with a C-C bond; Types of metal clusters and multiplicity of M-M bonds. Simple and condensed metal carbonyl clusters. Applications of PSEPT and Wade's-Mingo's and Lauhr's rule over metal carbonyl clusters. Metal halide and metal chalcogenide clusters: Bloomington schuffle in dinuclear tungsten clusters.

Module-3

Heteropoly and Isopoly acids: Structural principles and their applications

Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulphur-nitrogen, sulphur-nitrogen-fluorine compounds, - binary and multicomponent systems, haemolytic inorganic systems.

Recommended Books

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John-Wiley & Sons, New York.

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2. James E. Huheey, Inorganic Chemistry, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn. (1997), Butterworth Heinemann, London.

Specialization – IV: Inorganic chemistry
Special Topics in Inorganic Chemistry
TIU-PCH-T216

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

Module-1
Macrocyclic Complexes: Design and synthesis by coordination template effect, Applications of macrocyclic complexes.

Module-2
Supramolecular Chemistry: Concepts and terminology of supramolecular chemistry. Nature and types of supramolecular interactions (Hydrogen bonding, van der Waal interactions, π-stacking, C-H….π interactions etc.), Molecular recognition- Information and complementarity. Different types of receptors with special reference of Crown ethers, Cryptates and Calix[4]arene. Anion recognition and anion coordination chemistry. Molecular self-assembly formation and examples. Supramolecular chemistry of life, application of supramolecular chemistry.

Module-3
Molecular Magnetic Materials: types of magnetic interactions, inorganic and organic ferro-magnetic materials, low-spin–high-spin transitions, molecular magnets and applications.

Metallomesogens: Basic concepts, synthetic strategies, characterization and applications.

Recommended Books
1. Jean-Marie Lehn, Supramolecular Chemistry, VCH, Weinheim (1995).
2. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edition, John Wiley & Sons (Asia), Singapore (2003).
3. Oliver Kahn, Molecular Magnetism, VCH, Weinheim (1993).
4. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
5. R. S. Drago, Physical Methods in Inorganic Chemistry, 1st Edition (1971), Affiliated East-West Press, New Delhi.