



**SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING**  
(Deemed to be University)

**Syllabus for  
M.Sc. in Chemistry**

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**SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING**  
(Deemed to be University)

**Department of Chemistry**

**Syllabus for Two Year M.Sc. in Chemistry**

**Programme Objectives:**

The Masters Programme in Chemistry covers all aspects of the different branches of chemistry and lays emphasis on detailed understanding of the fundamental principles and on training in appropriate computational and experimental methods. This rigorous training in all the major branches of chemistry - theoretical, applied, instrumental, computational and experimental – sets the stage for electives in interdisciplinary areas as well as for an introduction to advanced emerging fields of research in the final semester.

**Programme Specific Objectives:**

The Masters course in chemistry will consist of seventeen papers in chemistry spread over four semesters. During this period all aspects of the different branches of Chemistry will be covered in a manner so that the students get as complete a picture as possible of the range and depth of the subject. The emphasis is on detailed understanding of the fundamental principles and giving training in appropriate computational and experimental methods. The objective is to provide a rigorous training in all the major branches of chemistry. In the final semester advanced emerging fields of research are being introduced in order to enable the students to have a fairly good knowledge of current trends in chemical research. Electives in frontier and inter disciplinary areas are being provided in the final semester. A special elective paper in the field of Biocatalysis is included so as to give the students an in depth understanding in Environment benign Chemistry. A student graduating with M.Sc. degree in Chemistry would have been exposed to almost every aspect of the subject- Theoretical, Applied, Instrumental, Computational and Experimental.

**DEPARTMENT OF CHEMISTRY**

**SCHEME OF INSTRUCTION AND EVALUATION**

**M.Sc. (CHEMISTRY)**  
(Effective 2018/19 batch onwards)

Paper Code	Title of the Paper	Credits	Hours	Modes of Evaluation	Types of Papers	Maximum Marks
<b>Semester I</b>						
PCHM-101(i)	Quantum Chemistry and Group Theory	<b>4</b>	4	IE2	T	100
PCHM-101(ii)	Mathematics for Chemistry	<b>Non-Credit</b>	2	-	T	-
PCHM-102	Analytical Chemistry	<b>3</b>	3	IE2	T	100
PCHM-103	Coordination Chemistry	<b>3</b>	3	IE2	T	100
PCHM-104	Advanced aspects of Organic structure and Stereochemistry	<b>3</b>	3	IE2	T	100
PCHM-105	Practicals: Coordination Chemistry (Preparation & Analysis)	<b>2</b>	6	I	P	50
PCHM-106	Practicals: Analytical Chemistry (Conductometry, Potentiometry, Voltammetry)	<b>2</b>	6	I	P	50
PCHM-107	Practicals: Organic Qualitative Analysis (mixture analysis & drug analysis)	<b>2</b>	6	I	P	50
PAWR-100	Awareness Course – I: Education for Life	<b>1</b>	2	I	T	50
		<b>20</b> credits	<b>35</b> hours			<b>600</b> marks
<b>Semester II</b>						
PCHM-201	Structural Inorganic and Bio-Inorganic Chemistry	<b>3</b>	3	IE2	T	100
PCHM-202	Chemical Kinetics and Surface Chemistry	<b>3</b>	3	IE2	T	100
PCHM-203	Thermodynamics and Electrochemistry	<b>3</b>	3	IE2	T	100
PCHM-204	Physical and Mechanistic aspects of Organic Chemistry	<b>3</b>	3	IE2	T	100
PCHM-205	Practicals: Inorganic Chemistry	<b>2</b>	6	I	P	50
PCHM-206	Practicals: Chemical Kinetics and Electrochemistry	<b>2</b>	6	I	P	50
PCHM-207	Practicals: Organic Synthesis (multistep) and Spectral Analysis	<b>2</b>	6	I	P	50
PAWR-200	Awareness Course – II: God, Society and Man	<b>1</b>	2	I	T	50
		<b>19</b> credits	<b>32</b> hours			<b>600</b> marks

Contd...

Paper Code	Title of the Paper	Credits	Hours	Modes of Evaluation	Types of Papers	Maximum Marks
<b>Semester III</b>						
PCHM-301	Organometallic Chemistry	3	3	IE2	T	100
PCHM-302	Polymer Chemistry and Special Topics from Physical Chemistry	3	3	IE2	T	100
PCHM-303	Elective-I	3	3	IE2*	T	100
PCHM-304	Elective-II (Inter-departmental Electives)	3	3	IE2*	T	100
PCHM-305	Practicals: Computational applications in chemistry-I	2	6	I	P	50
PCHM-306	Project work (Interim Review) **	Non-Credit	12	-	PW	50**
PAWR-300	Awareness Course -III: Guidelines for Morality	1	2	I	T	50
		<b>15</b> credits	<b>32</b> hours			<b>550</b> marks
<b>Semester IV</b>						
PCHM-401	Solid State Chemistry and Nano Materials	2	2	IE2	T	50
PCHM-402	Special Topics from Bio-organic Chemistry	2	2	IE2	T	50
PCHM-403	Medicinal Chemistry	2	2	IE2	T	50
PCHM-404	Elective-III (Inter-departmental Electives)	3	3	IE2*	T	100
PCHM-405	Elective-IV (Inter-departmental Electives)	3	3	IE2*	T	100
PCHM-406	Practicals: Computational applications in chemistry-II	2	6	I	P	50
PCHM-407	Project work ***	8***	12	E	PW	200***
PAWR-400	Awareness Course -IV: Wisdom for Life	1	2	I	T	50
		<b>23</b> credits	<b>32</b> hours			<b>650</b> marks
	<b>GRAND TOTAL</b>	<b>77</b> credits	<b>131</b> hours			<b>2400</b> marks

### Modes of Evaluation

Indicator	Legend
<b>IE1</b>	CIE and ESE ; ESE single evaluation
<b>IE2</b>	CIE and ESE ; ESE double evaluation
<b>I</b>	Continuous Internal Evaluation ( <b>CIE</b> ) only Note: 'I' does not connote 'Internal Examiner'
<b>E</b>	End Semester Examination ( <b>ESE</b> ) only Note: 'E' does not connote 'External Examiner'
<b>E1</b>	ESE single evaluation
<b>E2</b>	ESE double evaluation

Continuous Internal Evaluation (CIE) & End Semester Examination (ESE)

### Types of Papers

Indicator	Legend
<b>T</b>	Theory
<b>P</b>	Practical
<b>V</b>	Viva voce
<b>PW</b>	Project Work
<b>D</b>	Dissertation

PS: Please refer to guidelines for 'Modes of Evaluation for various types of papers', and Viva voce nomenclature & scope and constitution of the Viva voce Boards. **Contd...**

**Note: The electives offered are at the discretion of the Head of the Department.**

\*\* The Project Work topic would be finalized by the end of the second semester, and the Project Work starts thereafter, continues in the third semester and gets completed in the fourth semester. The Project Work done in the third semester is reviewed based on a preliminary report submitted by the student and is evaluated for 50 marks: which is later included as part of the total marks of 250 in the fourth semester.

\*\*\* Total marks for the Project Work would be **250 marks**, which would include **50 marks** for the review of the preliminary report submitted by the student at the end of the 3<sup>rd</sup> semester (please see\*\*) + **50 marks** for the Project Work viva-voce conducted at the end of the 4<sup>th</sup> semester + **150 marks** for the double evaluation of the Project Report submitted at the end of the fourth semester.

The elective papers are listed below:

### **Elective Papers offered in the Third and Fourth Semesters**

**THIRD SEMESTER (Choose any ONE paper from each of the following electives):**

#### **ELECTIVE -I.**

PCHM-303 E-I (i) Synthetic Organic Chemistry  
PCHM-303 E-I (ii) Novel Drug Delivery Systems

#### **ELECTIVE – II: (Interdepartmental elective)**

PCHM-304 E-II (i) Theory and Application of Physical Methods in Chemistry  
PPHY-304 EL-2 Concepts in Materials Science.

**FOURTH SEMESTER (Choose any ONE paper from each of the Electives listed below):**

#### **ELECTIVE – III: (Interdepartmental elective)**

PCHM-404 E-III (i) Environmental Chemistry  
PBIO-402 E-III (ii) BT-3 Environmental Biotechnology  
PCHM-404 E-III (iii) Advanced aspects of applications of group theory in Chemistry

#### **ELECTIVE – IV: (Interdepartmental elective)**

PCHM-405 E-IV (i) Biocatalysis for Industry and Environment  
PCHM-405 E-IV (ii) Organic chemistry of natural products  
PPHY-405 EL-11 Materials Characterization Techniques

NOTE: The students of the department during their third and fourth semesters may choose two electives in the Third semester (one each from electives-I & II) and two electives (one each from Electives – III & IV) in the Fourth semester out of the elective courses listed above, under the guidance and the recommendation of the Head of the Department.

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## Quantum Chemistry and Group Theory

**Schrodinger's equation** -it is the equation for the wave function of a particle – Classical mechanical quantities are represented by linear operators in quantum mechanics- -1 unit  
 The Schrodinger equation can be formulated as an eigenvalue problem -1 unit  
 Wave functions have a probabilistic interpretation-energy of a particle in a box is quantized - 1 unit  
 Wave function must be normalized-average momentum of a particle in a box is zero-  
 The uncertainty principle  $\sigma_p \sigma_x > h/ 2\pi$  -1unit

**Postulates of Quantum mechanics** – The state of a system is completely specified by its wave equation- postulate 1 - 1 unit  
 Quantum mechanical operators represent classical mechanical variables- postulate 2, postulate 3 and postulate 4 -1 unit  
 The commutators of two operators play a central role in the uncertainty principle-  
 Quantum mechanical operators must be Hermitian operators-postulate 2' -1unit  
 The Eigen functions of Hermitian operators are orthogonal - 1 unit  
 The probability of obtaining a certain value of an observable in a measurement is given by a Fourier coefficient - 1 unit  
 The time dependence of wave functions is governed by the time dependent Schrodinger equation- postulate 5 - 1 unit

**Application of Schrodinger's equation to the particle in a box** (one-dimensional and three-dimensional) with complete solution - average values - 1 unit  
 Expression for quantum mechanical tunneling - 1 unit

**Harmonic Oscillator:** Harmonic oscillator obeys Hooke's law-energy of a Harmonic oscillator is conserved - 1 unit  
 The equation for harmonic oscillator model of a diatomic molecule contains the reduced mass of the molecule—Harmonic oscillator approximation results from an expansion of an inter nuclear potential around its minimum -1 unit  
 Energy levels of a quantum mechanical harmonic oscillator- harmonic oscillator accounts for the infrared spectrum of a diatomic molecule - 1 unit  
 Overtones are observed in vibrational spectra- Harmonic oscillator wave functions involve Hermite polynomials Hermite polynomials are either even or odd functions—useful relations among Hermite polynomials - 1 unit  
 The vibrations of a polyatomic molecules are represented by normal coordinates-Harmonic oscillator selection rule - 1 unit

**Rigid rotator:** Energy levels of a rigid rotator-rigid rotator is a model for a rotating diatomic molecule - 1 unit  
 Rotational transitions accompany vibrational transitions-Rotation-vibration interaction accounts for the unequal spacing of the lines in the P and R branches of a rotation-vibration spectrum -1 unit

The lines of a pure rotational spectrum are not equally spaced-wave functions of a rigid rotator are called spherical harmonics-selection rule in the rigid rotator approximation -1 unit

**Hydrogen atom:** Schrodinger equation for a hydrogen atom can be solved exactly -1 unit  
Quantum numbers and their characteristics - Diagrams of orbital wave functions and probability distribution functions - their significance. -1 unit  
Spin-Orbit interaction affects the energies of a hydrogen atom - 1 unit  
Electronic levels of a hydrogen atom are described by term symbols - 1 unit  
The spectrum of atomic hydrogen in an external magnetic field is accounted for by the Zeeman effect- Schrodinger equation for a helium atom cannot be solved exactly - 1 unit

**The variational method and perturbation theory:** The variational method provides an upper bound to the ground state energy of a system -1unit  
A trial function that depends linearly on the variational parameters leads to a secular determinant -1 unit  
Trial functions can be linear combinations of functions that also contain variational parameters- Perturbation theory expresses the solution to one problem in terms of another problem that has been solved previously - 1 unit  
Perturbation theory consists of a set of successive corrections to an unperturbed problem- Selection rules are derived from time-dependent perturbation theory - 1 unit

**Many electron atoms:** Atomic and molecular calculations are expressed in atomic units - Both perturbation theory and the variational method can yield good results for a helium atom -1 unit  
Hartree- Fock equations are solved by a self consistent procedure-wave functions must be antisymmetric in the interchange of any two electrons - 2 units  
Antisymmetric wave functions can be represented by Slater determinants - Hartree –Fock method uses antisymmetric wave functions -1 unit  
Correlation energy is the difference between the Hartree- Fock energy and the exact energy - 1 unit

**Application of quantum mechanics to diatomic molecules.** Molecular orbital theory - Application to hydrogen molecule ion. - 1 unit  
Valence bond theory - Application to the hydrogen molecule. -Comparison of the MO and VB theories. -1unit  
Huckel  $\pi$  electron theory and its simple chemical applications. - 2 units

**Molecular symmetry and group theory:** Symmetry elements and Symmetry operations--1 unit  
Elementary properties of groups, Sub-groups, classes, Generator - 1 unit  
Point groups-classification - 1 unit  
Matrix form of symmetry operations, Great orthogonality theorem (Qualitative)-1 unit  
Irreducible and reducible representations, Bases of representation - 1 unit  
Character tables( $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$  in particular). - 2 units  
Understanding the character table-Reduction formula-Vanishing Integral Rule. – 1 unit

Applications - Symmetry adapted linear combination, Application to Molecular Orbitals ( $O_h$ ,  $T_d$ ,  $D_{4h}$ ), hybrid orbitals ( $\sigma$  and  $\pi$ ) - 2 units

Deductions of normal modes of vibrations for polyatomic molecules( non-linear)- Cartesian coordinates method, internal coordinates method-general method- - 2 units  
 -Linear molecules(Integration method, Cyvin-Schafer method and Sub-group method)-3units  
 Crystal field splitting of d orbitals in transition metal complexes,  $O_h$ ,  $T_d$ ,  $D_{4h}$  -2 units  
 Applications to IR and Raman spectra, Selection rules for electronic, IR and Raman spectra. -2 units  
 Delocalization energy for  $\pi$  electron system (Butadiene and benzene). -3 units

**PRESCRIBED BOOKS:**

1. Quantum Chemistry by Donald A. McQuarrie, Second edition, University Science Books, California, 2008
2. Chemical Applications of Group Theory by Cotton 3<sup>rd</sup> Ed., Wiley1990
3. Quantum chemistry by R.K.Prasad, Wiley Eastern 1992.
4. Group theory and its applications to chemistry by K.V. Raman Tata Mc Graw Hill, 1990

**REFERENCE BOOKS:**

1. Molecular Quantum Mechanics by P.W. Atkins, 2<sup>nd</sup> Ed. Oxford 1983.
2. Quantum Mechanics in Chemistry by M.W. Hanne, 2<sup>nd</sup> Ed. Benjamin 1969.
3. Symmetry and Structure by S.F.A. Kettle, Wiley 1985.
4. Quantum Chemistry by Levine, 5<sup>th</sup> Ed, PH 2000.
5. Ideas of Quantum Chemistry by Lucjan Piela, Elsevier Amsterdam 2007.

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**PCHM-101(ii)****Mathematics for Chemistry (Non-credit course)**

Introduction to numbers (real numbers, complex numbers)	...2 hrs
Functions: properties of functions-operations on functions-Dirac delta function	...2 hrs
Calculus: Basics of differentiation-Basics of integration-Differential equations	...6 hrs
Determinants and Matrices: Matrix operations-properties of matrices	...5 hrs
Operators: linear operators-Hermitian operators	...2 hrs
Review of vector space: Introduction to vectors-vector operations-vector space-basis vectors-linear transformations-orthogonality properties	... 5 hrs
Eigen values and Eigen functions	... 3hrs
Probability and statistics	... 2 hrs
Series and limits	... 2 hrs
Spherical coordinates	... 2 hrs

There should not be any external examination on this mathematics course.

**PRESCRIBED BOOKS:**

- 1) Quantum Chemistry by D.A. McQuarrie, Oxford University Press, Second edition, 2007.
- 2) Mathematics for Chemistry & Physics by George Turrell Academic Press (2001)
- 3) Mathematics for Physical Chemistry by Donald A. McQuarrie (Author), Mervin Hansen (Illustrator) University Science Books (2008)
- 4) The Chemistry Maths Book by Erich Steiner, Oxford University Press (2008)
- 5) Maths for Chemistry: A Chemist's Toolkit of Calculations by Paul Monk, Oxford University Press (2006)
- 6) Mathematics for Physical Chemistry, 3edn. by Robert G Mortimer, Academic Press (2005)
- 7) Mathematics for Quantum Chemistry by Jay Martin Andersen, Dover Publications (2005)

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**Analytical Chemistry****Evaluation of Analytical data:**

The uses of Statistics –the standard deviation of computed results - Method of least squares  
- Methods for reporting analytical data. -2 units

**Application of equilibrium calculations to complex systems**

A systematic method for deriving algebraic equations describing multi-equilibrium systems  
The calculation of solubility by the systematic method – -2 units  
Influence of complexing agents on solubility -2 units  
Effect of pH on solubility -2 unit

**Separation techniques:**

Super critical fluid chromatography- Principle and instrumentation-Applications  
of SCF -2 units  
Super critical extraction chromatography: Principles, advantages and applications.  
(2 unit)

Capillary electrophoresis - Capillary electro-chromatography- -2 units  
Solvent extraction - Multiple batch extraction – -2 units  
Countercurrent distribution- -2 units  
Solid phase extraction - flow injection analysis - reverse osmosis, electro dialysis. -2 units  
Affinity chromatography. -1 unit  
Ultra High Performance Liquid Chromatography (UHPLC) -1 unit  
Pyrolysis gas chromatography; Fast Protein Liquid Chromatography - 2 units

**Instrumental methods:**

Different types of electrodes – mercury electrode, solid electrodes,  
Chemically modified electrodes and microelectrodes- -1 unit.  
Voltammetry - pulse voltammetry (normal, differential, square wave, stair case voltammetry),  
AC voltammetry, - chronoamperometry-bi-amperometry – -2 units  
Cyclic Voltammetry- -2 units  
Stripping Methods (anodic, cathodic, adsorptive) and applications, -2 units

**Radio analytical methods:**

Principle of Radio analytical methods- -1 unit  
Isotope dilution analysis – Radiometric titrations – precipitation and  
complex formation titrations -2 units

**Photo Electrochemistry and electro-chemiluminescence:**

Introduction to Photo-electrochemistry at semiconductor electrodes - -2 units  
Photoemission from metal electrodes - Electro chemical monitoring of photolytic intermediates -  
Electro-chemiluminescence- -2 units

**Instrumentation:**

U.V. - visible, IR., luminescence, Raman	-3units
NMR, Mass spectrometer	-2 units
Atomic absorption spectrometry – flame photometry-principles and applications	-2 units.

**PRESCRIBED BOOKS:**

1. Principles of Instrumental Analysis, by D. A. Skoog, F. J. Holler and T. A. Nieman, 5<sup>th</sup> Ed., Saunders College publishing 1998.
2. Laboratory Techniques in Electro Analytical Chemistry by P. T. Kissinger and W. R. Heineman, Marcel Dekker Inc. New York 1984.
3. Radio Analytical Chemistry Vol I & II by J. Tolgyessy and M. Krys. Ellis Horwood Ltd, 1989
4. Fundamentals of Analytical Chemistry by D. A. Skoog, D. M. West and F. J. Holler Saunders College Publication, New York - 5<sup>th</sup> Ed., 1988.
5. Analytical Electrochemistry by Joseph Wang, Wiley VCH, 2006.

**REFERENCE BOOKS:**

1. Supercritical Fluid Chromatography by R. M. Smith, The Royal Society of Chemistry 1988.
2. Perspectives in Modern Chemical Spectroscopy by D. L. Andrews Springer Verlag, 1990
3. Analytical Chemistry G. D. Christian, 5<sup>th</sup> Ed. John - Wiley & Sons 1994.
4. Qualitative analysis by R. A. Day Jr., A.L. Underwood 5<sup>th</sup> Ed., Prentice Hall of India, 1988.
5. Vogel's textbook of Quantitative Chemical Analysis (revised copy), 5<sup>th</sup> Ed., ELBS, 1994.

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## Coordination Chemistry

### Theories of Metal-Ligand Bonding:

Crystal field theory: Important aspects of crystal field theory -	-1 unit
d-orbitals splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal geometries –	- 2 units
10Dq value and its calculation - CFSE in weak field and strong field cases	-1 unit
Factors affecting magnitude of 10Dq - Spectrochemical series –	-1 unit
Jahn-Teller Theory-applications of crystal field theory (colour and magnetic properties of complexes) Limitations of crystal field theory.	- 2 units
Molecular Orbital theory : Formation of molecular orbitals by LCAO method - Nephelauxetic effect –	- 1 unit
MO energy level diagrams for octahedral, tetrahedral and square planar complexes involving only $\sigma$ bonding and $\sigma$ and $\Pi$ bonding –	-2 units
Measurement of pi-bonding effects.	-1 unit

### Study of complexes in solution:

Introduction to stability constants –	- 1 unit
Factors affecting stability constants - Kinetic and thermodynamic stability - Irwing-William series –	- 1 unit
Concept of Hard and Soft acids and bases -	- 1 unit
Methods of determining stability constants (spectrophotometric, conductometric and pH-metric methods).	- 2 units

### Electronic spectra of metal complexes:

A term symbol gives a detailed description of an electron configuration-allowed values of J	- 1 unit
Hund's rules are used to determine the term symbol of the ground electronic state-atomic term symbols are used to describe atomic spectra, Term symbols of $d^n$ ions	-1 unit
Russel –Saunders coupling is most useful for light atoms	- 1 unit
Spectra of transition metal ions -- Orgel diagrams for $d^2$ to $d^9$ octahedral and tetrahedral complexes	- 2 units
Tanabe - Sugano diagram for $d^2$ ion complex –	- 1 unit
Charge transfer transitions - Selection rules and transition probabilities based on symmetry considerations.	- 1 unit

### Magnetic properties of complexes:

Types of magnetism (dia, para, ferro and anti-ferromagnetism) - Temperature independent paramagnetism –	- 1 unit
Magnetic susceptibility and its determination by Gouy and Faraday methods	-1 unit
Calculation of magnetic moment from magnetic susceptibility-	-1 unit
Spin-orbit coupling and its effect on magnetic moments –	-1 unit
Orbital contribution to magnetic moment-single molecule magnets-	-1 unit

### **Kinetics and Mechanisms of Reactions:**

Inert and labile complexes-substitution reactions in octahedral and square planar complexes –  
- 1 unit

D, I<sub>d</sub>, I<sub>A</sub> and A mechanisms – - 2 units

Bond making and Bond breaking- The Langford- Gray nomenclature- - 1 unit

Coordination number and substitution mechanisms- Stereochemistry of substitution-  
-2 units

Effect of non-participating ligands on the stability of complexes. Trans-effect in square - planar  
complexes – -2 units

Theories of Trans-effect (Polarization and pi-bonding theories)- Quantitative aspects of the Trans  
effect- - 1 unit

Dissociation mechanism-Substitution of non- coordinating and coordinating solvents Electron  
transfer reactions: Inner and outer sphere mechanisms -2 units

Marcus Cross relationship - Template effect. - 1 unit

### **Photochemistry of Coordination compounds:**

Introduction to Photochemical reactions - Laws of Photochemistry - excited states of metal  
complexes - 1 unit

Relaxation processes of excited states - emission from excited states: [Cr(en)<sub>3</sub>]<sup>3+</sup> ion, [Ru(bpy)<sub>3</sub>]<sup>2+</sup>  
ion excited state electron transfer processes – - 1 unit

Brief account on Photo-substitution, photo-dissociation - 1 unit

Photo-oxidation, Photo-reduction and Photo-isomerisation reactions of complexes. -2 units

### **PRESCRIBED BOOKS:**

1. Fundamental Concepts of Inorganic Chemistry, Asim.K.Das, second edition  
(volumes:1-7), CBS Publishers and Distributors Pvt.Ltd. **2010**.
2. Inorganic chemistry by J.E. Huheey, E.A. Keiter and R.L. Keiter, Harper collins, 4<sup>th</sup> Ed.,  
1993.
3. Advanced Inorganic Chemistry by F.A. Cotton and G.W. Wilkinson, John Wiley, 5<sup>th</sup> Ed.,  
1988.
4. Mechanisms of Inorganic Reactions by F. Basolo and R.G. Pearson, Wiley Eastern, 2<sup>nd</sup> Ed.,  
1977.
5. Coordination Chemistry by F. Basolo and R. Johnson, W. A. Benjamin Inc., 1964.
6. Coordination Chemistry by D. Banerjee, Tata-McGraw-Hill 1993.
7. Complexes and First Row Transition Elements by David Nicholls, Macmillan 1974.
8. Molecular Magnetism by O. Kahn, Wiley VCH, 1993

## REFERENCE BOOKS:

1. Photochemistry of Coordination Compounds by V.Balzani & V.Carasitti, Academic Press, New York 1970.
2. Concepts and Models of Inorganic Chemistry by B. Douglas, D.H Mc Daniel & J.J. Alexander, 2<sup>nd</sup> Ed., John Wiley, New York 1983.
3. Transition Metal Chemistry by M. Gerloch & E.C Constable, VCH Publications New York, 1994.
4. Kinetics and Mechanisms of Reactions of Transition Metal Complexes by R.G Wilkins, 2<sup>nd</sup> Ed., VCH publications, 1991.
5. Inorganic Reaction Mechanisms by Martin L.Tobe and John Burgess, Longman, 1999.
6. Reaction mechanisms of Inorganic and Organometallic systems, 2<sup>nd</sup> Ed; by Robert B.J ordan, Oxford University Press, Oxford, 1991.
7. Inorganic Chemistry by Gary Wulfsberg, USB, California, 2000.
8. Electronic Structure and Properties of Transition Metal Compounds, 2<sup>nd</sup> Ed., Issac B Bersuker, Wiley (2010).

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**Advanced aspects of Organic Structure and Stereochemistry****Resonance and Aromaticity**

The concept of resonance as distinct from the phenomenon of tautomerism - a review with appropriate examples.	-1 unit
Less-common conjugative interactions such as hyperconjugation and homo-conjugation - evidences and illustrative examples.	-1 unit
Structure and chemistry of Dendralenes and Radialenes.	-2 units
Different criteria for aromaticity and different methods for determining aromatic character - concept of anti-aromaticity - Huckel's rule - Mobius system –	-1 unit
An introduction to computer assisted energy calculations of aromatic, anti-aromatic and non aromatic systems using ab initio molecular orbital packages/programs (PC Spartan & Hyperchem lite)	- 2 units.
Further illustrations of Huckel's rule - The simplest aromatic system - The cyclopropenyl carbocation.	-1 unit
Cyclobutadiene and cyclooctatetraene - Molecular orbital pictures to demonstrate their anti-aromaticity - Jahn Teller effect.	-1 unit
Non-benzenoid aromatic hydrocarbons derived from cyclo pentadienyl carbanion - The Fulvenes and Fulvalenes.	-1 unit
Cycloheptatrienyl carbocation - tropone and tropolones.	-1 unit
Annulenes - aromatic and anti - aromatic systems - ring current and its effect on proton magnetic resonance spectra.	-1 unit
Bicyclic and polycyclic aromatic systems - Azulenes.	-1 unit
Dewar's perturbation of molecular orbitals approach to the prediction of aromaticity, non-aromaticity and anti-aromaticity of conjugated cyclic systems. Alternate and non-alternate hydrocarbons and the concept of union.	-2 units
Heteroaromatic compounds - comparative aromaticity of five membered and six membered heterocyclic compounds containing one heteroatom. - An introduction with sydnones as example.	-2 units

**PRESCRIBED BOOKS:**

1. The Modern Structural Theory of Organic Chemistry by L.N. Ferguson, Prentice Hall 1966.
2. Advanced Organic Chemistry by J.March, 4<sup>th</sup> Edition, John Wiley & Sons, 1992.
3. Physical and Mechanistic Organic Chemistry by R.A.Y. Jones 2<sup>nd</sup> Ed., Cambridge University Press, 1984.
4. Highlights of Organic Chemistry, William J.Le Noble, Marcel Dekker Inc. New Yark, 1974.

**REFERENCE BOOKS:**

1. Chapters 6 and 13 in "Organic Chemistry" by S.H.Pine, J.B.Hendrickson, C.J.Cram and G.S.Hammond 4<sup>th</sup> Ed., Mc Graw Hill, Kogakusha ,1980.
2. Molecular Orbital Theory for Organic Chemists by A.Streitweiser Jr., John Wiley & Sons, 1961.

3. A Laboratory Book of Computational Organic Chemistry by W. J. Hehre, A.J.Shusterman, W.W.Huang, Wavefunction Publications, 1996.

**Valence bond tautomerism and rigid structures:**

Explanation of the phenomenon of valence - bond tautomerism fluxional molecules illustrated by homotropyliene and bullvalene. -1 unit  
The chemistry of fullerenes with particular reference to buckminsterfullerene - C<sub>60</sub>  
Determination of structure, reactions and applications. -1 unit

**PRESCRIBED BOOK:**

1. Advanced Organic Chemistry by Michael B. Smith & J. March, 5<sup>th</sup> Ed., John Wiley & Sons, Inc, New York, 2001.

**Conformational Analysis:**

Conformations of cyclic compounds - small ring systems (Cyclopropane, Cyclobutane and Cyclopentane) - A review. -1 unit  
Conformations of cyclohexane and cyclohexanone, and monosubstituted cyclohexanes-disubstituted cyclohexanes - Conformational and configurational isomerism - Relative order of stabilities - preferred conformations. -2 units  
Conformational analysis of cyclohexanes - Dynamic aspects- typical reactions which bring out the differences between stereoisomers. -2 units  
Medium - size ring systems - Conformations of Cyclopentane, Cyclooctane, and Cyclononane. -1 unit  
Conformations of cyclodecane - transannular reactions with particular reference to the cyclodecane system. -2 units  
Bicyclic compounds with particular reference to decalin -1 unit  
Strained bicyclic systems. -1 unit  
Application of PMR spectral data(coupling constants in conformational analysis) -1 unit

**Advanced aspects of configurational isomerism:**

Sequence rule and its applications to a wide range of situations. -2 units  
Stereochemistry of compounds containing two and more unequal chiral centers - Concept of pseudo-chirality. -1 unit  
Stereochemistry of allenes and spirans. -1 unit  
Optical isomerism due to restricted rotation. Atropisomerism, Isomerism exhibited by Biphenyls. -2 units  
Further examples of atropisomerism - polyphenyls, "Ansa" compounds, "paracyclophanes" and hexahelicene. -1 unit  
Determination of absolute configuration - chemical interconversions - classical examples of (+) tartaric acid, (-) Lactic acid and related compounds. -1 unit  
Chemical correlations involving diastereoisomers - Determination of the absolute configuration of shikimic acid. -1 unit  
Configurational assignments based on asymmetric synthesis - Applications of Cram's rule and Prelog's rule - illustrative examples. -2 units



Chiro-optical methods-principles of optical rotatory dispersion and circular Dichroism- -1 unit  
Applications of the O.R.D. and C.D techniques - plain and cotton effect curves- -1 unit  
The alpha - halo - ketone rule and their applications – -1 unit  
Electrophilic and Nucleophilic additions in Substituted cyclohexene and cyclohexyl epoxide systems. -1 unit

### **PRESCRIBED BOOKS:**

1. Stereochemistry of carbon compounds by Ernest L. Eliel, Tata McGraw-Hill Publishing Company Ltd.; 14th Reprint edition, 1990.
2. Stereochemistry of organic compounds principles and applications by D. Nasipuri, Wiley Eastern, January 1994.
3. Organic chemistry by J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, Sec. Ed. 2005. (Pg no 468-470, 858-861).

### **REFERENCE BOOKS:**

1. The Modern structural theory of organic chemistry by L.N. Ferguson, Prentice Hall of India, 1966.
2. Stereochemistry and conformational analysis by J. Dale, Verlag Chemie, 1978.
3. Stereochemistry by E.B. Ramsay, Heyden, 1981.
4. Carbon-carbon and carbon - Proton NMR couplings - Applications to Organic Stereochemistry and Conformational analysis by J.A. Marshall, Florida Verlag Chemie, 1983.
5. Stereochemistry by K. Mislow, Benjamin Cummings Publications, 1965.
6. Stereospecificity in organic chemistry and Enzymology by J. Reney and J.A. Robinson, Florida, Verlag Chemie-Monographs in Modern Chemistry, 1982
7. Fullerenes, Ed George S Mammond, Valerie J Cook, ACS symposium series, 4 :1 , 1982.

\* \* \*

**PCHM-105**

2 CREDITS

**Practicals: Coordination Chemistry (Preparation and Analysis)**

Preparation of inorganic complexes of transition metals with common oxygen and nitrogen, donor ligands and determination of metal content of these complexes by standard analytical methods.

Potassium tri(oxalato)ferrate(III)trihydrate.

Sulphatotris(thiourea)zinc (II)

Hexammine nickel(II) chloride

Tris (en)nickel(II) chloride.

Chloropentamine cobalt(III) chloride.

Potassium bis(oxalato)cuprate(II)dihydrate.

Polarographic determination of 1) cadmium and 2) zinc.

Analysis of spectra of a few typical coordination complexes.

**PRESCRIBED BOOKS:**

- 1) A text book of quantitative inorganic analysis by A.I.Vogel 4 Ed., ELBS, 1978.
- 2) Practical Inorganic Chemistry by G. Pass and H. Sutcliffe, 2 Ed., Science Paperbacks.
- 3) Inorganic Experiments, Ed., by J. Derek Woolins, 3<sup>rd</sup> Revd. Ed., Wilry-VCH, 2010.

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**PCHM-106**

2 CREDITS

**Practicals: Analytical Chemistry  
(Conductometry, Potentiometry, Voltammetry)**

Dissociation constants of a polyprotic acid -pH titration.

Simultaneous spectrophotometric determination of chromium and manganese.

Fluoride determination by null point method.

Manganese determination by titrating with permanganate in neutral pyrophosphate solution.

Estimate concentration of H<sub>2</sub>SO<sub>4</sub>, CH<sub>3</sub>COOH and CuSO<sub>4</sub> by conductometric titration with NaOH.

Titration of Ferrous ammonium Sulphate with Cerium Sulphate.

Titration of pure solutions of KI, KCl and KBr and their mixtures against AgNO<sub>3</sub>.

Variation of refractive index with mixtures of CCl<sub>4</sub> and ethyl acetate.

Hydrolysis constant of aniline hydrochloride

Titration of Ferrous ammonium sulphate with potassium dichromate using bimetallic electrode.

Determination of indicator constant.

Determination of ionisation constants.

Differential pulse voltammetric analysis of trace ions present in natural samples

**PRESCRIBED BOOKS:**

1. Chemistry experiments for Instrumental Methods by Donald T.Sawyer, William R.Heineman & Jalice M.Beebe, John Wiley & Sons, 1984.
2. Vogels Textbook of Quantitative Chemical Analysis (revised copy) 5<sup>th</sup> Ed., ELBS, 1994.
3. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.

\* \* \*

**Practicals: Organic Qualitative Analysis**  
**(Mixture analysis & drug analysis)**

Separation of mixtures containing 2 organic compounds and their characterisation by qualitative analysis.

TLC analysis of some patent medicines.

**PRESCRIBED BOOKS:**

- 1) Elementary Practical Organic chemistry Part II, Qualitative Organic analysis by A.I Vogel 2<sup>nd</sup> Ed, CBS publications, 1987.
- 2) Thin Layer chromatography - Laboratory Work book edited by Eigen Stahl, Springer International student edition, 1969.
- 3) Chromatography in Organic micro-analysis - A laboratory guide by Raphael Ikan, Academic press, 1982.
- 4) Quantitative analysis of Drugs in Pharmaceutical preparations by P.D. Sethi, 3<sup>rd</sup> Ed., CBS publishers, 1997.
- 5) Experimental Organic Chemistry by P.R. Singh, D.S. Gupta and K.S. Bajpai, Vols I & II, Tata Mc Graw Hill, 1980.

\* \* \*

**Structural Inorganic and Bio-Inorganic Chemistry****Structural Inorganic Chemistry:****Synthesis, Reactions, Structure and Bonding in:****Catenated compounds:** Catenation - Heterocatenation, Intercatenation - 2 units

Isopolyanions and Heteropoly anions. - 2 units

**Ring compounds:** Borazines - Phosphazines, Polyphosphazines-sulfur-nitrogen rings and other Heterocyclic systems - 2 units

Homocyclic inorganic ring systems (S, Se &amp; P and oxocarbon anions). - 2 units

**Cage compounds:** Phosphorous cage compounds with oxygen, sulfur and arsenic atoms- 1 unit

Boron cage compounds: Boranes, Synthetic strategies in Boron cage chemistry, Pharmacologically active Boron analogues of amino acids, - 2 units

The Pyrazoboles, Carboranes and Metallocarboranes. - 1 unit

**Inorganic polymers:** Synthesis, structure and applications of the polymers

Polyphosphazenes, - 1 unit

Polysilanes - 1 unit

Polysiloxanes - 1 unit

Metal chelate polymers. - 1 unit

Inorganic polymers that contain phosphorous, Boron and Sulphur - 1 unit

**Bio-Inorganic chemistry:**

New perspectives and biological roles of essential trace elements. - 2 units

**Oxygen carriers:** Transport and storage of dioxygen – -1 unit

Reactions of dioxygen- structure and functioning of hemoglobin and myoglobin - 2 units

Hemerythrins Hemocyanin - 1 unit

Model compounds for oxygen carriers (Vaska's iridium complex, cobalt - DMG complex). -1 unit

**Biological nitrogen fixation:** Nitrogen fixing organisms - structure and function of nitrogenase enzyme - Chemistry of nitrification – -2 units

Fixation via nitride formation – - 1 unit

Dinitrogen complexes as biological models. -1 unit

**Metalloproteins - Metalloenzymes:** The characterization of metal - binding sites -1 unit

Carbonic anhydrase – Carboxy peptidase – -2 units

Super oxide dismutase - Structure and biochemical functions of B<sub>12</sub> Coenzyme. - 1 unit**Alkali metal transport in Biological systems:**

Introduction - Coordination chemistry of alkali metal ions- - 2 units

Ion transport - Modes of passage – - 1 unit

Sodium dependent transport. - 1 unit

**Metal ions toxicity and Chelation therapy:**

Toxicity of metal ions particularly heavy metal ions –	- 1 unit
Chelating agents-chelation therapy –	- 1 unit
Therapeutic uses of metals, ligands and complexes with special reference to anti-cancer activity.	- 2 units

**Metal ion folding and cross-linking of biomolecules:**

Metal-ion stabilisation of protein structure and nucleic acid structure	- 2 units
Protein binding to metallated DNA	- 2 units
Metal-organised structures as probes for conformation	-1 unit

**PRESCRIBED BOOKS:**

1. Inorganic Chemistry by J.E. Huheey, E.A. Keiter and R.L.Keiter, Harper collins, 4<sup>th</sup> Ed., 1993.
2. Advanced Inorganic chemistry by F.A. Cotton and G. Wilkinson, 5<sup>th</sup> Ed., John Wiley, 5<sup>th</sup> Ed., New York, 1988.
3. Structural Inorganic chemistry by A.F Wells 5<sup>th</sup> Ed., Oxford science publications, 1987.
4. Chemistry of the elements by N.N. Greenwood and A. Earnshaw, 2<sup>nd</sup> Ed., Butterworth-Heinemann, 1997.
5. Inorganic Polymers, J.E. Mark, H.R. Allcock and R. West, Prentice Hall 1992.
6. Inorganic Reactions of biological processes by M.N. Hughes, John-Wiley, 2<sup>nd</sup> Ed., New York 1981.
7. Bioinorganic Chemistry by Wolfgang Kaim and B. Schwederski, John Wiley, New York, 1994.
8. Inorganic Biochemistry - An Introduction by J.A.Cowan, VCH, 1993.
9. Principles of Bioinorganic Chemistry by S.J.Lippard and J.M.Berg, University Science Books, California, 1994.

**REFERENCE BOOK:**

1. Advances in Boron and the Boranes, A. Reenberg and R.E. Williams, VCH, 1988.
2. Inorganic and Organometallic Polymers, Vadapalli Chandrasekhar, Springer, 2005.

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## Chemical Kinetics and Surface Chemistry

### CHEMICAL KINETICS:

#### Theories of Reaction rates:

Kinetic theory of collisions	-1 unit
Rate theories based on thermodynamics and statistical mechanics-conventional transition state theory some applications of conventional transition state theory	-2 units
Thermodynamic formulation of conventional transition state theory - assumptions and limitations of conventional transition state theory	-2 units
Extensions of transition state theory - microscopic reversibility.	-1 unit

#### Elementary Gas - Phase Reactions:

Bimolecular reactions - Trimolecular reactions - Unimolecular reactions.	-2 units
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#### Elementary Reactions in Solutions:

Solvent effects on reaction rates - Factors determining the reaction rates in solution - Reactions between ions - Ion-dipole and Dipole - Dipole reactions	-2 units
Extra thermodynamic relationships - Isokinetic relationship	-2 units

#### Composite Reactions:

Types of composite mechanisms - rate equations for composite mechanisms	-1 unit
Chain reactions - Some inorganic mechanisms - Hydrogen - Bromine, Hydrogen - Chlorine and Hydrogen - Iodine reactions	-2 units
Organic decompositions - Goldfinger - Letort - Ni clause rules - Inhibition mechanisms - Acetaldehyde decomposition –	-2 units
Gas - Phase combination -Hydrogen - oxygen reaction.	-1 unit

#### Photochemical and Radiation chemical Reactions:

Photochemical reaction - Laser photochemistry - Photosensitisation - Radiation Chemical reactions.	-2 units
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#### Homogeneous Catalysis:

General catalytic mechanisms - Acid-base catalysis -	-1 unit
Catalysis by enzymes - influence of concentration (single substrate, double substrate), inhibition,	-2 units
Transient - Phase kinetics, Sigmoid kinetics - kinetics of bacterial growth.	-1 unit

#### Isotope Effects:

Equilibrium isotope effects - Primary kinetic isotope effects - Secondary kinetic Isotope effects.	-2 units
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#### Reaction Dynamics:

Molecular dynamical calculations - The reactions $H+H_2$ , $Br+H_2$ and more complex reactions - chemiluminescence.	-2 units
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**Fast Reactions :**

Relaxation kinetics - Basic principles of chemical relaxation methods - chemical relaxation in two step and multi-step synthesis – -2 units

Experimental methods for the study of relaxation kinetics and applications. Temperature jump method – Diffusion controlled reactions - Fluorescence quenching – Common ion inhibition -2 units

Flash photolysis and introduction to Time resolved Pico/femto second methods (e.g. introduction to Time Correlated Single Photon Counting) -1 unit

**Surface Chemistry:**

Adsorption of gases and vapors on solids: Adsorption time - the Langmuir adsorption isotherm - kinetic derivation – -1 unit

Statistical derivation of Langmuir adsorption isotherm -1 unit

Adsorption entropies - lateral interaction - The BET and related isotherms - derivation of the BET equation - properties of the BET equation - -2 units

Langmuir Blodgett Films structure and characterization mixed LB film, studies of the LB deposition process- thermodynamics of adsorption -2 units

Chemisorption and Catalysis - Chemisorption - the molecular view - Chemisorption isotherms - kinetics of Chemisorption - The Chemisorption bond. -1 unit

Electrical aspects of surface chemistry - electrical double layer - Stern treatment of the electrical double layer, -1 unit

Free energy of a diffuse double layer - Repulsion between two plane double layers - zeta potential - -1 unit

Electrophoresis, Electro-osmosis, Streaming potential and Sedimentation potential -3 units

**PRESCRIBED BOOKS:**

1. Chemical Kinetics - K.J. Laidler, 3<sup>rd</sup> edition, Pearson Education Inc., 1987.
2. Chemical Kinetics - The study of reaction rates in solution, K.A. Connors – VCH Publishers, New York 1990.
3. Chemical Kinetic Methods, C. Kalidas, New Age International Publishers, New Delhi, 1996.
4. Introduction to molecular dynamics and chemical kinetics. G.D. Billing and K.V. Mikkalsen, John Wiley & Sons 1996.
5. Physical chemistry with biological application by K.J.Laidler, Benjamin Cummings Publications Company Inc., Menlo Park, California 1978.
6. Physical chemistry of surfaces, 6th Ed. A.W. Adamson and A.P. Gast, John Wiley & Sons 1997.

## REFERENCE BOOKS:

1. Fundamentals of Chemical relaxation by H. Strehlow and W. Knoche, Verlag Chemie, Weinheim 1977.
2. Physical organic chemistry, The fundamental concepts, C.D. Ritchie, Marcel Dekker, Inc, 1990.
3. Modern Electrochemistry, Volume 2A – Fundamentals of Electrode Processes, 2<sup>nd</sup> ed., by J. O. M Bockris, A. K. N. Reddy, M. Gamboa-Aldeco, Kluwer Academic Publishers, New York 2002.
4. Principles of colloids and surface chemistry, 2<sup>nd</sup> edition, P.C. Hiemenz. Marcel Dekker, INC. 1986.

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## Thermodynamics and Electrochemistry

### Statistical Thermodynamics:

Introduction: The distribution laws - negative absolute temperatures –	- 2 units
Partition function - Thermodynamic functions in terms of the partition function-	1 unit
Molecular interpretation of the basic laws of thermodynamics –	-1 unit
Evaluation of the partition function - Translational partition function –	-2 units
Rotational partition function -	-2 units
Vibrational partition function –	-2 units
Electronic partition function - Nuclear partition function –	-1 unit
Statistical thermodynamics of gaseous mixtures –	-1 unit
Statistical interpretation of the equilibrium constant –	-1 unit
Statistical thermodynamics of an ideal crystal -	-2 units
Ideal lattice gas – Electron gas	-1 unit
Statistical derivation of the equation of state for nonideal fluids -.	-2 units

### Non Equilibrium Thermodynamics

Introduction - Entropy production in Chemical reactions - Entropy production and Entropy flow in open systems –	-2 units
Transformation properties of rates and affinities - Onsager's theory - Irreversible Thermodynamics and biological systems - Oscillatory reactions.	-2 units

### Electrochemistry:

Debye-Huckel Onsager equation-Derivation-	- 1 unit
Electrodics - Introduction - The basic electrodic equation - The Butler - Volmer equation –	-2 units
The current potential laws at other types of charged interfaces –	-1 unit
The quantum aspects of charge transfer reactions at electrode solution inter faces -	1 unit
Electrode reactions and chemical reactions – multistep reactions – transient behavior of interfaces – transport in the electrolyte effects, charge transfer at the interface.	-2 units
Determining the step wise mechanism of an electrodic reaction, current potential laws for Electro chemical systems.	-2 units
Electrodic reactions of special interest – Electro catalysis – Electro growth of metals on electrodes – hydrogen – evolution reaction – electronation of oxygen.	-2 units
Electro chemical systems of technological interest, technological aspects of electrochemistry – corrosion and the stability of metals.	-2 units
Electrochemical energy conversion – Electricity storage.	-1 unit
Photo electrochemistry: Introduction-Band bending at the semiconductor/solution interface- Photoexcitation of electrons by absorption of light-Surface effects in photoelectrochemistry-	-2 units
Photoelectrocatalysis-The photoelectrochemical splitting of water-The photoelectrochemical reduction of CO <sub>2</sub> .	-1 unit
Bioelectrochemistry: Bioelectrodics-Membrane potentials-Electrochemical communication in biological organisms-	-2 units

Enzymes as electrodes.	-1 unit
Electrochemical sensors-electrochemical biosensors-gas sensors-solid state devices and sensor arrays.	- 2 units
Electrochemical impedance spectroscopy	- 1 unit

**PRESCRIBED BOOKS:**

1. Physical chemistry, by Robert G. Mortimer, Third edition, Academic press, 2008.
2. Physical Chemistry by U.Fried, H.F.Hameka and U.Blukis Macmillan Publication, 1977.
3. Modern Electrochemistry, Volumes 1 & 2, JOM Bockris and AKN Reddy Plenum Press, New York. 1988.
4. Chemical Thermodynamics P.A.Rock, University Science Books, 1983.
5. Modern Electrochemistry 2B, 2<sup>nd</sup> edition, JOM Bockris and AKN Reddy, Kluwer Academic/Plenum Publishers, New York, 2000.
6. Thermodynamics by J. Rajaram and J. C. Kuriacose, 2<sup>nd</sup> Ed., SLNC & Co., 1993.
7. Electrochemical methods –Fundamentals and Applications by A.J. Bard and L.R. Faulkner, Second edition, John Wiley and Sons

**REFERENCE BOOKS:**

1. Electrochemistry theoretical foundation - J. Goodieman John Wiley sons 1987.
2. Spectro electrochemistry - Theory and Practice R.J.Gale, Plenum Press New York, 1988.
3. Principles of colloids and surface chemistry, 2<sup>nd</sup> edition, P.C. Hiemenz. Marcel Dekker,INC. 1986.
4. Physical chemistry of surfaces, 6<sup>th</sup> Ed. A.W. Adamson and A.P. Gast, John Wiley & sons 1997.
5. Introduction to Thermodynamics of Irreversible Processes by I. Prigogine, 3<sup>rd</sup> Ed. Interscience Publishers, 1967.

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**Physical and Mechanistic aspects of Organic Chemistry****Nucleophilic addition to the carbonyl group:**

Hydride transfer reactions, stereochemistry of hydride reduction –	-1 unit
Clemmenson & Wolff Kishner reductions-	-1 unit
Crossed and intramolecular Cannizzaro reactions-	-1 unit
Mechanism of benzoin condensation and crossed aldol condensations-	-1 unit
Reformatsky reaction, Claisen and related condensation reactions -	-1 unit
Thorpe reaction, Stobbe condensation-	- 1 unit
Acyloin condensation and its usefulness in the synthesis of large ring compounds -	1 unit
Mannich reaction and Ritter reaction –	- 1 unit

**Elimination reactions:**

Chugaev reaction, cleavage of quaternary ammonium hydroxides, quaternary ammonium salts with strong bases –	- 2 units
Amine oxides, sulfoxides & selenium oxides –	- 1 unit
Conversion of epoxides to olefins - Shapiro reaction - decomposition of p-toluene - sulfonyl hydrazones –	- 1 unit
Cis - elimination - pyrolytic eliminations - Stereochemistry.	- 1 unit
1,4 - Addition of organometallic compounds to activated double bonds.	- 1 unit

<b>Aromatic substitution reactions:</b> A review of the generalized mechanism - directive and rate controlling factors – Substituent effects ,Partial rate factors-	- 2 units
Gattermann formylation, Vilsmeier - Hack formylation and related reactions-	- 1 unit
Nucleophilic aromatic substitution reactions going through the benzyne mechanism -- and Meisenheimer complex –	1 unit
SR <sub>N1</sub> aromatic substitution reactions - Aromatic homolytic substitution reactions,	-1 unit
Substitution reactions of thiophene, furan, pyrrole –	- 2 units
pyridine, pyridine oxide- quinoline and isoquinoline –	- 2 units
Addition reactions of furan & thiophen - Chichibabin reaction, Skraup syntheses & Fisher indole synthesis-	- 2 units
Modifications to Hammett equation, Brown and Taft equations -	-2 units

<b>Pericyclic reactions:</b> Electrocyclic reactions	- 1 unit
Cycloaddition reactions: 2+2 photochemical and-[2+2] Thermal Pericyclic reactions suprafacial and antarafacial additions-	- 1 unit
Stereochemistry of Diels - Alder reaction-	- 1 unit
Sigmatropic rearrangements –	-1 unit
Claisen, abnormal Claisen and Cope rearrangements-	-1 unit
FMO approach and aromatic transition state theory in pericyclic reactions	
Examples and problems on pericyclic reactions-	-1 unit

**Molecular rearrangements:** Benzilic acid and Demjanov rearrangements- 1 unit  
 Favorskii and Wolff rearrangements (Arndt - Eistert synthesis), dienone - phenol (thermal and photochemical)- - 2 units,  
 Stevens, Somelet and Wittig rearrangements- - 1 unit  
 The benzidene rearrangement. Intramolecular migrations from nitrogen to carbon - the Orton, Fisher - Hepp and related rearrangements. Hoffman - Loffer Freytag reaction and Hauser rearrangement- -2 units

**Free radical reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism of an aromatic substrate, neighboring group assistance- -1 unit.  
 Reactivity for aliphatic and aromatic substrates at a bridged head. Reactivity in the attacking radicals. The effect of radicals on reactivity- -1 unit.  
 Allylic halogenation (NBS), Oxidation of aldehydes to carboxylic acids – -1 unit,  
 Auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts - 1unit; Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction- -1 unit  
 McMurray Coupling, Barton Reaction, AIBN with (Bu)<sub>4</sub>Sn-H -1 unit

**PRESCRIBED BOOKS:**

1. Advanced organic chemistry by Carey and Sundberg, 5<sup>th</sup>. Ed., Part B, Plenum Press, 2012.
2. Organic chemistry by J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, Sec. Ed. 2005.
3. Advanced organic chemistry by J.March, 5<sup>th</sup> Ed. Wiley - Interscience, 1991.
4. Physical and Mechanistic Organic Chemistry by R.A.Y. Jones, 2<sup>nd</sup> Ed., Cambridge University Press, 1984.
5. Modern Synthetic Reactions by Herbert O. House, Benjamin/Cummings, 2<sup>nd</sup>. Ed. 1972.
6. Pericyclic reactions by S.N.Mukerji, Macmillan, 1979.
7. Organic reactions and mechanisms by P.S. Kalsi, 3<sup>rd</sup> Edition, New age international Publishers 2010.

**REFERENCE BOOKS:**

1. Organic reactions, Eds. William D. Dauben et al., Vol.1 to 6 and 28 - 31 John Wiley & Sons, 1947 -1984.
2. Principles of organic syntheses: by R.O.E Norman, 2<sup>nd</sup> Ed., part B, Methusan, 1978.
3. The Physical basis of organic chemistry: by H.Maskill, Oxford science publications, 1985.

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**Practicals: Inorganic Chemistry**

Semi-micro qualitative inorganic analysis of mixture of three salts containing three anions and three cations including interfering ions.

**PRESCRIBED BOOKS:**

- 1) Applied Chemistry (Theory & Practice), O.P.Vermani & A.K.Narula, Wiley Eastern, 1989.
- 2) Vogel's text book of macro and semimicro Qualitative Inorganic Analysis Ed G.Svehla Orient Longman 1982.

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**Practicals: Chemical Kinetics and Electrochemistry**

1. To investigate the mutarotation of glucose catalysed by acid or base.
2. To study the kinetics of hydrolysis of ethylacetate by NaOH at two temperatures by conductance measurements and hence the energy of activation of the reaction.
3. To study the kinetics of hydrolysis of t-butyl chloride and determine the order and energy of activation of the reaction.
4. To study the kinetics of the reaction between  $K_2S_2O_8$  and KI, determine the rate constant and order of the reaction, study the influence of ionic strength on the rate constant
5. To investigate the reaction between acetone and iodine.
6. To study the kinetics of decomposition of complex formed between sodium sulphide and sodium nitroprusside.
7. To study the decomposition of oxalic acid in solution photosensitized by uranyl sulphate
8. To plot a polarogram for mixture of  $Cd^{2+}$ ,  $Zn^{2+}$  and  $Mn^{2+}$  ions
9. Determination of formula of a complex by voltammetric analysis.
10. Cyclic voltammetric analysis of natural samples
11. Electrochemical of corrosion current and corrosion potential of any system which undergoes corrosion.
12. Determination of corrosion current and corrosion potential of any system which undergoes corrosion.
13. Electrochemical studies with modified electrodes.
14. Electrochemical synthesis of conducting polymers.
15. Determination of rates of hydrolysis of some organic esters and verification of Hammett equation.

**PRESCRIBED BOOKS:**

- 1) Modern Experiments for Introductory Chemistry, compiled by Neidig and Stratton, 2<sup>nd</sup> Ed., Reprinted from Journal of Chemical Education, 1990.
- 2) Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.
- 3) Experimental Physical Chemistry by A.M. Halpern, 2<sup>nd</sup> Ed., Prentice Hall, 1997.

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**Practicals: Organic Synthesis (multistep) and Spectral Analysis**

Multi-step preparations of organic compounds illustrating the preparative uses of reactions such as aldol condensation, mannich reaction, enamine reaction, claisen condensation etc., and rearrangements such as Claisen, Fries, Beckmann, Wolff etc.,-Preparation of amino acetone semi-carbazone hydrochloride, ethyl  $\gamma$ -bromo butyrate.

Design and synthesis of organic compounds possessing novel features.

Experiments involving - enamine reactions, Robinson annelation, Wittig reaction and protection - deprotection sequence (use of cyclic acetals in the protection of carbonyl - use of ester in the protection of alcohols or phenols etc.,)

Preparative organic photochemistry - preparation of phenanthrene - 9-carboxylic acid and benzpinacol.

Use of polymer supported organic synthesis (Silica supported reagents, alumina supported reagents etc.)

Zeisel's estimation, Zeriwittinoff's estimation

**PRESCRIBED BOOKS:**

1. Experimental technique in Organic Chemistry by D.J Pasto, C.R.Johnson and M.J.Miller, Prentice Hall, 1992.
2. Experimental Organic Chemistry: Principles and Practice by L. M. Harwood and C.J. Moody, Blackwell Scientific Publications, 1989
3. Reactions and Syntheses by L.F. Tietze and Th. Eicher, University Science Books, California, 1989.
4. Vogels Textbook of Practical Organic Chemistry revised by B. S. Furniss et al., 5<sup>th</sup> Ed., ELBS, 1989.

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**Organometallic Chemistry****Transition Metal Carbon Monoxide Compounds:**

Introduction-the 18-electron rule and its limitations-	-1 unit
Preparation of metal carbonyls - Structures of metal carbonyls (mononuclear, binuclear, trinuclear, tetra nuclear and poly nuclear) –	-2 units
Bonding features: semibridging CO groups (in cyclic sets, in unsymmetrical environments and caused by steric crowding) –	-2 units
Side-on bonding of CO - oxygen to metal bond -	- 1 unit
Vibrational spectra of metal carbonyls (detection of bridging of CO groups, molecular symmetry, bond angles,mixture of conformers, force constants) –	- 2 units
Reactions of metal carbonyls:CO substitution reactions, photochemical reactions, Nucleophilic and electrophilic attacks on CO.	-2 units

**Transition Metal Dinitrogen and Nitrosyl complexes:****Dinitrogen complexes:**

Preparation of dinitrogen complexes-	- 1 unit
Structure and bonding of dinitrogen complexes-	- 1 unit
Comparison of stability of isoelectronic CO and N <sub>2</sub> complexes-	- 1 unit
Dinitrogen complexes in chemical fixation of nitrogen.	- 1 unit

**Nitrosyl complexes:**

Preparation of nitrosyl complexes of Ir., Ru, Cr. and Mn	- 1 unit
Structure of nitrosyl complexes of Ir., Ru, Cr. and Mn	-1 unit
Bonding in nitrosyl complexes of Ir., Ru, Cr. and Mn	-1 unit
Linear and bent nitrosyl groups.	- 1 unit

**Clusters and Metal-Metal Bonds:**

Introduction -metal carbonyl clusters: Low nuclearity carbonyl (M <sub>s</sub> and M <sub>4</sub> ) clusters -	
Isoelectronic and Isolobal relationships –	- 2 units
High nuclearity carbonyl clusters (HNCC <sub>s</sub> ) –	- 1 unit
Hetero atoms in metal atom clusters (carbide and nitride containing clusters) - Electron counting schemes for HNCC <sub>s</sub> - The capping rule.	- 2 units

<b>Lower halide and chalcogenide clusters:</b> Octahedral metal halide and chalcogenide clusters –	- 1 unit
Triangular clusters - Solid state extended array systems.	-1 unit

<b>Compounds with M-M multiple bonds:</b> Major structural types - Quadrupole bonds in clusters –	-2 units
One dimensional solids.	-1 unit

**Transition Metal Complexes of Hydrocarbons:**

Metal alkyls, carbenes, carbynes and carbides –	- 1 unit
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Nonaromatic alkene and alkyne complexes –Metal carbenes-Fisher and Schrock carbenes-  
 -2 units  
 Applications in olefin metathesis, particularly Grubb’s catalyst -1unit  
 Allyl and pentadienyl complexes - Metallocenes: synthesis and structures of cyclopentadienyl  
 compounds – -1unit  
 Arenes and other Alicyclic Ligands- stability of Polyene and polyenyl complexes-1unit.

### Reactions of Organometallic Complexes:

Oxidative addition reactions: Concerted additions-SN<sup>2</sup> reactions and radical mechanisms  
 -2 units  
 Hydrogen addition and HX additions - Reductive elimination reactions -  $\sigma$  -bond  
 metathesis-Oxidative coupling-reductive cleavage – -2 units  
 Insertion reactions: CO insertion into M - C and M-H bonds - Cyclometallation reaction.  
 -2 units

### Catalysis by Organometallic Compounds:

Synthetic gasoline - Polymerisation (Ziegler Natta Catalyst) – Oligomerisation -2 units

### Applications of Organometallic compounds

in a) Agriculture and Horticulture,  
 b) Industry and c) Medicine - 3 units

### PRESCRIBED BOOKS:

1. Inorganic Chemistry by E. Huheey, E.A. Keiter and R.L. Keiter. 4<sup>th</sup> Ed., Harper Collins 1993
2. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson. 5<sup>th</sup> Ed., Wiley 1988
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, 2<sup>nd</sup> Ed., Butterworth, 1997.
4. Organometallic Chemistry by R.C. Mehrotra and A. Singh, Wiley Eastern Ltd, 1991.
5. Reaction Mechanisms of Inorganic & Organometallic systems by R.B. Jordan , 2<sup>nd</sup> Ed., Oxford University Press, New York 1998.
6. Organometallic Chemistry of Transition metals by R.H. Crabtree.
7. Basic Organometallic Chemistry, I. Haiduc and J.J. Zuckerman, WDeG Publishers, 1985.
8. Concepts and Models of Inorganic Chemistry- 2<sup>nd</sup> Ed; - B. Douglas, D. McDaniel and J. Alexander, Wiley and Sons, New York (1983)

### REFERENCE BOOKS:

1. Inorganic Chemistry, K.F. Purcell and J.C. Kotz ., W.B. Saunders Co.,1977.
2. Structural Inorganic Chemistry, 5<sup>th</sup> Ed; A.F. Wells, OSP, Oxford, 1987
3. Comprehensive Organometallic chemistry, edited by G. Wilkinson, F.G.A. Stone and E.W. Abel (9 volumes), 1982

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## Polymer Chemistry and Special Topics from Physical Chemistry

### POLYMER CHEMISTRY:

**Step Polymerisation:** Mechanism of step polymerisation - kinetics of step polymerisation - molecular weight control in linear polymerisation – -3 units  
 Molecular weight distribution in linear polymerisation polyfunctional step reaction polymerisation - Newer types of step polymerisation. -2 units

**Radical Chain Polymerisation:** Nature of radical chain polymerisation - Rate of radical chain polymerisation - -2 units  
 Initiation - molecular weight - chain transfer - inhibition and retardation - Determination of absolute rate constants - energetic characteristics - auto acceleration – -2 units  
 General considerations on Living Radical Polymerisation - Introduction to ATRP and RAFT -2 units

**Emulsion polymerisation:** Qualitative picture - quantitative aspects - other characteristics of emulsion polymerisation. -2 units

**Ionic chain polymerisation:** Comparison of radical and ionic polymerisations - kinetics - cationic polymerisation of the carbon - carbon double bond -2 units  
 Anionic polymerisation of the carbon - carbon double bond - Block copolymers. -2 units

**Chain copolymerisation:** Copolymer composition – -1 unit  
 Radical co-polymerisation - ionic co-polymerisation - kinetics of co-polymerisation. Applications of co-polymerisation. -1 unit

**Ring opening polymerisation:** General characteristics - Cyclic ethers - Cyclic amides. -1 unit

**Stereochemistry of polymerisation:**  
 Types of stereo isomerism in polymers - Properties of stereo regular polymers -1 unit  
 Forces of stereoregulations in alkene polymerisation, - kinetics -2 units

**Polymer structure and physical properties:**  
 Crystalline melting point - Glass transition temperature – Factors affecting  $T_m$  and  $T_g$  - Property requirements and polymer utilizations. -3 units

**Mechanical behaviour of polymers:** -2 units

*Mechanism of deformations and for strengthening of polymers:*

Deformation of semi crystalline polymers: mechanism of elastic deformation and mechanism of plastic deformation. Factors that influence the mechanical properties of semi crystalline polymers  
 Deformation of elastomers

**Conducting polymers:** General characteristics with examples. -1 unit

**Polymer molecular weight** –different types – their determination. - 2 units

## **SPECIAL TOPICS FROM PHYSICAL CHEMISTRY**

### **Photo electron spectroscopy:**

Introduction - experimental aspects of PES - Ionisation energies and orbital energies - the importance of Koopman's rule - - 1 unit

Core electron PES: X- PES (ESCA) elemental analysis - chemical shift in X-PES - X-PES as structural technique - problems of solid state X PES - 1 unit

Auger electron spectroscopy - spin orbital coupling in PES - Fine structure in the spectra of open - shell molecules. -2 units

### **Valence - electron (UV - PES):**

Atoms and diatomic molecules - the noble gases - spin - orbit coupling -1 unit

Hydrogen halides - vibrational fine structure in PES - halogens, nitrogen and carbon monoxide, -2 units

UV (valence electron) PES - small polyatomic molecules -H<sub>2</sub>O-CH<sub>4</sub>-NH<sub>3</sub>. -2 units

Trends in the isoelectronic series CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O, HF, Ne, Relationship between PES and the valence bond description of electronic structure. -1 unit

UV - (valence electron) PES of large molecules - localized molecular orbitals - Effects of substituents on localized orbitals in organic molecules – non-bonded interactions in molecules - Donor - acceptor interactions - PES of transition - metal complexes. -2 units

### **Ion cyclotron Resonance spectroscopy:**

Introduction Techniques and theory - principles of operation Instrumentation Detection by radio frequency energy absorption -1 unit

### **Photoacoustic spectroscopy:**

Basic principles of PAS, PAS- gases and condensed systems, chemical and surface application. -1 unit

## **PRESCRIBED BOOKS:**

1. Principles of Polymerisation by G. Odian, 4<sup>th</sup> Ed., John Wiley & Sons., New Jersey, 2004.
2. Contemporary Polymer Chemistry by H R Allcock, F.W. Lampe and J. E. Mark, 3<sup>rd</sup> ed., Pearson Education Inc. New Jersey 2003.
3. Text Book of Polymer Science by F.W. Billmeyer, Jr., 3<sup>rd</sup> ed., John Wiley & Sons, New York 1984.
4. Introduction to Polymers by R.J. Young and P.A. Lovell, 2<sup>nd</sup> ed., Chapman & Hall, London 1991.
5. Materials Science and Engineering – An Introduction by Callister and Rethwisch, 9<sup>th</sup> edition, 2014, Wiley NJ.

6. Unit 20: Photoelectron spectroscopy in Physical Methods and Molecule Structure 2, 2<sup>nd</sup> ed.; As part of series Science: A third Level Course - The Nature of Chemistry, The Open University Press, Milton Keynes 1980
7. Photoelectron Spectroscopy – Principles and Applications by Stefan, 3rd edition, Springer-Verlag GmbH 2003 Berlin Heidelberg
8. Physical Methods in Modern Chemical Analysis, Vol II by Theodore Kuwana, Academic Press, 1980.
9. Edward P. C. Lai, Becky L. Chan & Mohammadreza Hadjmohammadi (1985) Use and Applications of Photoacoustic Spectroscopy, Applied Spectroscopy Reviews, 21:3, 179-210

**REFERENCE BOOKS:**

1. Seymour/Carraher's Polymer Chemistry by C.E. Carraher Jr., 5<sup>th</sup> ed., Marcel Dekker Inc., New York 2000.
2. Polymer Chemistry by M.P.Stevens, 2<sup>nd</sup> ed., Oxford University Press 1990.
3. Introduction to Physical Polymer Science by L. H. Sperling, 4<sup>th</sup> ed., John Wiley & sons, New Jersey 1993.
4. Photoelectron and Auger Spectroscopy by Thomas A Carlson, Plenum Press, 1975.

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## ELECTIVE-I

PCHM-303 E-I (i)

3 CREDITS

### Synthetic Organic Chemistry

**Synthetic Organic Chemistry** - Concept and use of Protection & deprotection of sensitive functional groups in organic synthesis :

Alcohol	-1 unit
Carbonyl –carboxyl –	-1 unit
Amine –lactone and thiols- problem solving -	-1 units.

**Newer synthetic reagents** - Polymer supported reagents and their applications in Peptide synthesis –

Solution phase synthesis versus solid supported synthesis –	-1 unit
Sheppard synthesis of peptides –	-1 unit
Introduction to reactions on inorganic solid supports – Alumina –	- 1 unit,
Silica & zeolites –	- 1 unit
Introduction to combinatorial synthesis-Library synthesis on resin beads(only solid phase)-1unit	
Mitsunobu Reaction (Diethyl azodicarboxylate-DEAD)	-1 unit

**Reductions in organic synthesis** - uses of complex metal hydrides in organic syntheses (NaBH<sub>4</sub>, LiAlH<sub>4</sub>, DIBAL, LiAlH<sub>4</sub>, NaBH<sub>3</sub>(CN), AlH<sub>3</sub>) –

	- 2 units
Hydroboration and its applications –	- 2 units
Metal / liquid ammonia reactions (Birch and related reductions) - catalytic reductions (Pd, Pt, Ni, Copper chromite & wilkinsons catalyst) - Catalytic transfer hydrogenation - Problem solving	- 2 units

<b>Oxidations in organic synthesis</b> –Alcohol Oxidations	-1 unit
Alkene oxidations (Sharpless and other epoxidations), Prevost, Woodward and other Hydroxylations	-2units
Reactions with DDQ and Chloranil.	-1unit

<b>Planning a synthesis</b> - the basis for retrosynthetic analysis –	-1 unit
Disconnections of C=C-, synthons, chiron, transform based strategies-	-1 unit
Strategic bond approach- with suitable example –cis-Jasmone - Problem solving-	-1 unit

**Diastereoselectivity**- Stereo selective reactions – Prochirality-Diastereoselective addition to carbonyl group without rings

-2 units

<b>Asymmetric synthesis:</b> Chirality- chiral pool- resolution of enantiomers	-1 unit
chiral auxiliaries - alkylation of enolates	-2 units
enantiomeric excess - asymmetric formation of c-c bonds-asymmetric conjugate addition - organo catalysis	- 2 units

**Electro - organic syntheses –**

Electrode reactions classified by reaction type – - 1 unit

**Organic Photochemistry –**

Alkenes: Isomerization, cycloaddition, di- $\Pi$  methane reaction, ring closure – - 1 units

Carbonyl compounds: Norrish type I & II reactions, Paterno-Buchi reaction – - 2 units

Aromatic photochemistry: Isomerizations, photoaddition, cycloadditions to the aromatic ring -  
singlet oxygen oxidations – -2 units.

**Organo metallic reagents in synthetic chemistry –**

Use of organometallic compounds - iodomethyl zinc iodide,- - 1 unit

Organo selenium oxidations and selenium dioxide oxidation – -1 unit

Palladium catalysed vinylic substitutions- Stille coupling reactions, Suzuki coupling-- 1 unit.

**Biosynthesis** - a brief introduction to acetate malonate, acetate mevalonate and shikimic acid pathways- -1 unit

Problem Solving – -1 unit.

**Total Synthesis of selected Natural Products – Reserpine** - 2 units,

Cholesterol – - 2 unit

Gilvocarcin-M – -1 unit

**PRESCRIBED BOOKS:**

1. Guidebook to Organic Synthesis by Raymond. K. Mackie & David M. Smith, ELBS, Sec.Ed. 1990.
2. Organic chemistry by J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, Sec. Ed. 2005
3. Modern Methods of Organic Synthesis by W. Carruthers, Cambridge University Press, 1987.
4. Organic Electro chemistry edited by Heming Lund, 2<sup>nd</sup> Ed.,New York, Marcel Decker, 1983.
5. Organic Photochemistry by Jan Kopecky, VCH, 1991.
6. The Chemical Synthesis of Peptides by John Jones, Oxford University Press, 1991.
7. Advanced Organic Chemistry by F. Carey and R.J. Sundberg, Part-B, Plenum Press 2<sup>nd</sup> Ed., 1984.
8. Principles of Organic Synthesis by R.O.C. Norman, 2<sup>nd</sup> Ed., Chapman and Hall, 1978.

9. Organic reactions and mechanisms by P.S. Kalsi, 3<sup>rd</sup> edition, New age international Publishers 2010.

10. Combinatorial chemistry by R.O.C. Norman, 2<sup>nd</sup> edition, Chapman and Hall, 1978.

**REFERENCE BOOKS:**

1. Bio-transformations in Organic Chemistry by Kurt Faber, Springer Verlag, Berlin, 1992.

2. Designing organic synthesis by S. Warren, John Wiley Sons 1982.

3. Modern synthetic reactions by House, 2<sup>nd</sup> Ed., Benjamin Cummins Publications, 1972.

4. The Logic of Chemical Synthesis by E.J. Corey and Xue-Min Cheng, John Wiley and Sons, 1989.

5. Photochemistry in Organic Synthesis by Ed. J.D.Coyle, RSC, 1986.

6. Synthetic Organic Electrochemistry, by Albert J. Fry, 2<sup>nd</sup> Ed., John Wiley and Sons, 1989.

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### Novel Drug Delivery Systems

**1 Fundamentals of Controlled Release Drug Delivery:** Influence of drug properties and routes of drug administration on the design of sustained and controlled release systems.

2 units

**2. Oral controlled drug delivery systems:** Formulation, fabrication and evaluation of various oral controlled drug delivery systems including gastro retentive, colon targeted and pulsatile drug delivery.

3 units

**3. Parenteral controlled release system:** Scope, terminology & techniques used, injectable controlled release, formulation. Long acting contraceptive formulations. Implantable drug delivery, micro spheres liposomes & quality control.

3 units

**4. Mucosal drug delivery models:** Buccal, rectal, nasal, mucosal & vaginal drug delivery

2 units

Mechanisms of transports of drugs through mucosal routes, penetration enhancers, formulation development, in-vitro, ex-vivo and in-vivo methods of evaluation (for each route).

3 units

**5. Transdermal drug delivery system:** Permeation through skin including mechanism, permeation enhances,

3 units

In-vitro skin permeation, technologies for developing transdermal drug delivery system & evaluation parameters.

3 units

**6. Site specific drug delivery system:** Active & passive targeting, resealed erythrocyte, monoclonal antibodies drug targeting particulate carrier system, specific drug delivery to targeted organs like brain & colon, freeze drying of Parenteral, environmental controlled Parenteral manufacturing.

3 units

3 units

**7. Ocular Drug Delivery:** Ocular delivery mechanisms & development of Ocular controlled release systems.

2 units

2 units

**8. Protein & peptide drug delivery system:** Physical aspects, biochemistry of protein drug (structure, properties & stability- Mechanisms of destabilization.

3 units

Techniques of stabilization of Proteins and Peptides.) General methods of analysis of protein & peptide drugs, barrier to transport & Pharmacokinetics,

3 units

Different route of delivery, practical considerations.

1 unit

Importance of pre-formulation & formulation considerations, toxicity immunogenicity, stability & regulatory perspective.

3 units

**9. Regulatory consideration in controlled release:** Modification requirements to demonstrate safety, efficiency & controlled release nature.

3 units

Bioavailability, assurance, WHO & Indian condition.

3 units

### **PRESCRIBED BOOKS:**

1. Remington's pharmaceuticals sciences. 21<sup>st</sup> Edition, Lippincott Williams and Wilkins- Vol. I & II
2. Novel drug delivery system – Marcel Dekker N.Y. Second Edition, Revised and Expanded by Yie W. Chien. Vol- 50.
3. Controlled drug delivery system – Vicent H.L., Marcel Dekker Second Edition, Revised and Expanded by J. R. Robinson and Vincent H. L. Lee. Vol- 29.
4. Bentley's textbooks of pharmaceuticals – E.A. Rawlin
5. Novel and controlled drug delivery systems – N.K. Jain
6. Advances in Novel and Controlled Drug Delivery- N.K. Jain

### **REFERENCE BOOKS:**

1. Chien, Y.W.: Novel Drug Delivery Systems, Marcel Dekker, New York and Basel
2. Robinson, J.R. & Lee, V.H.I.,: Controlled and Novel Drug Delivery Marcel Dekker, New York.

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## ELECTIVE-II

PCHM-304 E-II (i)

Interdepartmental elective

3 CREDITS

### Theory and Applications of Physical Methods in Chemistry

#### Applications in organic and Biochemistry.

Use of shift reagents – -1 unit  
in U.V. spectral analysis, with examples chosen from chemistry of naturally occurring flavonoids- where such methods have been particularly successful. -2 units

I.R.spectra with regards to study of hydrogen bonding – -2 units  
and resonance effects in organic compounds – -2 units

Use of paramagnetic shift reagents – -1 unit  
NOE effect, FT NMR its advantage- -1 unit  
Double resonance, with particular reference to spin - spin decouplings, solvent effects in PMR spectra -2 units  
13C NMR – Introduction and theory – -1 unit  
Applications – -1 unit  
High resolution mass spectral fragmentation mechanism, chemical ionisation spectra –2 units  
and extensive analysis of problems based on integrated spectral data with examples chosen from natural products – -4 units.

#### New dimensions in NMR :

Introduction - Theory and applications of DEPT spectra and Homo COSY – -2 units  
Applications of Hetro COSY- HMQC and HSQC -1 unit  
Incredible natural abundance double quantum transfer experiment (2-D INADEQUATE)-  
Problem solving. – -1 unit

#### Theoretical principles and Applications in Inorganic chemistry.

**Introduction:** A brief review of the selection rules for absorption of radiation by molecular vibrations, Intensity and line width of spectral line. Population of various states and intensity. Doppler broadening and life time broadening, factors affecting coupling, degeneracy. –2 units

**Infrared spectroscopy** vibrations of polyatomic molecules- fundamental vibrations and their symmetry- overtone and combination frequencies- Fermi resonance- -1 unit  
The influence of rotation on the spectra of linear (polyatomic) molecules – -1unit  
Effect of co-ordination on spectra due to change in symmetry – -1 unit

#### Microwave spectroscopy –

Rotation of molecules and rotational spectra - Diatomic molecules - the rigid rotor – -2 units  
intensity of spectral lines - effect of isotopic substitution - -1 unit  
Non-rigid rotator, spectrum of non-rigid rotator - poly atomic molecules - linear, symmetric top and asymmetric top molecules (only spectral features) – -2 units  
Basic outline of the instrumentation of microwave technique- -1 unit

Applicable from June 2018 onwards

**Raman Spectroscopy** - Raman scattering - theory of Raman effect - pure rotational Raman spectra of linear, spherical, symmetric top and asymmetric top molecules -2 units  
Raman activity of vibrations - Structure determination CO<sub>2</sub>, N<sub>2</sub>O, SO<sub>2</sub>, NO<sub>3</sub><sup>-</sup>, ClO<sub>3</sub><sup>-</sup> and ClF<sub>3</sub> using Raman spectroscopy – -1 unit  
Basic instrumentation – -1 unit

**Applications of NMR spectroscopy** in inorganic chemistry with special reference to <sup>31</sup>P, <sup>19</sup>F, <sup>11</sup>B nuclei – -2 units  
and NQR spectroscopy – -1 unit

**Electron paramagnetic resonance:** Theory and applications to Nickel (II) & Copper(II) compounds, magnetic exchange process in dinuclear complexes - -2 units.

**Mossbauer spectroscopy:** Origin and interpretation of Mossbauer effect-  
Mossbauer chemical shift - 1 unit  
Application of Mossbauer spectroscopy to Fe and Sn systems - 1 unit

#### **PRESCRIBED BOOKS:**

1. Introduction to Spectroscopy, A Guide to students of Organic Chemistry, by Pavia, Lampman and Kriz, 3<sup>rd</sup> Ed, 2007.
2. Spectrometric identification of Organic Compounds by Silverstein, Bassler and Morrill, 6<sup>th</sup> Ed., Wiley, 2013.
3. Basic One and Two-Dimensional NMR Spectroscopy by Horst Friebolin, 5<sup>th</sup> Ed. Wiley-VCH, 2011.
4. Fundamentals of Molecular Spectroscopy by C.N. Banwell, 3<sup>rd</sup> Ed., T.M.H. Publishing Co 1980.
5. Physical Methods in Inorganic Chemistry by R.S. Drago, East - West Press 1968.
6. Structural Methods in Inorganic chemistry by E.A.V. Ebsworth, 2<sup>nd</sup> Ed. D.W.H. Rankin and S. Craddock, 1991.
7. NMR in Chemistry - multinuclear introduction by W. Kemp, Mcmillan 1986.
8. IR Spectroscopy by Nakanishi and Solomon, 2<sup>nd</sup> Ed, Holden Day 1977.
9. Organic Spectroscopy - Principles and applications by Laszolo and Stale, Harper and Row 1971.

#### **REFERENCE BOOKS:**

1. Spectroscopic Techniques for Organic Chemistry, by J.W. Cooper, Wiley 1980.
2. Introduction to Molecular Spectroscopy by G.M. Barrow, McGraw - Hill 1962.
3. Spectral problems in Organic Chemistry, by J. Devis and C.H.J. Well, Chapman and Hall (1984).
4. NMR of newly accessible nuclei, P. Lazalo Vols: 1&2, Academic Press 1983
5. NMR and Chemistry by J.W. Akitt, 2<sup>nd</sup> Ed., Chapman and Hall 1984 .
6. Carbon -13 NMR spectroscopy by Levy, Lichter and Nelson, 2<sup>nd</sup> Ed., Chapman and Hall 1980

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**PPHY-304 EL-2**

**Concepts in Materials Science**

3 CREDITS

**(Interdepartmental elective)**

(The title of the paper and the syllabus are same as the Elective paper offered by the department of Physics)

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**PCHM-305**

2 CREDITS

**Computational applications in chemistry – I**

Introduction to Molecular Modeling; MO Theory: Ab initio From the Beginning. Potential Energy Surfaces & Optimization Methods;	4 units
Introduction to python	3 units
Methods for Electron Correlation; Semi-Empirical Molecular Orbital Methods	4 units
Density Functional Theory (DFT);	3 units
Introduction to Hyperchemlite, Gaussian, Autodock, MOE	5 units
Various applications of the above levels to organic reactions (like conformational analysis)	
Lab problem	4 units
Studying reaction pathways using Intrinsic reaction coordinate method	2 units
Natural Bond Orbital and Atoms in Molecule analyses	1 units
Calculating the thermodynamic properties, HOMO, LUMO, Ionization potentials, chemical hardness, softness, dipole moment, polarizability	4 units

**References:**

1. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems.
2. David C. Young Copyright (2001) John Wiley & Sons, Inc.
3. Computational Chemistry of Solid State Materials -A Guide for Materials Scientists, Chemists, Physicists and others by Richard Dronskowski, WILEY-VCH Verlag GmbH & Co. KGaA.
4. A Chemist's Guide to Density Functional Theory - Koch, W., Holthausen, M. C. 2001, ISBN 3-527-30372-3
5. Essentials of Computational Chemistry Theories and Models, Cramer, C. J. 2004 ISBN 0-470-09182-7

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**Project work (Interim Review)**

**At the end of the 3<sup>rd</sup> semester assessment of the project work will be done along with the literature review.**

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**Solid State Chemistry and Nano Materials**

**Preparative methods:** Solid state reactions general principles, experimental procedure,- 1 unit  
 Co-precipitation as a precursor to solid state reactions, - 1 unit  
 Kinetics of solid state reactions- -1unit  
 Crystallizations of solutions, melts, glasses and gels, vapour phase transport methods, ion exchange reactions, electro chemical reduction methods and thin film preparation, growth of single crystals - 1 unit

**X-Ray Diffraction:** X-rays and their generation-an optical grating and diffraction of light, crystals and diffraction of x-rays - 2 units  
 X-ray diffraction experiment, the powder method-principles and uses, single crystal methods-principle and uses- - 2 units  
 High temperature X-ray diffraction, electron diffraction and neutron diffraction- -2 units.

**Electronic properties and band theory-** Introduction- metals, insulators and semiconductors- 1 unit  
 Electronic structure of solids- band theory- -1 unit  
 colour in inorganic solids.- -1 unit.

**Electrical properties-** Hall effect, dielectric materials, ferro-pyro-piezo electricity and its applications- -1unit

**Magnetic properties:** Classification of materials -Dia, para, ferro, ferri, and antiferro magnetic types - -2 units  
 Selected magnetic materials such as spinels, garnets and perovskites- -1 unit

**Superconductivity:** Theory, discovery and recent high T<sub>c</sub> materials - -2 units

**Organic solids state chemistry-**Topochemical control of organic solid state reactions – 2 units  
 Electrically conducting solids, organic charge transfer complex, organic metals, new super conductors- -1 unit

**Carbon Nanomaterials** - Synthesis of Nanomaterials: Top down and bottom up synthesis approach, physical and chemical techniques for nanomaterial synthesis- sol-gel and hydrothermal methods - 3 units  
Carbon Nanotubes and carbon clusters- -2 units  
Applications of carbon nanotubes- -1 unit

**PRESCRIBED BOOKS:**

1. Solid state chemistry and its applications, by A. R. West, W. S. E. Wiley.2003.
2. Introduction to Nanotechnology byPoole and Owens ,Wiley,2003
3. Nanochemistry: A Chemical Approach to Nanomaterials. by Geoffrey A Ozin (Author), André C Arsenault (Author)Royal Society of Chemistry, 2005.
4. Introduction to solids. L.V. Azaroff, Tata Mcgraw Hill, 1977.
5. Solid state chemistry, L. Smart and E. Moore, Chapman Hall 1992.

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### Special Topics from Bio-Organic Chemistry

<b>The molecular logic of life</b> - principles of bio catalysis –	-1 unit
Factors responsible for enzyme efficiency (Bruice's proximity effect, Koshland's Orbital steering, Multifunctional catalysis)-	-2 units.
<b>Host - Guest complexation chemistry</b> – Basic concepts, molecular recognition, complex formation and host design-	-2 units
Macrocycles, clefts and open chain host structures, thermodynamics of multi-site host-guest complexation.-	-1 unit.
Non-covalent interactions and organic host- guest complexes – Ionic, hydrogen bonding, cation – pi electron interactions-	-2 units
Van der waals' stacking and charge transfer interactions and their quantification-	-1 unit
<b>Ionophores for cations and anions:</b> chelate, macrocyclic and cryptate effects, complexation selectivity, thermodynamics (enthalpy, entropy and heat capacity changes),-	-2 units
Macrocycles with secondary binding sites, effect of solvent-	- 1 unit
<b>Crown ethers</b> - synthesis of all oxygen –	-1 unit,
all nitrogen, all sulphur & oxygen - nitrogen bridged systems –	- 2 units
Use of crown ethers in Organic Synthesis –	-1 unit
Binaphthyl crown ethers (CPK models) in racemic resolution –	-1 unit.
Cyclodextrins - ester hydrolysis, model of carbonic anhydrase (Tabushi's model)	--2 units
Micelles, their use in organic Synthesis –	- 1 unit
Breslow's remote functionalization using substituted benzophenones –	-1 unit
<b>Bio - organic chemistry of the Phosphates</b> - biological role of phosphate macromolecules	-1 unit
General properties, experimental evidences for DNA double helix-	-1 unit
Chemical synthesis of polynucleotides (trinucleotide)-	-1 units
Role of other nucleotide phosphates (NADP, FAD, CAMP & CGMP) –	-2 units
<b>Selected applications:</b> Synthetic classification of organic electron transfer reactions - Marcus Theory	– 1 unit
Photo-induced intramolecular electron transfer systems - introduction to molecular switches – optical devices, electrochemical devices-	- 2 units
<b>Nanobiotechnology</b> – Introduction, - applications in medicine.	- 1 unit

#### PRESCRIBED BOOKS:

1. Bio organic chemistry - Hermann Dugas, Christophur penney, Springer Verlag, New York 1981.

2. Principles and methods in Supramolecular Chemistry – Hans-Jorg Schneider and Anatoly Yatsimirsky, John Wiley & Sons, LTd., England, 2000.
3. Handbook of Organic Conductive Molecules and Polymers, Ed. By Hari Singh Nalwa, John Wiley & Sons, England, 1977.

**REFERENCE BOOKS:**

1. Biological chemistry - Henery R. Mahler, Engene H. Cordes 2<sup>nd</sup> Ed., Harper Row Publication 1971.
2. Clinical chemistry - Donald F. Calbreath, W.B. Saunder's Company, 1992.
3. Principles of Biochemistry - 2<sup>nd</sup> Ed., Worth Publishers New York 1993.
4. Advances in Physical Organic Chemistry, Vol.18, Academic Press, 1982.
5. Topics in Carboxylic Chemistry, Ed. Douglas Lloyd, Plenum Press, p269, 1969.
6. The Chemistry of Functional Groups, Ed. Saul Patai, Supplement E, Part 1, John Wiley and Sons, 1980.
7. Rodd's Chemistry of Carbon Compounds, Ed. S.Coffey and M.F.Ansell, Elsevier. 2<sup>nd</sup> Ed., 1964.

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**Medicinal Chemistry****Drug Design:**

The drug discovery process - conceptual back-ground - Drug receptors –	- 2 units
Drug target binding forces-	-1 unit
History and development of QSAR-	-1 unit
Effect of physical properties of the drug on its action ( Ferguson and related theories)-	2 units
Concept of lead structure & pharmacophore – Concept of isosterism and bioisosterism-	2 units
Three dimensional structure - aided drug design (use of Hyperchem lite and Autodoc to get hands on experience)-	-1 unit

**Pharmacokinetics & Pharmacodynamics:**

Introduction of drug absorption, bioavailability (factors effecting and dosage determination)-	- 2 units
and metabolism -Phase I & Phase II –	- 2 units

**A study of antibiotics:**

Chemistry and pharmacology of streptomycin-	- 2 units;
Structure and Pharmacology of tetracyclines (detailed structure elucidation of tetracycline)	- 2 units,
gramicidin, a survey of anticancer antibiotics –	-1 unit

**Dietary factors:**

Study of water-soluble vitamins(Structure elucidation, synthesis)	
Chemistry and biological functions of thiamine –	- 2 units,
riboflavin –	- 2 units,
pyridoxine –	- 2 units,
pantothenic acid and folic acid –	- 2 units.

**Drugs from medicinal plants:**

A study of active ingredients of some well-established Indian medicinal plants –	- 2 units;
A survey of Chinese medicinal plants-	- 2 units

**PRESCRIBED BOOKS:**

1. Burger's Medicinal chemistry, Volume I, Ed. - M.E. Wolff, 5th Ed., John Wiley & Sons, 1995.
2. Principles of Medicinal Chemistry, Edited by N.O. Foye, Lea and Febiger; Philadelphia, 1976.
3. Comprehensive Medicinal Chemistry Vol 4 , Edited by C. Hansch, P.G. Sammes and J. B. Taylor, Quantitative Drug Design, Pergamon Press, 1990.



4. Molecular Recognition of Amiloride Analogs: A Molecular Electrostatic Potential Analysis, J. Med. Chem., 35, p 1643, 1992.
5. Harper's Biochemistry, Robert K. Murry, D.K. Granner, P.A. Mayes and V.W. Rodwell, 25<sup>th</sup> Ed. Mc Graw Hill, Lange medical books, 1999

**REFERENCE BOOKS:**

1. Introductory Medicinal Chemistry by J.B. Taylor and P.D. Kennewell, Ellis Horwood, 1981.
2. Modern Drug Research, Vol.12, Paths to better and safer drugs edited by Yvonne Connloy Martin, Eber Hard Kutter, Volkhard Sustel., Marcel Dekker. Inc, 1989.
3. Kirk Othmer's Encyclopaedia of Chemical Technology 3<sup>rd</sup> edition, Wiley Interscience Publication. 1978 - 84
4. Ullmann's Encyclopaedia of Industrial Chemistry VCH Publishers, Wurzburg, Federal Republic of Germany, 1987-89.
5. Remington's Practice of Pharmacy, 13<sup>th</sup> Ed., The Mach Publishing Company, Eastern P.A. 1979.

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## ELECTIVE – III:

**PCHM-404 E-III (i) Environmental Chemistry 3 CREDITS**  
**(Inter departmental elective)**

### **Air Pollution:**

Air pollutants - Air quality standards - -1 unit  
Production, fate, effects and control of gaseous pollutants - Oxides of carbon, nitrogen and Sulphur - Organic air pollutants – 2units  
Photochemical reactions, photochemical smog, Greenhouse effect, - 2 units  
Acid rain and Ozone depletion. -1 unit  
Particles in the atmosphere - physical behaviour - physical and chemical processes for particle formation - 1unit  
Composition of inorganic and organic particles- toxic metals and radioactive particles Effects and control of particles  
- 1 unit

### **Water Pollution:**

Water quality - Water pollutants (inorganic and organic) - Sources, fate, effects and controlling measures - Chemical speciation – - 2 units  
Pollution by radionucleides - Biochemical oxygen demand-Chemical oxygen demand,-2 units  
Eutrophication, Biodegradation of pollutants. - 2 units

### **Water treatment:**

Hardness of water and its removal - removal of solids and other toxic materials - 1 unit  
Treatment of water for drinking - Electrodialysis, ion exchange, - 1 unit  
Reverse osmosis, desalination processes, - 1 unit  
Removal of iron, manganese, phosphorous, calcium and nitrogen - 1unit  
Treatment of water for industrial purposes – - 1 unit  
Sedimentation, coagulation, flocculation, filtration, - 2 units  
Adsorption, disinfection of water – - 1 unit  
Sewage treatment (physical and chemical methods) – - 1 unit  
Health effects of drinking water treatment technologies –  
Impact of detergents, pesticides and other additives on sewage treatment. - 1 unit

### **Oils in fresh & marine water:**

Sources of oil pollution -Chemistry and fate of hydrocarbons –  
Oil in run off and ground water – -1 unit  
Biodegradation - effect on aquatic organisms and communities – -1 unit  
Treatment and disposal technology. -1 unit

### **Soil Pollution:**

Soil pollutants -Inorganic, organic,  
Pesticides, radionuclides – -1 unit  
Sources and effects on nature and properties of soil, crops, plants and terrestrial animals. -1 unit

**Hazardous Wastes :**

Nature and sources of hazardous wastes –	- 1 unit
Classification, characteristics & constituents –	- 1 unit
Transport and effects –	- 1 unit
Hazardous wastes in Geosphere, Hydrosphere, Biosphere and Atmosphere	- 2 units
Reduction, treatment by physical and chemical methods –	-1 unit
Thermal treatment methods –	-1 unit
Biodegradation of wastes –	- 1 unit
Disposal of hazardous wastes. Waste management and Industrial by-products	-1 unit
Natural hazards and management- control of subsurface migration of Hazardous Waste	-1 unit
E-Waste: effect on environment: Sources-constituents and their effects-pollution of water, soil and air-Methods of treatment and disposal-Extraction of gold and other precious metals from E-waste.	- 3 units

**Values in Environment:**

The philosophy and Technology of living in tune with nature and its assets	- 2 units
Nature-A silent teacher, Ecology-The Indian Approach	- 1 unit

**PRESCRIBED BOOKS:**

1. Environmental Chemistry by Stanley E. Manahan, 5<sup>th</sup> Ed., Lewis, 1991.
2. Oil in Fresh Water - Ed., Vander Meulen and Hruday, Pergamon, 1987.
3. Chemical Contamination in The Human Environment by Lippmann and Schlesinger, OUP, Oxford, 1979.
4. Environmental Pollution by H.M. Dix., Wiley, 1981.
5. Environmental Chemistry by A.K. De, 2<sup>nd</sup> Ed., Wiley Eastern 1989.
6. Water Treatment - Principles and Design by J.M. Montgomery., Wiley, 1985.
7. Pollution: Causes, Effects and Control by R.M. Harrison, 3<sup>rd</sup> Ed., Royal Society of Chemistry, London, 1996.

**REFERENCE BOOKS:**

1. Atmospheric Chemistry by B.J. Finlayson – Pitts and N.N. Pitts Jr., Wiley, 1986.
2. Hazardous and Industrial Wastes – Ed., M.M. Varma, HMCRI, 1988.
3. Water Treatment - Principles and Design by J.M. Montgomery., Wiley, 1985.

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**PBIO-402 E-III (ii) (BT-3) (Inter Departmental Elective)**

**3 Credits**

### **Environmental Biotechnology**

(The title of the paper and the syllabus are same as the core paper offered by the department of Biosciences)

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**PCHM-404 E-III (iii)**

**Interdepartmental elective**

3 credits

### **Advanced aspects of applications of group theory in chemistry**

**Concept of symmetry in molecules:** symmetry elements, Cartesian coordinate system and symmetry elements -more about symmetry elements, -2 units  
mathematical requirements for a point group. -1 unit

**Molecular point groups:** molecules of low symmetry and high symmetry, molecules of special symmetry-notation of point groups-descent in symmetry in molecules with substitution, -3 units

Symmetry criteria for optical activity-symmetry restrictions on dipole moments and stereo isomerism. -2 units

**Infra-red and Raman spectroscopy of molecules:** symmetry based selection rules of IR, Raman,-symmetry requirements for overtones, binary and ternary combination bands, Fermi resonance. -3 units

**Molecular orbital theory of metal complexes:** linear combination of atomic orbitals theory-MO energy level diagram for a diatomic molecules- -3 units  
Molecular orbitals and hybrid orbitals and their symmetry species-hybrid orbitals for sigma, pi bonding-projection operation method and the ligand group orbitals, -3 units  
MO theory of coordination compounds, MO theory of sandwich complexes - 3 units

**Free ion configuration terms and states:** inter electronic repulsion parameters- spin orbit coupling parameters- -2 units  
symmetry of atomic orbitals and the spectral terms and correlation tables- -3 units  
Molecular term symbols derivation notation and selection rules for transition -3 units

**Ligand field theory of coordination compounds:** simple crystal field theory of  $ML_5$  complexes, effect of weak crystal field on terms, ligand field term diagrams, -3 units  
Orgel diagrams, correlation diagrams, -3 units  
Tanabe-Sugano diagrams of different d-orbital configurations -3 units

**Electronic spectra of metal complexes:** selection rules for electronic spectra-electric dipole transitions, magnetic dipole transitions, nature of electronic spectral bands, -3 units  
classification of electronic spectra, charge transfer spectra, -2 units  
evolution of  $Dq$ ,  $B'$  and  $\beta$  parameters, graphical method, Konigs numerical method electronic spectra of lanthanides and actinides. - 3 units

**Prescribed books:**

1. The theory of transition metal ions, J S Griffith Cambridge university press, Cambridge-1961
2. Theory and applications of UV spectroscopy. H H Gaffe and M Orchin Wiley New York 1962
3. Symmetry orbitals and spectra, Morchin, H H gaffe Wiley (inter science) New York 1970
4. Symmetry and spectroscopy of molecules K. Veera reddy New age international (P) ltd, publishers Second revised edition 2009
5. Inorganic electron spectroscopy, ABP lever second edition Elsevier Amsterdam(1984)
6. Comprehensive coordination chemistry, edited by G Wilkinson. Rd Gillard and JaMc Cleverty, volumes 1-7 Pergamon press, New York 1987
7. Introduction to ligand fields, B N Figgis
8. Chemical Applications of Group Theory by F.A. Cotton 3rd Ed., Wiley1990

**Reference Books:**

1. Introduction to infrared and Raman spectroscopy, NB Colthup, LH Daly and SE Wiberley Second edition, Academic Press, New York(1975)
2. Molecular orbital theory for organic chemists, A. Streitweiser, Jr, John Wiley & Sons Inc., New York (1961)
3. Symmetry through the eyes of a chemist, I. Hargittai and M.Hargittai, Verlagsgesellschaft, Germany(1986)

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## ELECTIVE – IV

**PCHM-405 E-IV (i) (Inter Departmental Elective) 3 Credits**

### **Biocatalysis for Industry and Environment**

#### **Bio transformation, Biocatalyst and Chemical Industry:**

Basic organic reaction mechanism, common prejudices against enzymes, advantages and disadvantages of biocatalysts, isolated enzyme versus whole cell systems, Enzymatic and Microbial Reactions	- 5 units
Application in Organic Synthesis: Hydrolytic Reactions, Reductions, Oxidations, Formation of C-C Bonds,	- 2 units
Additions and Eliminations Reactions.	- 2 unit
Special Techniques Involving the use of Enzymes and Microorganisms: Extending and Improving Bio-transformations, Purified Enzymes/ Crude Enzymes, Extracts, substrate Modifications.	- 3 units
Effects of Temperature on Enzyme Selectivity, Enzymes in Organic Solvents, Advantages of Bio-transformations in Organic Solvents.	- 1 unit
Designing a Solvent System for Enzyme Catalyzed Reactions.	- 1 unit
Immobilized Enzymes and Immobilized Microorganisms, Principal Immobilization techniques, Lipase powders.	- 2 units
Enzymes Covalently Bonded on Neutral Polymers, Cross-Linked Enzyme Crystals (CLEC). Cofactor Regeneration Techniques-	- 1 unit
<b>Microbial Kinetics</b> Reaction theory and kinetics, Cell growth and kinetics.	-1unit
Yield and maintenance, coefficient concepts, Determination of microbial kinetics from batch data.	- 1 unit
Substrate utilization and product formation kinetics.	- 1 unit
Enzyme inhibition, reversible inhibition,	- 1 unit
noncompetitive/uncompetitive inhibition, irreversible inhibition.	- 2 units
pH effects on enzyme kinetics .	- 1 unit

#### **Bioreactor Operation**

Batch, fed-batch and chemostat operation of bioreactors, Evaluation of kinetic and yield parameters in chemostat culture, Bioreactor configurations, Fermentor operation – initiation, operation and harvest of batches	- 2 units
Application of Biotechnology to Chemical Production, Single-step Reactions of Commercial Importance, Multi-step Reactions of Commercial Importance	-2 units
Biomass hydrolysis, enzymatic conversion of biomass components(cellulose, hemicellulose and lignin) to sugars and other value added products. Enzymes commonly used in processing systems: Carbohydrases, proteases, lipases and oxidoreductases.	-2 units
Biological Routes to Optically Active Epoxides, The Production of Optically Pure Natural and Unnatural Amino Acids, hydro-xylation of steroids at unactivated carbon centers, Case Study.	-3 units

### **Bioremediation and Biological Method for Pollution Control:**

Environmental remediation: Bioremediation and biodegradation - molecular biological approaches to sustainable development. - 2 units

Bioremediation of fossil fuels like oil, coal, pesticides and pcb's. - 1 unit

Anaerobic and aerobic degradation, site characterization, treatability assessment, remediation technology selection - 2 units

Design of in situ remediation techniques, phyto remediations, Case Study. - 2 units

Environmental enhancement: Positive intervention: molecular biological approaches to increasing biochemical tolerance (crop protection, fertilizers) - 2 units

Clean technologies: biotechnological alternatives to present energy sources and commodity production; - 1 unit

### **PRESCRIBED BOOKS:**

1. Biotransformations and Bioprocesses, Doble Mukesh, Anil Kumar & Vilas Gajanan Gaikar, Marcel Dekker, New York, USA, 2004.
2. Biotreatment of Industrial Effluents, Doble Mukesh and Anil Kumar, Elsevier, USA, 2005.
3. Biotransformations in Preparative Organic Chemistry, H. G. Davies, D. R. Kelly, R. H. Green and Stanley M. Roberts, Academic Press, New York, 1989.
4. Bio-transformations in Organic Chemistry by Kurt Faber, Springer Verlag, Berlin, 1992.
5. Bioprocess Engineering Principles by Pauline M. Doran, Academic Press. 1995, ISBN-13: 978-0-12-220856-0
6. Bioprocess Engineering, Basic concepts by Michael L. Shuler and Fikret Kargi, Second Edition, PTR Prentice Hall. 2001, ISBN 0-13-081908-5.
7. Biocatalysis: Biochemical fundamentals and applications by Peter Grunwald, Imperial college Press, 2009, ISBN-13 978-1-86094-771-1; ISBN-10 1-86094-771-9
8. Practical biotransformations: A beginners' guide by Gideon Grogan, First edition, John Wiley & Sons, 2009, ISBN 9781405193672.

### **REFERENCE BOOKS:**

1. Combinatorial Chemistry by Nicholas K. Terrett, Oxford Chemistry Masters, Oxford University Press, 1988.
2. Designing organic synthesis by S. Warren, John Wiley Sons 1982.
3. The Logic of Chemical Synthesis by E.J. Corey and Xue-Min Cheng, John Wiley and Sons, 1989.

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### Organic Chemistry of Natural Products

<b>Methods in Natural product chemistry:</b> Techniques used in isolation	- 1 unit
Determination of structures of different types of plant secondary metabolites-	- 2 units
<b>Biosynthesis</b> - a brief introduction to acetate malonate pathway	- 1 unit
Acetate mevalonate pathway	- 2 units
Shikimic acid pathway	- 2 units
<b>Terpenes and steroids:</b> Structure elucidation of citral-	- 2 units
Photochemistry of santonin	- 2 units
Synthesis of longifolene	- 2 units
Total synthesis of steroid hormones	- 2 units
Synthesis of Prostaglandins (PGF <sub>2α</sub> )-	- 2 units
<b>Alkaloids:</b>	
Biosynthesis of opium alkaloids: Stereochemistry and rearrangements of morphine	- 2 units
Determination of structure of strychnine and its total synthesis	- 2 units
Stereochemistry and synthesis of quinine –	- 2 units
Photochemistry of Colchicine-	- 2 units
<b>Oxygen heterocyclic compounds:</b> Structure elucidation of flavonoids with a suitable example (use of colour reactions, UV, MS, <sup>13</sup> C & <sup>1</sup> H NMR)-	- 2 units
Determination of structure of scandenin by spectral methods	- 2 units.
<b>Antibiotics:</b> Reactions & synthesis of penicillin	- 3 units
Total synthesis of anti-cancer antibiotics such as daunorubicin	- 3 units
<b>Chemical Ecology:</b> An introductory study: chemistry of insects with particular reference to chemical defense mechanisms, pheromones	-2 units
Plant defense chemicals - Allelo - chemicals and Phytoalexins – (examples and their use in agriculture)	- 2 units
<b>Problem-Solving sessions:</b> critical analysis and interpretation of data from current literature concerning natural products	- 5 units

#### PRESCRIBED BOOKS:

1. Chemistry of Natural Products – A Unified Approach, by N. R. Krishnaswamy, University Press, Hyderabad, 1999.
2. Natural Products Ed., by K. Nakanishi et al, Vols 1, 2 and 3, Academic press 1974, 1975 and 1983.
3. Classics in Total Syntheses by K. C. Nicolaou and E. J. Sorensen, VCH, 1996.



4. Natural Products by J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne, Addison Wesley Longman Limited, 1994.

**REFERENCE BOOKS:**

1. Rodd's Chemistry of Carbon Compounds, Ed. by Coffey, Vols 2 C, D, and E with supplements and volumes 4E, G and H, Elsevier 1974 to 1985.
2. Comprehensive Organic Chemistry Ed., by Barton Oilis, Vol 5, Biological compounds, Ed., by E. Hasiam, Pergamon press, 1979.
3. Total synthesis of Natural products Ed., J. Apsimon, Vols I, V and VI Academic Press, 1973, 1983 and 1984,
4. Natural Products by J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne, Addison Wesley Longman Limited, 1994.

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**PPHY-405 EL-11                      (Interdepartmental elective)                      3 Credits**

**Materials Characterization Techniques**

**(The title of the paper and the syllabus are same as the Elective paper offered by the department of Physics)**

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**Computational applications in chemistry – II**

Introduction to Molecular Mechanics	2 units
Introduction to various force fields	2 units
Force field parameterization	2 units
Basics of Molecular Dynamics Simulation	2 units
Setting up of the MD simulations and running the minimization, optimization and trajectory generation	4 units
Using Molecular Dynamics to Compute Properties	6 units
Introduction to Gromacs	7 units
Electrostatics & Solvation in Biomolecules	2 units
Calculation of Free Energy	2 units
Quantum Mechanics/Molecular Mechanics (QM/MM)	1 unit

**References:**

1. Computational Chemistry and Molecular Modeling Principles and Applications by K. I. Ramachandran · G. Deepa, K. Namboori, 2008 Springer-Verlag Berlin Heidelberg, ISBN-13 978-3-540-77302-3.
2. COMPUTATIONAL CHEMISTRY Introduction to the Theory and Applications of Molecular and Quantum Mechanics Errol Lewars, 2004 Kluwer Academic Publishers New York, Boston, Dordrecht, London, Moscow, ISBN: 1-4020-7285-6
3. Understanding Molecular simulations From algorithms to applications by Frenkel D and Berend S, 2002 Academic Press New York,
4. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young Copyright (2001) John Wiley & Sons, Inc.

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**Project work –Part II****Submission of Dissertation and evaluation of the dissertation submitted**

SSS