Syllabus
Ph.D. Course Work

Department of Chemistry and Chemical Sciences

CENTRAL UNIVERSITY OF JAMMU
Rahya-Suchani (Bagla), District-Samba
Jammu-181143, (J&K) India

Course Matrix for Ph.D. Program in Chemistry

The credits assigned to the Ph.D. course work are 16. Students have to opt for four courses. The proposed course matrix for Ph.D. program in Chemistry is given below:

Module-I: Compulsory

S. No.	Course	Code	Type	Credits	L-T-P
1	Research Methodology and Computer Applications	PHCHM1C001T	C	4	3-1-0

Module-II: Research Area Specific (Any three)

S. No.	Course	Code	Type	Credits	L-T-P
1	Characterization Techniques	PHCHM1C002T	E	4	3-1-0
2	Stereochemistry and Asymmetric Synthesis	PHCHM1C003T	E	4	3-1-0
3	Organic Synthesis	PHCHM1C004T	E	4	3-1-0
4	Green Chemistry	PHCHM1C005T	E	4	3-1-0
5	Application of Group Theory and Inorganic Spectroscopy	PHCHM1C006T	E	4	3-1-0
6	Advanced Topics in Inorganic Chemistry	PHCHM1C007T	E	4	3-1-0
7	Bioinorganic and Organometallic Chemistry	PHCHM1C008T	E	4	3-1-0
8	Advanced Quantum Mechanics and Computational Chemistry	PHCHM1C009T	E	4	3-1-0
9	Spectroscopy and Group Theory	PHCHM1C010T	E	4	3-1-0
10	Computer Programming and Numerical Methods	PHCHM1C011T	E	4	3-1-0
11	Thermodynamics, Kinetics and Electrochemistry	PHCHM1C012T	E	4	3-1-0

Note:

1. Students have to opt for any three courses from Module-II to make a total of 16 credits.
2. C: Core, E: Elective

Course Name: Research Methodology and Computer Applications
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Research methodology: Research, Definition, Need of research, Identification of the problem, Research evaluation methods, Various indexes (*h*-index, *i*-index, etc.), Issues related to plagiarism, ethics, Intellectual property rights, Copyright, Copyleft, Patents, Industrial designs, Trademarks, Literature survey (Chemical abstracts, Scopus, Scifinder etc.), Research report, review, thesis writing.

UNIT – II 12 hours

Chemistry laboratory safety: Safety rules, Chemical safety, Workplace Hazardous Material Information System (WHMIS), Material Safety Data Sheets (MSDS), Science laboratory safety signs, Emergency procedures, First aid, Rules specific for the organic chemistry laboratories, Waste management.

UNIT – III 12 hours

Statistics: Introduction, Probability theories, Conditional probability, Poisson distribution, Binomial distribution and Properties of normal distributions, Estimates of Means and Proportions, Chi-Square test, Association of attributes, t-Test, Anova, Standard deviation, Co-efficient of variations, Correlation and regression analysis, Mathematical and statistical analysis using software tools MATLab, SPSS, PsiLAB etc.

UNIT – IV 12 hours

Computer applications: Computer basics, Data representation, Computer generation and classification, Computer languages, Operating systems, Computer networks.

Spreadsheet tool: Introduction to spreadsheet and its features and functions, Using formulae and functions, Generating charts/graphs and other features (Tools: Microsoft Excel, Libre office, Open office etc.)

Presentation tool: Introduction to presentation tool and its features and functions, Preparation of presentations (Microsoft PowerPoint, Libre office, Open Office etc.).

UNIT – V 12 hours

Quantitative and Separation methods: Chromatographic techniques, High performance liquid chromatography (HPLC), Gas Chromatography (GC), Thin Layer chromatography (TLC), Column Chromatography (CC), Reversed phase chromatography (RPC), Chiral chromatography.

REFERENCES

1. J. Anderson, B. H. Dursten and M. Poole, *Thesis and Assignment Writing*, Wiley Eastern.
2. D. C. Harris *Quantitative Chemical Analysis*, 2007, W. H. Freeman and Company
3. R. Panneerselvan, *Research Methodology,* PHI, New Delhi.
4. Michael M. Marda, *Research Methods of Science*, 1st Ed., Cambridge University Press, New York.
5. C. C. Kothari and Gourav Garg, *Research Methodology*, 3rd Ed., New Age Internationa.
6. S. K. Muthu, *Probability and Error for Physical Science*, Orient Lougman.
7. P. R. Majhi and P. K. Khatua, *Research Methodology*, Himalaya Publication House.

Course Name: Characterization Techniques
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

UV-VIS spectroscopy: Interaction of electromagnetic radiation with matter, Types of electronic transition, Beer-Lambert law, Selection rules, Allowed and forbidden transitions, Effect of conjugation, Applications of UV-VIS spectroscopy in organic chemistry, Woodward-Fieser rules.

IR Spectroscopy: Principle, Molecular vibrations, Characteristic functional group absorptions, Factors influencing group frequencies, Hydrogen bonding, Overtones, Combination bands, Fermi Resonance.

UNIT – II **14 hours**

NMR spectroscopy: ^{1}H-NMR: Introduction, Shielding, Chemical shift, Diamagnetic anisotropy, Integration, Exchangeable hydrogens, Chemical equivalence, Magnetic equivalence, Spin coupling, Non-first order spectra, Spin systems (AB, AX, AB_2, AX_2, AMX, ABX, ABC etc), Geminal, Vicinal and Long range coupling, Coupling constants, Spin decoupling, Relaxations, Nuclear Overhauser effect, NMR shift reagents, Variable temperature ^{1}H-NMR, Coupling of proton with ^{13}C, ^{19}F, ^{31}P and ^{29}Si.

^{13}C-NMR: Proton-decoupled and off-resonance, Chemical shifts, DEPT (45, 90 and 135).

2D NMR: Introduction, HOMOCOSY, HETCOR, HMQC, HMBC, INADEQUATE and NOESY.

UNIT – III **12 hours**

Mass spectrometry: Mass spectrometry, Principle, Basic instrumentation, Ionization techniques – EI, CI, FD and FAB, Fragmentation, Molecular ion peak, Base peak, Metastable ions, Isotopes, Nitrogen rule, McLafferty rearrangement, Retro Diels-Alder, Characteristic fragmentation patterns of hydrocarbons, ethers, alcohols, phenols, ketones, aldehydes, carboxylic acids, amides, HRMS, Introduction to ESI-MS and MALDI-TOF.

UNIT – IV **10 hours**

Applications of spectroscopic techniques: Problems on the structural elucidation of organic compounds using UV, IR, NMR and Mass techniques.

UNIT – V **12 hours**

Thermal analysis: General principles and applications of Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Thermo Gravimetric Analysis (TGA), ThermoMechanical Analysis (TMA).

Microscopic techniques: General principles and applications of Scanning Electron Microscopy (SEM), Environmental SEM, Transmission Electron Microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM).

REFERENCES

1. R. M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th Ed., Wiley, 2004.
2. P. S. Kalsi, *Spectroscopy of Organic Compounds*, New Age International, 6th Ed., 2006.
3. W. Kemp, *Organic Spectroscopy*, Palgrave, 2008.

4. H. Friebolin, *Basic One and Two Dimensional NMR Spectroscopy*, 5th Ed., Wiley-VCH, 2010.
5. A. Upadhyay, K. Upadhyay and N. Nath, *Biophysical Chemistry – Principles and Techniques*, 4th Ed., Himalaya Publishing House, 2010.
6. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, 7th Ed., CBS Publishers & Distributors, 2004.

Course Name: Stereochemistry and Asymmetric Synthesis
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Conformational analysis: Conformational analysis of acyclic and cyclic compounds, Effect of conformation on reactivity in acyclic compounds and cyclohexanes: Stereoelectronic and steric factors, Oxidation of cyclohexanol, Esterification of cyclohexane carboxylic acid, Solvolysis of tosylates, E2 and *cis* eliminations, Formation and cleavage of epoxide ring, Neighboring group participation, Molecular rearrangements.

Conformation of cyclohexene and cyclohexanone, Conformation and stereochemistry of *cis*- and *trans*-decalins and 9-methyl decalin, Conformation of perhydrophenanthrene and perhydroanthracenes.

UNIT – II 12 hours

Stereochemistry: Optical activity and chirality, Stereochemistry of molecules with more than one asymmetric carbon (up to five), Homotopic and heterotopic ligands and faces, Heterotopicity and NMR, Enantiotopic and diastereotopic atoms, groups and faces, Stereotopic ligands and NMR spectroscopy, Prochiral centers: Chiral methyl, phosphate, sulphate and thiophosphate groups, Chirality of molecules devoid of chiral centers: Biphenyls, allenes, spiranes, molecules with planar chirality, Chiroptical properties, Applications of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD).

UNIT – III 12 hours

Introduction to asymmetric synthesis: Importance of asymmetric synthesis, Basic principles of asymmetric synthesis, Stereospecific and stereoselective reactions, Enantioselectivity and diastereoselectivity, Conditions for an efficient asymmetric synthesis, Energetic considerations, Strategies for asymmetric synthesis, Analytical methods for determining enantiomeric excess, Resolving agents and resolution of racemic compounds having common functional groups such as alcohol, amine and acid.

UNIT – IV 12 hours

Asymmetric synthesis on chiral substrate: Nucleophilic addition to α-chiral carbonyl compounds, Prediction of stereochemistry-Cram's rule and related modifications, Double stereo-differentiation, matched pair and mismatched pair, Examples from aldol condensation and hydroboration reactions, Electrophilic addition to α-chiral olefins-epoxidation, Cyclopropanation, Hydroboration-oxidation, Alkylation of enolates of β-chiral carbonyl compounds.

UNIT – V 12 hours

Asymmetric synthesis using chiral reagents: Chiral organoboranes, Chiral modification of lithium aluminum hydride, BINAL-H, Asymmetric Michael addition to α,β-unsaturated carbonyl compounds, TS model.

Asymmetric synthesis using chiral auxiliary: Chiral auxiliaries derived from proline, camphor, menthol and other chiral pool sources, Pyrrolidine, Oxithiane, Oxazolidine-2-one, Thiazolidine-2-one, Phenylethylamine, 2-Phenylcyclohexanol, 8-Phenyl menthol.

Asymmetric synthesis using chiral catalysts: Asymmetric alkylation and allylation of carbonyl compounds, Asymmetric hydrogenation, Proline mediated aldol reactions, Sharpless asymmetric epoxidation, Dihydroxylation, Aminohydroxylation of alkenes.

REFERENCES

1. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, Wiley, New York, 2008.
2. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 2nd Ed., New Age International, 2002.
3. P. S. Kalsi, *Stereochemistry: Conformation and Mechanism*, 9th Ed., New Age International, 2009.
4. J. D. Morrison, *Asymmetric Synthesis*, Vol 1-5, Academic press, 1983.
5. *Comprehensive Asymmetric Catalysis,* E. N. Jacobsen, A. Pfaltz, H. Yamamoto, Eds., Springer, 2000.
6. R. Noyori, *Asymmetric Catalysis in Organic synthesis*, Wiley-New York, 1994.
7. I. Ojima, *Catalytic Asymmetric Synthesis*, VCH-NY, Pergamon, 1998.
8. *Methods for the Asymmetric Synthesis of Complex Organic Molecules*, D. J. O'Leary, Lecture Notes 2001.
9. H. B. Kagan, *Aymmetric Synthesis*, 1st Ed., Thieme Medical Publishers, 2003.

Course Name: Organic Synthesis
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Oxidation reactions: Swern oxidation, HIO_4, $Pb(OAc)_4$, $Hg(OAC)_2$, I_2/AgOAc, Woodward and Prevost reactions, Sharpless asymmetric epoxidation and Peroxyacids, Ozone, PCC, PDC, Etards reagent, MnO_2, OsO_4, SeO_2, DDQ, RuO_4, Jones reagent, Copper chromite and Wacker's reagent ($PdCl_2$), Iodobenzenediacetate, IBX, Dess-Martin periodinane.

UNIT – II **12 hours**

Reduction reactions: Metal hydrides: $LiAlH_4$, $NaBH_4$, $Na(CN)BH_3$, $Zn(BH_4)_2$ and Trialkyltin hydrides, DIBAL, Metals in acidic medium (alkali metals, tin and zinc), H_2/metal catalysts (hydrogenation), $SnCl_2$ and Lawessonn reagent, $TiCl_4$/Zn-Cu (McMurray reagent), Wilkinson's catalyst, Lindlar catalyst, BH_3/THF, 9-BBN and Optically active boranes.

UNIT – III **12 hours**

Organometallic reagents: Organozinc and copper reagents: Preparation, Functionalized zinc and copper reagents, Synthetic applications, Gilman reagents, Reformatsky reaction, Simmons-Smith reaction, Grignard and organolithium reagents in organic synthesis, Organoboron reagents, Synthetic application of Sn and Si reagents, Wittig, Horner-Wadsworth-Emmons Reactions, Cross-coupling reactions (Suzuki, Heck), Ring closing metathesis.

UNIT – IV **12 hours**

Protecting groups in organic synthesis: Importance, Protection and deprotection of hydroxyl groups: Methyl, ethyl and benzyl ethers (MOM, MTM, SMOM, MEM, SEM, THP and MPM ethers), Silyl ethers (TMS, TES, TIPS, DEIPS, TBDMS, TBDPS, DPMS, DTBMS and TBMPS ethers), Protection for 1,2- and 1,3-diols, Protection and deprotection of carbonyl compounds: Acyclic and cyclic acetals and ketals, monothio and dithioacetals and ketals, Monoprotection of dicarbonyl compounds, Protection of amines, Boc, Cbz, PMB, Bn, Ac, Bz and Ts. Selective protection of secondary amines-MIBK, Common protecting groups for carboxylic acids and thiols.

UNIT – V **12 hours**

Retrosynthetic analysis: Introduction, Target molecule, Linear and convergent synthesis, Disconnection approach, Synthons and synthetic equivalents, Nucleophilic, Electrophilic, Electro-neutral and Free radical synthons, Transform, Functional group interconversion, Umpolung, Chemo-, regio- and stereoselectivities, Protecting groups, One group disconnection: Alcohols and carbonyl compounds, Two group disconnection: 1,2-, 1,3-, 1,4-, 1,5-, and 1,6-difunctional compounds, Diels-Alder reactions, Robinson annulation, Michael addition, Retrosynthetic analysis of simple organic molecules.

REFERENCES

1. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2nd Ed., Wiley, 2008.
2. S. Warren and P. Wyatt, *Organic Synthesis: Strategy and Control*, Wiley, 2007.
3. E. J. Corey and X.-M. Cheng, *The Logic of Chemical Synthesis*, Wiley, 1995.
4. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6th Ed., Wiley, New Jersey, 2007.

5. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part A: Structure and Mechanisms*, 5th Ed., Springer, New York, 2007.
6. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part B: Reactions and Syntheses*, 5th Ed., Springer, New York, 2007.
7. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
8. M. B. Smith, *Organic Synthesis*, 2nd Ed., McGraw-Hill, New Delhi, 2004.
9. F. A. Carey, *Organic Chemistry*, McGraw-Hill, New Delhi, 2000.
10. J. McMurry, *Organic Chemistry*, 5th Ed., Brooks/Cole, New York, 2000.

Course Name: Green Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Introduction to green chemistry: Definition, Principles of green chemistry, Ideal synthesis, E-factor, Atom economy, Atom economic (rearrangement and addition reactions) and uneconomic reactions (substitution and elimination reaction), Need, development and vision of green chemistry, Advantages over conventional methods, Modern variants in green synthesis, Step economy, Introduction to multicomponent reactions (MCRs) and Domino reactions (DRs).

UNIT – II **12 hours**

Green synthesis/reactions: Comparative study of conventional and green protocols of Wittig, Bouveault, Heck, Michael addition, Darzen, Diels-Alder reaction, Thiamine mediated acyloin condensation, Baeyer-Villiger oxidation, Claisen rearrangement, Hantzsch synthesis, Ugi reaction, Click reactions, Combinatorial chemistry, Green synthesis of nanoparticles, Selected examples from US Presidential Green Chemistry Challenge Award Winners.

UNIT – III **12 hours**

Reactions in unconventional medium: Pollution due to solvents, Global effect of solvent usage, Need for green solvents, Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability, Ionic liquids, Glycerol, Polyethylene glycol, Supercritical fluids, Solvent-free reactions, Fluorous phase reactions.

UNIT – IV **12 hours**

Heterogeneous catalysis: Introduction to green catalysis, Heterogeneous catalysts, Advantages of solid catalysts or reagents, Use of zeolites, silica, alumina, clay, amberlyst, montmorillonite, polymers, cyclodextrin supported catalysts, Solid acids, Ion exchange resins, Advantages of solid acids over mineral acids, Supported metal oxides, Rare earth triflates, Physisorbed and Chemisorbed solid acid catalysis, Biocatalysts, Baker's yeast.

UNIT – V **12 hours**

Nonconventional energy sources: Microwave assisted reactions, advantage of microwave exposure, specific effects of microwaves, selected microwave-assisted condensations reactions, oxidations, reductions reactions and multicomponent reactions, Ultrasound assisted reactions, Ball milling, Continuous flow reactor, Photochemical reactions.

REFERENCES

1. P. Tundo, A. Perosa and F. Zucchini, *Methods and Reagents for Green Chemistry*, Wiley, New Jersey, 2007.
2. M. Rai and C. Posten, *Green Biosynthesis of Nanoparticles Mechanisms and Application* CABI, 2013.
3. A. S. Matlack, *Introduction to Green Chemistry*, Marcel Dekker, Inc., New York, 2001.
4. A. Patti, *Green Approaches to Asymmetric Catalytic Synthesis*, Springer, 2011.
5. V. K. Ahluwalia, *Green Chemistry: Environmentally benign reaction*, Boca Raton, FL: CRC, Taylor & Francis, 2008.
6. P. T. Anastas and R. H. Crabtree, *Handbook of Green Chemistry, Green Catalysis, Homogeneous Catalysis*, Wiley, 2014.

Course Name: Application of Group Theory and Inorganic Spectroscopy
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Symmetry and group theory: Symmetry elements, Symmetry operations, Schoenflies symbols, Reducible and irreducible representations, Properties of irreducible representation, Direct product representation, Orthogonality theorem and its consequences, Construction of character tables, Direct product, Symmetry adapted linear combinations, Projection operators, Derivation of character tables for C2v, C3v and C2h.

Use of character tables: Molecular vibrations, Symmetry of vibrations in non-linear molecules (CH_4, H_2O, XeF_4, BF_3, SF_6 and NH_3), Application of Group theory in IR, UV-Vis and Raman spectroscopy of Inorganic complexes.

UNIT – II 12 hours

Electron spin resonance spectroscopy: Theory of ESR Spectroscopy, Zeeman equation, g-value, Nuclear hyperfine splitting, Spin densities and McConnell relationship, Factors affecting the magnitude of g and A tensors in metal species, Zero-field splitting and Kramers degeneracy, Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes, Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions and inorganic free radicals such as PH_4, F_2^- and $[BH_3]^-$.

Nuclear magnetic resonance spectroscopy: Principle, The contact and pseudo-contact shifts, Factors affecting nuclear relaxation, Nuclear magnetic resonance ($^{10,11}B$, ^{19}F, ^{31}P, NMR), Application of NMR in the structural elucidation of inorganic compounds, ^{31}P NMR spectra of P_4S_3, H_3PO_3, H_3PO_2 and HPF_2, ^{19}F NMR spectra of ClF_3, BrF_5 and equimolar mixture of TiF_6^{2-} and TiF_4 in ethanol, Fluxional behavior of molecules lanthanide shift reagents, ^{10}B and ^{11}B resonance studies.

UNIT – III 12 hours

UV-visible spectroscopy: Origin of spectra and electronic transitions, Quantitative aspects of UV-Visible absorption measurement, Term-symbols, Calibration graph for quantitative analysis, General design of instruments for absorbance measurements, Use of UV spectroscopy in distinguishing geometrical isomers

Infrared spectroscopy: The vibration of diatomic molecule and polyatomic molecules, Harmonic and anharmonic oscillators, Types of molecular vibrations, Rotational vibrational spectrum of linear and symmetric top molecules, Applications: Skeletal vibrations of inorganic molecules, Factors influencing vibrational frequency of bonds, Hydrogen bonding, Electronic effect, Mass effect.

Raman spectroscopy: Classical and quantum theory of Raman effect, Rotational Raman spectra, Linear and symmetric top molecules, Vibrational raman spectra, Raman activity of vibrations, Rule of mutual exclusion, Rotational fine structures, Polarized and depolarized Raman lines, Application of Raman active vibrations on H_2O, CNS^-, NO_3^-, CN^- and SO_4^{2-}.

UNIT – IV 12 hours

Mossbauer spectroscopy: Basic principles, Spectral parameters and spectrum display, Isomer shifts, Magnetic interactions, Mossbauer emission spectroscopy, Applications to iron and tin complexes.

NQR spectroscopy: Characteristics of quadrupolar nucleus, Effects of field gradient and magnetic field upon quadrupolar energy levels, NQR transitions, Applications of NQR spectroscopy.

Spectroscopic methods for optically active complexes: Introduction to theory, Optical rotatory dispersion (ORD) and ORD curves, Positive and negative cotton effect, Circular dichroism (CD), Comparison between ORD and CD - their inter relationships.

UNIT – V **12 hours**

X-ray diffraction: X-ray diffraction by single crystal, Space groups, Systematic absences in X-ray data and identification of lattice types , Glide planes and screw axes, X-ray intensities, Structure factor and its relation to intensity and electron density, Phase problem, Structure solution by Heavy atom method and direct method, Determination of absolute configuration of molecules, A brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB).

Electron diffraction by gases: Scattering intensity vs Scattering angle, Wierl equation, Measurement technique, Elucidation of structure of simple gas phase molecules.

Neutron diffraction by crystals: Magnetic scattering, Measurement techniques, Elucidation of structure of magnetically ordered unit cell.

REFERENCES

1. K. V. Reddy, *Symmetry and Spectroscopy of Molecules,* 2nd Ed., New Age International, 2009.
2. S. F. A. Kettle, F. Albert Cotton, *Symmetry and Structure, Chemical Applications of Group Theory,* 3rd Ed., Wiley, 2003.
3. Robert L. Carter, *Molecular Symmetry and Group Theory,* Wiley, 1998.
4. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, Elsevier, Amsterdam, 1984.
5. C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, 3rd Ed., TMH, New Delhi, 1983.
6. B. P. Straughan and S.Walker, *Spectroscopy*, Vol. 3, Chapman Hall London, 1976.
7. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, New York, 1964.
8. P. K. Ghosh, *Introduction to Photoelectron Spectroscopy*, John Wiley New York, 1989.
9. P. M. Silverstein and F. X. Wester, *Spectroscopic Identification of Organic Compounds*, 6th Ed., Wiley, 1998.
10. W. Kemp, *Organic Spectroscopy*, 3rd Ed., MacMillon, 1994.
11. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, 1965.
12. Y. R. Sharma, *Elementary Organic Spectroscopy-Principles and Chemical Applications*, S.Chand, 1992.

Course Name: Advanced Topics in Inorganic Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Magneto chemistry: Definition of magnetic properties, Types of magnetic bodies, Diamagnetism and Pascal's constant, Russell-Saunders coupling, Multiple widths, Stereochemical applications of magnetic properties of the first transition series, Lanthanides and actinides, Determination of magnetic susceptibility by Gouy's method, Derivation of Van-Vleck formula for susceptibility.

UNIT – II **14 hours**

Metal organic frameworks: Polymeric coordination compounds, Coordination polymer, Coordination network, Metal-organic framework, Carboxylate ligands, Introduction to MOFs, Design, Synthesis, Structure and reactivity, Importance of large-pore crystalline open frameworks, Post Polymer MOF hybrid membranes (Crystals and Chains), Luminescent MOFs, Ligand-based luminescence in MOF, Metal based luminescence, LMCT, MLCT and MMCT in MOFs, Applications: Gas separation and storage (H_2, methane), CO_2 capture (from Flue gases, Natural gas and Syngas), Future aspects of MOFs, MOCAs, Custom tailored metal organic complex arrays.

UNIT – III **14 hours**

Inorganic photochemistry: Principle of light absorption, Physical and chemical processes, Bimolecular reactions, Stern-Volmer relationship, Properties of d-d, d-π*, π-π* and π-d energy states, Photochemical reactions of metal complexes (Substitution reaction), Adamson's rules, Rearrangement, Isomerisation, Racemisation, Aquation and Annation, Redox reactions, Electron counting schemes, Capping rule, Mechanism of CTTM photoreduction, Compounds with metal-metal bonding, Reinecke's salt, Chemical actinometer.

Applications: Importance of solar energy conversion and storage, Cleavage of water using $[Ru(bpy)_3]^{2+}$, Cadmium sulphide colloidal particles and titanium dioxide semiconductor, $[Ru(edta)H_2O]$ catalysed ammonia production.

UNIT – IV **10 hours**

Photovoltaic materials: Dye-sensitized solar cells (DSSC), Introduction, Operating principles of the DSSC, Device fabrication, Photon to current efficiency, Open circuit photovoltage, Molecular sensitizers, Spectral response, Surface chelation of metal complexes onto the TiO_2, Photovoltaic properties, Stability, Ruthenium and osmium metal complexes for DSSCs, Inorganic materials, Pervoskites.

UNIT – V **10 hours**

Organic light-emitting diodes (OLEDs) and Light emitting electrochemical cells (LEECS): Introduction, Types of luminescent, Standard OLED and LEECS, Device architecture principle, OLEDs Vs LEECS, Transport properties, Photophysical properties, Tuning of phosphorescence colours, Controlling quantum yields, Iridium, platinum and copper complexes for OLEDs and LEECs.

REFERENCES

1. Alan Earnshaw, *Introduction to Magnetochemistry*, Academic Press.
2. Bond C. Chapman, *Heterogeneous Catalysis*, 2nd Ed., 1987.

3. J. M. Thomas and W. J. Thomas, *Introduction to the Principles of Heterogeneous Catalysis*, Academic press, New York, 1967.
4. S. K. Kulkarni, *Nanotechnology: Principles and Particles*, Capital Publication Co.
5. A. W. Adamson and P. D. Fleischauer, *Concepts of Inorganic Photochemistry*, Wiley, New York, 1975.
6. J. Ferraudi, *Elements of Inorganic Photochemistry*, Wiley, New York, 1988.
7. A. W. Adamson and P. D. Fleischauer, *Concepts of Inorganic Photochemistry*, Pub. Co. Inc. Florida, 1984.
8. D. Farrusseng, *Metal-Organic Frameworks*, Wiley, 2011.
9. L. R. Mac Gillivray, *Metal-Organic Frameworks: Design and Application*, Wiley, 2010.
10. B. Chen and G. Qian, *Metal-Organic Frameworks for Photonics Applications*, Springer, 2014.
11. V. W. W. Yam, *WOLEDs and Organic Photovoltaics Recent Advances and Applications*, Springer, 2010.
12. K. Kalyanasundaram, *Dye-Sensitized Solar Cells*, CRC Press, Taylor &. Francis Group, 2010.
13. H. Yersin, W. J. Finkenzeller, *Triplet Emitters for Organic Light-Emitting Diodes: Basic Properties, Highly Efficient OLEDs with Phosphorescent Materials*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2007.

Course Name: Bioinorganic and Organometallic Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Introduction to bioinorganic chemistry: Metals in biology-Metalloenzymes, Hydrolases, Carboxypeptidase, Carbonic anhydrase, Alkaline phosphatase and other dinuclear phosphatases and hydrolases, Electron transfer proteins: Blue copper, Iron-sulphur proteins, Ferridoxins, Rubredoxin and Cytochromes, Redox enzymes: Cu, Zn SOD and Cytochrome P450, Manganese enzyme and Xanthine oxidase, Heme-enzymes: Peroxidase and Catalase.

Metalloporphyrins: Porphyrin nucleus and Classification of porphyrins, Important metalloporphyrins occurring in nature, Detection of porphyrins spectrophotometrically and by fluorescence, Bile pigments, Chemical nature and their physiological significance, Haemoglobin and myoglobin, Oxygen transport and storage, Hemerythrin and Hemocyanin, Bohr effect.

UNIT – II 12 hours

Metal complexes in biological studies: Therapeutic applications of *cis*-platin, Theory and mode of action of therapeutic chelating agents, Single ligand chelation therapy, Aminopolycarboxylic acids, Desferrioxamine, Pencillamine, Triethylenetetramine, Mixed ligand chelation therapy, Detoxification by metal chelation, Drugs that act by binding at the metal sites of metalloenzyme.

Chemotherapy: Chemotherapy with compounds of certain non-essential elements, Platinum complexes in cancer therapy, Cisplatin and its mode of action, Gold containing drugs as anti-rheumatic agents and their mode of action, Radiopharmaceuticals, Metallothionens in detoxification, Anti-viral chemotherapy and Metal peptide interaction.

UNIT – III 12 hours

Supramolecular chemistry-I

Molecular recognition: Introduction to recognition, Information and complimentarily, Molecular receptors, Design principles, Spherical recognition, Cryptates of metal cations, Tetrahedral recognition by macrocyclic cryptands, Recognition of ammonium ions and related substrates, Recognition of neutral molecules, Recognition of anionic substrates (anionic coordination).

Transport processes and carrier design: Carrier-mediated transport, Cation transport processes, Cation carriers, Anion transport processes, Anion carriers, Coupled processes, Molecular and supramolecular devices, Supramolecular photochemistry, Supramolecular electronic devices, Supramolecular ionic devices.

UNIT – IV 12 hours

Supramolecular chemistry-II

Concepts and languages of supramolecular chemistry: Supramolecular devices, Various types of supramolecular devices, Molecular and supramolecular ionic devices, Tubular mesophases, Molecular protonics, Switching devices, Photo switching and electro switching, Supramolecular sensors, Ion and molecule sensors.

Supramolecular reactivity and catalysis: Catalysis by reactive macrocyclic cation and anionic receptor molecules, Catalysis with cyclophane type receptors, Supramolecular metallocatalysis, Cocatalysis, Catalysis of synthetic reactions, Biomolecular and abiotic catalysis, supramolecular chemistry in solution, Cyclodextrin, Micelles, Dendrimmers, Gelators, Classification and typical reactions, Applications.

UNIT – V **12 hours**

Advanced organometallic chemistry: Metal alkyl and aryls, 18 electron rule, Dewar-Chatt approach to bonding in olefins, Cyclopentadiene, Benzene and Cyclobutadiene complexes of transition metals, Their preparations, bonding and reactions, Fluxional organometallic compounds, Fluxionality and dynamic equilibria in compounds such as η2-olefin, η3-allyl and dienyl complexes, Activation of small molecules by complexation, Agostic interaction, Insertion, Alkyl migration, Insertion and elimination, Stereochemical change.

Organometallic reactions and catalysis: Monsanto acetic acid process, Wacker process, Olefin metathesis, Cross coupling reactions (Suzuki and Heck) and Amination, Water splitting reactions using organometallic catalyst.

REFERENCES

1. Nelson, David and Cox, *Lehninger's Principles of Biochemistry*, Macmillan, New York.
2. Willium Elliott and Daphne Elliott, *Biochemistry and Molecular Biology*.
3. M. N. Hughes, *The Inorganic Chemistry of Biological Processes*, 2nd Ed.
4. A. W. Addison, W. R. Cullen, D. Dolphin and B. R. James, *Biological Aspects of Inorganic Chemistry*.
5. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publishing Company, New Delhi, 1997.
6. R. W. Hay, *Bio-Inorganic Chemistry*, Ellis Horwood, 1987.
7. R. M. Roat-Malone, *Bio-Inorganic Chemistry*, John Wiley, 2002.
8. W. Kaim and B. Schwederski, *Bio-InorganicChemistry: Introduction Elements in the chemistry of Life*, John Wiley & Sons, 1994.
9. J. M. Lehn, *Supramolecular Chemistry*, VCH, Wienheim, 1995.
10. J. M. Lehn, *Transition Metals in Supramolecular Chemistry*, John Wiley and sons, New York, 1999.
11. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, John Wiley and Sons, New York.
12. S. E. Kegley and A. R. Pinhas, *Problems and Solutions in Organometallic Chemistry*, University Science Books, Oxford University Press.
13. P. Powell, *Principles of Organometallic Chemistry*, 2nd Ed., Chapman and Hall, London.
14. J. P. Collman, L. S. Hegedus, J. R. Nortan and R. G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books, Mill Valley, California.
15. R. C. Mehrotra and A. Sing, *Organometallic Chemistry. A Unified Approach*, New Age Internationals, 2006.
16. P. Powell, *Principles of Organometallic Chemistry*, Springer-Sciencet Business Media, B. V., 1988.
17. R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 2007

Course Name: Advanced Quantum Mechanics and Computational Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Basics of quantum mechanics: Operator formalism and its application to quantum mechanics, Eigenvalue problem, Expectation values, Wave function, Time dependent and time independent Schrödinger wave equation and its importance, Probabilities, Orthogonal and orthonormal functions, Postulates of quantum mechanics.

UNIT – II 12 hours

Applications of quantum mechanics: Particle in a one, two and three-dimensional box, Particle in a ring, Delta function, Degeneracy and its applications, Schrödinger wave equation for H-atom and its solution in terms of the variables r, θ, φ, quantum numbers.

UNIT – III 12 hours

Advanced quantum mechanics: Approximation methods, Variational theory and perturbation theory, Many electron atoms and Hartee-Fock theory, Application to the helium atom, Antisymmetry and Exclusion Principle, Spin of electron, Terms symbols and spectroscopic states, Born-Oppenheimer approximation, Hydrogen molecule ion, post Hartee-Fock theory, Density functional theory.

UNIT – IV 12 hours

Computational chemistry-I: Computational modeling, The concepts of Potential Energy Surface, Chemical bonding, Reactivity, Molecular properties, Spectroscopy from the electronic structure perspective, Optimizations, Frequency calculations, The basic principles of quantum chemistry and understand the potential, Limitations of computational techniques, Use of common computational chemistry software.

UNIT – V 12 hours

Computational chemistry-II: Knowledge of methods and basis sets, Comparative study of QM, MM and semi-empirical methods, Finding minima and maxima, Potential energy surface scanning, Intrinsic reaction coordinate, Charge analysis: Mullikan, *Hireshfield,* NBO; HOMO-LUMO diagram analysis, Study of reaction mechanism, Basic idea of molecular modeling and other computational techniques.

REFERENCES

1. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, 1st Ed., Viva, 1999.
2. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Ed., Tata McGraw Hill. 1998.
3. I. N. Levine, *Quantum Chemistry*, 7th Ed., Pearson, 2013.
4. C. J. Cramer, *Essentials of Computational Chemistry*, 2nd Revised edition, Wiley-Blackwell, 2004.
5. F. Jensen, *Introduction to Computational Chemistry*, 2 Ed., Wiley, 2007.
6. On-line manual of *Gaussian 16* and *GAMESS.*

Course Name: Spectroscopy and Group Theory
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Rotational spectroscopy: Linear, symmetric rotor, spherical rotor and asymmetric rotor molecules, Diatomic and linear polyatomic molecules, Selection rules, Transition frequencies or wavenumbers, Intensities, Centrifugal distortion, Diatomic molecules in excited vibrational states, Stark effect in diatomic, linear and symmetric rotor molecules, Rotational Raman spectroscopy, Spectrum of non-rigid rotator, Polyatomic molecules, Determination of bond length, Isotope effect.

UNIT – II **12 hours**

Vibrational spectroscopy: Infrared spectrum, Energy levels of simple harmonic oscillator, Selection rules, Pure vibrational spectrum, Intensity, Determination of force constant and qualitative relation of force constant and bond energies, Concept of polarizability, Raman Spectrum, Pure vibrational Raman spectra of diatomic molecules, Selection rules, Anharmonicity, Electrical anharmonicity, Mechanical anharmonicity, Vibration-rotation spectroscopy: Infrared spectra and Raman spectra, Polyatomic molecules, Group vibrations, Anharmonicity and potential energy surfaces, Local mode treatment of vibrations, Vibrational potential functions with more than one minimum.

UNIT – III **12 hours**

Electronic spectroscopy: Atomic spectroscopy, Angular momenta and magnetic moments, Coupling of angular momenta, Russell–Saunders coupling approximation, Term symbol, Electronic spectroscopy of diatomic molecules, Franck-Condon principle, Classification of electronic states, Electronic selection rules, Vibrational coarse structure, Rotational fine structure, Electronic spectroscopy of polyatomic molecules, Molecular orbitals and electronic states, Electronic and vibronic selection rules, Fluorescence and Phosphorescence, Internal conversion and intersystem crossing, Photoelectron spectroscopy.

UNIT – IV **12 hours**

Group theory: Molecular symmetry, Symmetry elements and symmetry operation, Point group symmetry, Matrix representation of symmetry operations, Character and Character tables, Reducible and irreducible representations, The great orthogonality theorem, Decomposition of reducible representation and the direct product.

UNIT – V **12 hours**

Application of group theory: Character tables and their applications, group theory and quantum mechanics: Wave function as bases of irreducible representation, Direct product, Symmetry adopted linear combination, Symmetry and molecular vibrations: Determination of IR/RAMAN active modes of molecular vibrations, Symmetry and Molecular orbital theory.

REFERENCES

1. C. Banwell and E. McCash, *An Introduction to Molecular Spectroscopy*, 4th Ed., McGraw Hills, 1994.
2. C. Banwell and C. McCash, H. Chaudhury, *Fundamentals of Molecular Spectroscopy,* 4th Ed., McGraw Hill Education, 2013.
3. J. Michael Hollas, *Modern Spectroscopy*, 4th Ed., Wiley, 2004.
4. F. A. Cotton, *Symmetry and Group Theory*, 3rd Revised edition, Wiley, 1990.

5. Daniel C. Harris, Michael D. Bertolucci, *Symmetry and Spectroscopy: Introduction to Vibrational and Electronic Spectroscopy*, New edition, Dover Books, 1989.

Course Name: Computer Programming and Numerical Methods
Course Code: 4 Credits (3-1-0)

UNIT – I 10 hours

Basics: Basic architecture of computers, Software, Hardware, OS: Operating Computer using GUI based operating system, I/O, Basic knowledge of Linux OS and '*vi* editor' and simple command for operations using terminal, *sftp* and *ssh* protocol.

Programming language: Learning a language for expressing computations, Types of language: FORTRAN, C, C++, Python (object oriented programming), Basic knowledge of Fortran 90, Types of errors: Syntax errors, Logical errors and Run-time errors.

UNIT – II 14 hours

Programming with FORTRAN: Data statements, Logical and arithmetic expressions, Implicit and explicit data typing, Mix-mode arithmetic, Library functions, I-O statements, Implementation of loops, Nested loops, Control statements, Functions and subroutines, Array, strings and character processing, Format specifications, Example for small programs.

UNIT – III 12 hours

Numerical methods-I: Finding roots of an equation, Newton-Raphson method, Basic ideas of interpolation, Newton's forward and backward interpolation, Secant method, Bisection methods.

UNIT – IV 14 hours

Numerical methods-II: Numerical differentiation: 1st and 2nd order, Numerical integration of a definite integral, Quadrature rule, Trapezoidal and Simpson's one-third rule, Numerical solution of coupled differential equation using Runge-Kutta and Relaxation techniques, LU factorization, Pivoting.

UNIT – V 10 hours

Numerical methods-III: Gaussian elimination, Gauss-Jordan elimination, Jacobi method, Matrix diagonalization: Jacobi iteration, QR and LR methods.

REFERENCES

1. K. V. Raman, *Computers in Chemistry*, 1st. Ed., Tata McGraw Hill, 2004.
2. V. Rajaraman, *Computer Programming in Fortran 90 and 95*, 1st Ed., Prentice Hall, 1997.
3. M. Schatzman, *Numerical Analysis: a Mathematical Introduction*, 1st Ed., Oxford University Press, 2002.
4. R. L. Burden and J. D. Faires, *Numerical Analysis*, 10th Ed., CENGAGE Learning Custom Publishing, 2015.
5. Arnold Robbins, Elbert Hannah, Linda Lamb, O'Reilly, *Learning the vi and Vim Editors*, 7th Ed., O′Reilly, 2008.
6. S. A. Mollah, *Numerical Analysis and Computational Programming*, 5th Revised edition, Books and Allied (P) Ltd., 2000.

Course Name: Thermodynamics, Kinetics and Electrochemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 10 hours

Chemical kinetics-I: Methods of determining rate laws, Temperature dependence of chemical reactions, Consecutive and parallel reactions, Steady-state approximation, Collision theory, Steric factor, Treatment of unimolecular reactions, Transition state theory, Erying and Arrhenius equations, General features of fast reaction, Study of kinetics by stopped flow technique, Relaxation method, Flash photolysis.

UNIT – II 12 hours

Chemical kinetics-II: Autocatalysis, Flow techniques, Kinetic equations of flow systems, Relaxation techniques for different order reactions, Potential energy surface, Reaction coordinates and paths, Absolute rate theory, Reactions in solution, Statistical approach to rate theory, Hinselwood, RRK and RRKM theories.

UNIT – III 12 hours

Electrochemistry: Debye-Hückel limiting law and its extension, Pitzer ion-interaction approach for osmotic and activity coefficients of electrolyte solutions, Debye-Hückel-Onsager theory and its limitation, Shedlovsky equation, Poisson-Boltzmann cell model of polyelectrolyte solutions, Osmotic and activity coefficients of polyelectrolytes, Electrical conductivity of polyelectrolyte solutions.

UNIT – IV 12 hours

Thermodynamics: Statistical interpretation of entropy, Thermodynamic potentials, Chemical potential, Thermodynamic properties of ideal gases and mixtures of ideal gases, Thermodynamic treatment of non ideal gases.

Reaction equilibrium: Reactions involving gases, Reactions involving pure condensed phases and a gaseous phase, Ellingham diagrams.

Measurement of thermodynamic properties: Concepts, Properties of ideal solution, Non-ideal systems, Excess functions for non-ideal solutions, Partial molar quantities, Determination of partial molar volume and enthalpy, Dilatometric and density measurement methods, Flow calorimeters, Marsh as well as Gibbs and VAN Ness static vapour methods for measuring vapour pressure of liquid and hence Gibbs free energy of mixing, Excess isentropic compressibility, Determination of excess isentropic compressibility.

UNIT – V 14 hours

Statistical thermodynamics: Concept of distribution, Thermodynamic probability, Ensemble averaging, Canonical, grand canonical and micro canonical ensembles, Statistical mechanics for systems of independent particles and its importance in chemistry, Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Idea of microstates and macro states, Thermodynamic probability (W) for the three types of statistics, Evaluation of translational, rotational and vibrational partition functions for monatomic and diatomic gases.

REFERENCES

1. P. W. Atkins, *Physical Chemistry*, 10th Ed., Oxford, 2014.
2. H. B. Callen, *Thermodynamics and Introduction to Thermostastics* 2nd Ed., Wiley, 2006.
3. S. Glasstone, *Thermodynamics for Chemists*, 1st Ed., Read Books, 2007.

4. D. A. McQuarrie, *Statistical Mechanics,* Viva Books Pvt. Ltd., New Delhi, 2003.
5. John O'M. Bockris, Amulya K. N. Reddy, *Modern Electrochemistry: Ionics,* 2nd Ed., Springer, 1998.

****