ST. JOSEPH'S COLLEGE (AUTONOMOUS), DEVAGIRI, CALICUT 8

Syllabus for

M.Sc. CHEMISTRY PROGRAMME

(UNDER SJCCSS SYSTEM)

(Effective from 2016 Admission)

St. Joseph's College, Devagiri (Autonomous)
M.Sc. CHEMISTRY

<u>Regulations and Syllabus with effect from 2016 admission</u>

The Board of Studies in Chemistry (PG) at its meeting held on 11-02-2016 considered the revision of M.Sc. Chemistry syllabus under Credit Semester System (CSS) and resolved to implement the revised syllabus from 2016 admission onwards. The revised programme pattern; syllabus, distribution of credits and scheme of evaluation, etc. approved by the Board of studies in Chemistry (PG) at its meeting held on 03-03-2016 are given below:

Pattern of the Programme

a) The name of the programme shall be M.Sc. Chemistry under CSS pattern.
b) The programme shall be offered in four semesters within a period of two academic years.
c) Eligibility for admission will be as per the rules laid down by the Calicut University from time to time.
d) Details of the programme offered for the programme are given in Table (page 7). The programme shall be conducted in accordance with the programme pattern, scheme of examination and syllabus prescribed. Of the 25 hours per week, 15 hours shall be allotted for theory and 10 hours for practical. Total credits of the programme is 92.

Theory Courses

There will be four theory courses during all the four semesters. All the theory courses in the first and second semesters are core courses. In the third and fourth semesters there will be three core theory courses and one elective theory course. Students can choose any one of the elective courses given in the table. Only one elective course chosen by the department both in the third and fourth semesters will be considered for calculating the workload of teachers. However, a student is permitted to choose any other elective course in the third and fourth semesters, without having any lecture classes. The credits of the theory courses are given in the table and the total credit for theory courses is 60.

Practical Courses

In each semester, there will be three core practical courses. However the practical examinations will be conducted only at the end of second and fourth semesters. Each practical examination will be of six hour duration and 4 credits. The total credit for practical courses is 24.

Project and Viva Voce

Each student has to perform an independent research project work during the programme under the guidance of a faculty member of the college/ scientists or faculties of recognised research institutions. No time is specially allotted for conducting the project work in the time table. Projects done in the quality control or quality analysis division of the industries will not be considered. At the same time, projects done in the R & D division of reputed industry can be considered. Each student has to submit three copies of the project dissertation for valuation at the end of fourth semester. After the valuation one copy may be returned to the student, one may be given to the project supervisor and the third one should be kept in the department/college library. Evaluation of the project work (4 credits) will be done on a separate day at the end of fourth semester, after the theory examinations. Viva voce on the project will also be done on the same day. Viva voce examinations, based on the theory and practical courses, will be conducted at the end of second and fourth semesters (2credits each, total 4 credit), on a separate day.

Grading and Evaluation

(I) Accumulated minimum credit required for successful completion of the course shall be 92.

(II) A project work of 4 credits is compulsory and it should be done during the programme. However no specific hours are given for the project work. Project evaluation should be conducted by one external examiner, one internal examiner (shall not be the guide of the project) from the specific branch (inorganic/organic/physical/theoretical) and HoD, at the end of IV semester, on a separate day.

(III) A comprehensive Viva Voce may be conducted by three external examiners, one each from inorganic chemistry, organic chemistry and physical chemistry area, at the end of II and IV Semesters on a separate day and carries 2 credits each.

(IV) Evaluation and Grading should be done by 7 point indirect grading system.

Mark Distribution and Indirect Grading System

Mark system is followed instead of direct grading for each question. After external and internal evaluations the marks obtained in the respective examinations are forwarded to the controller's office. All other calculations, including grading, will be done by the office of the controller of examinations using the software. Indirect Grading System in 7 point scale is followed. The performance in each course is evaluated by assigning a letter grade (A^+, A, B^+, B, C, D or F) to that course by the method of indirect grading

The Seven Point Indirect Grading System

$$\text{Grade Point (G)} = \frac{\textit{Percetage of Marks Obtained} \in \textit{a course}}{10}$$

Grade point is expressed in a 10.0 point scale varies from 0.0 to 10.0

1. Letter Grade: Based the grade point Letter Grade is awarded as given in the following table

% of Marks (IA + ESE)	Range of Grade Point (G)	Letter Grade
90 - 100	9.0 - 10.0	A^+
80 - 89	8.0 -8.9	A
70 - 79	7.0 -7.9	B^+
60 - 69	6.0 -6.9	B
50 - 59	5.0 - 5.9	C
40 - 49	4.0 - 4.9	D
Course incomplete	0.0- 3.9 = 0.0	F

2. The minimum Grade Point required for passing a course is 4.0. The grade point for marks in the range 0 to 39 is taken as 0.0.

3. Credit Point (P) = Grade Point (G) x Credit of the Course (C)

4. Semester Grade Point Average (SGPA) =

$$\frac{\sum \textit{of credit points} (P) \textit{ obtained by the studentin} \in \textit{the various courses of the semester}}{\textit{Total Credit of the semester}}$$

If P_1, P_2 --- P_n are the Credit Points (rounded off to the first decimal place) scored by the student in various courses of the semester and C_1,C_2 --- C_n are the credits of the respective courses, then, Semester Grade Point Average (SGPA) = $\frac{P_1+P_2+------+P_n}{C_1+C_2+------+C_n}$

5. Cumulative Grade Point Average (CGPA) =

$$\frac{\sum of\ credit\ points\,(P)\,obtained\ by\ the\ studentin \in the\ various\ courses\ of\ the\ Programme}{Total\ Credit\ of\ the\ Programme}$$

CGPA shall be rounded off to the first two decimal places.

Example

Course Code	Course Name	Marks						Credit **C**	% Score	Grade Point **G**	grade	Credit Point **C** x **G**
		Internal		External		Total						
		Scored	Max.	Scored	Max.	Scored	Max.					
xxxxx	xxxxx	16	20	62	80	78	100	4	78	7.8	B	31.2
xxxxx	xxxxx	14	20	58	80	72	100	4	72	7.2	B	28.8
xxxxx	xxxxx	14	20	66	80	80	100	4	80	8.0	A	32.0
xxxxx	xxxxx	16	20	72	80	88	100	4	88	8.8	A	35.2
xxxxx	xxxxx	14	20	66	80	80	100	4	80	8.0	A	32.0
xxxxx	xxxxx	14	16	60	64	74	80	2	93	9.3	A	18.6
Total						**472**	**580**	**22**				**177.8**

SGPA =

$$\frac{\sum of\ credit\ points\,(P)\,obtained\ by\ the\ studentin \in the\ various\ courses\ of\ the\ semester}{Total\ Credit\ of\ the\ semester}$$

$= \frac{177.8}{22}$

= 8.08

A Grade

Note: In the event a candidate fails to secure D grade (40 % marks) in any Course in a semester, consolidation of SGPA and CGPA will be made only after obtaining a minimum pass, D grade (40 % marks) in the failed Course in a subsequent appearance.

(V) Weightage of Internal and External valuation:

The evaluation scheme for each course shall contain two parts:

(a) internal evaluation and (b) external evaluation. Its weightages are as follows:

Internal 20% External 80%

Both internal and external evaluation will be carried out using indirect Grading System, in 7 point scale

(VI) Internal evaluation (must be transparent and fair):

Theory: Maximum marks: 20

Item	Internal Exam	Seminar	Assignment	Attendance
Mark	8	4	4	4

Practical: Maximum marks: 20

Item	Model Exam	Record	Attendance	Viva
Mark	8	4	4	4

Project: Maximum marks: 20

Item	Commitment	Research attitude	Performance	Viva
Mark	8	4	4	4

Project internal evaluation of each student should be done by the supervising faculty in the department.

Viva Voce:

No internal evaluation for viva voce

Attendance:

% of attendance	Above 90	85-89.9	80-84.9	75-79.9	Below 75
Mark	4	3	2	1	0

Internal Examination:

% of marks in the internal exam	Above 90	80 -89.9	70-79.9	60-69.9	50-59.9	40-49.9	30-39.9	20-29.9	Below 20
Internal mark	8	7	6	5	4	3	2	1	0

(VII) External evaluation:

a) Theory: In all semesters the theory courses have examination of three hours duration and 80 marks.

Division	Type	No. of questions	Marks per question	Total Marks per section
Section A	Paragraph	12	2	24
Section B	Short essay	8 out of 12	4	32
Section C	Essay	2 out of 4	12	24

b) Practicals: At the end of II and IV semesters.

There will be three practical examinations of six hours duration (Organic, Inorganic and Physical) at the end of second semester as well as at the end of fourth semester. Each examination has 80 marks and 4 credits

c) Viva Voce: At the end of II and IV semesters on a separate day (50 marks and 2 credits each).

Viva voce will be based on both the theory and practical courses during the year.

d) Project Evaluation: Total marks is 80 and credit for project is 4.

The evaluation will be done at the end of IV semester on a separate day. Evaluation is based on:

i) Sigificance and relevance of the project - Marks 15
ii) Project report - Marks 35
iii) Presentation - Marks 15
iv) Viva Voce - Marks 15

Credit Distribution		
Name of Course		Credits
1. Core Theory (14 Courses, 14 Examinations) 2. Core Practical(12 Courses, 6 Examinations) 3. Elective Theory(2 Courses, 2 Examinations) 4. Viva Voce (2 Examinations) 5. Research Project		54 24 06 04 04
Total	**16 Theory Examinations, 6 Practical Examinations, 2 Viva Voce, 1 Investigatory Project**	**92**

(VIII) Course code

Each course has a course code

eg., DCHE1B01T The letters/ numbers in the course should be interpreted as ;

D - The revision status of the syllabus. Even letters are reserved for PG syllabus. D represent first revised syllabus.

CHE – Chemistry

1 – Semester number

B – Core course (E for elective courses)

01 – Serial number of the course

T – Theory course (P for practical course)

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Board of Studies in Chemistry,
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Courses offered for M.Sc. Chemistry Programme under CSS Patten

Semester	Course Code	Name of Course	Hours/ Week	Credit	Mark
I	DCHE1B01T	Theoretical Chemistry I	4	4	100
	DCHE1B02T	Inorganic Chemistry I	3	3	100
	DCHE1B03T	Organic Chemistry I	4	4	100
	DCHE1B04T	Physical Chemistry I	4	4	100
	DCHE2B09P	Inorganic Chemistry Practical I	3	No Exam in Sem I	
	DCHE2B10P	Organic Chemistry practical I	3		
	DCHE2B11P	Physical Chemistry Practical I	4		
II	DCHE2B05T	Theoretical Chemistry II	4	4	100
	DCHE2B06T	Inorganic Chemistry II	4	4	100
	DCHE2B07T	Organic Chemistry II	3	4	100
	DCHE2B08T	Physical Chemistry II	4	4	100
	DCHE2B09P	Inorganic chemistry practical II	3	4	100
	DCHE2B10P	Organic chemistry Practical II	4	4	100
	DCHE2B11P	Physical chemistry practical II	3	3	100
	DCHE2B12V	Viva Voce	-	2	50
III	DCHE3B13T	Inorganic Chemistry III	4	4	100
	DCHE3B14T	Organic Chemistry III	4	4	100
	DCHE3B15T	Physical Chemistry III	4	4	100

	DCHE3E01T	Synthetic organic chemistry (Elective)	Select One	3	3	100
	DCHE3E02T	Computational chemistry (Elective)				
	DCHE3E03T	Green and Nanochemistry (Elective)				
	DCHE3E04T	Industrial Catalysis (Elective)				
	DCHE4B19P	Inorganic chemistry practical III		4	No Exam in Sem III	
	DCHE4B20P	Organic chemistry Practical III		3		
	DCHE4B21P	Physical chemistry practical III		3		
IV	DCHE4B16T	Advanced Inorganic Chemistry		4	4	100
	DCHE4B17T	Advanced Organic Chemistry		4	4	100
	DCHE4B18T	Advanced Physical Chemistry		4	4	100
	DCHE4E05T	Analytical Chemistry (Elective)	Select One	3	3	100
	DCHE4E06T	Petrochemicals and Cosmetics (Elective)				
	DCHE4E07T	Natural Products & Polymers (Elective)				
	DCHE4E08T	Material Science (Elective)				
	DCHE4B19P	Inorganic chemistry practical IV		3	4	100
	DCHE4B20P	Organic chemistry Practical IV		4	4	100
	DCHE4B21P	Physical chemistry practical IV		3	4	100
	DCHE4B22V	Viva Voce		-	2	50
	DCHE4B23D	Investigatory Project		-	4	100
		Total		**25Hr/ Week**	**92**	**2400**

SEMESTER I

Theory Course I

DCHE1B01T –THEORETICAL CHEMISTRY - I

(4Credits, 72 hrs)

Unit 1: Introduction to Quantum Mechanics (18hrs)

Historical Aspects: The ultraviolet catastrophe of classical physics and birth of quantum theory – support of quantum theory by photo electric effect – dual nature of light- de Broglie matter wave equation – dual nature of electrons: Electron diffraction. Wave function and Born interpretation of it

Operator algebra: Linear and nonlinear operators, Laplacian operator, Hamiltonian operator, eigen functions and eigen values of an operator, commutative operators and eigen value determination. The uncertainty principle and its justification using operator algebra. Hermitian operators and their properties.

Stationary waves on a clamped string: Boundary conditions and generation of quantum number. Derivation of Schrodinger wave equation from classical stationary wave equation, well behaved wave functions and ortho normality.

Postulates of quantum mechanics: The operator postulate, The eigen value postulate, The expectation value postulate and The postulate of time dependence. Conservative and non conservative systems.

Unit 2: Quantum Mechanics of Translational & Vibrational Motions (18hrs)

Free particle in one-dimension: Particle in a one-dimensional box with infinite potential walls: Setting up of Schrodinger equation and solution of it- eigen value- normalisation and orthogonality- Expectation values of energy, momentum and position. Particle in a one-dimensional box with one finite potential wall-Significance of the problem, Introduction to tunnelling.

Particle in a three dimensional box: Separation of variables, degeneracy, relation between degeneracy and Symmetry

One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, rodregues formula, even and odd functions, zero point energy

Quantization of angular momentum: Quantum mechanical operators corresponding to angular momentum ($\hat{L}_x, \hat{L}_y, \hat{L}_z$) - commutation relations between these operators - commutation relations between $\hat{L}^2$ and $\hat{L}_z$ - Ladder operator method for angular momentum – raising and lowering angular momentum operators ($\hat{L}_{¿}+¿,$ $\hat{L}_{¿}-¿$

Unit: 3 Quantum Mechanics of Rotational Motion (18hrs)

Planar rigid rotor (or particle on a ring): the Φ -equation, real and imaginary solutions of the Φ -equation, cos and sine combinations of wave functions – normalisation of the solutions -angular momentum of rotating particle, polar plots.

Non planar rigid rotor (or particle on a sphere): spherical polar coordinates and their relation with Cartesian coordinates. Schrodinger equation in spherical polar coordinates and separation of variables in to $\Theta \wedge \Theta$ equations. Solution of Φ equation

Solution of Θ equation: Expression of Θ equation as associated Legendre equations.- Legendre equation and lender polynomial- associated Legendre polynomial (Derivation of the solution is not expected) – recursion and rodregues formula to obtain the polynomials and their application – relation between values of magnetic quantum number (m_l) and azimuthal quantum number(l).

Spherical harmonics: Spherical harmonics in real and complx forms - Spherical harmonics as eigen functions of angular momentum operators L^2 and L_z . Eigen values of L and L_z – space quantisation of angular momentum vector, Zeeman effect. Degeneracy of energy levels

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (18hrs)

Potential energy of hydrogen-like systems: the wave equation in spherical polar coordinates, separation of variables, the R, Θ and Φ equations and their solutions, (Derivation of the solutions are not expected)

Radial functions: Laguerre and associated Laguerre polynomials- Recursion formula to calculate associated Laguerre polynomial - Principal and subsidiary quantum numbers-degeneracy-letter symbols of atomic orbitals

Atomic orbitals: wave functions and energies of hydrogen-like atoms, Radial plots, Radial density plots, Angular plots or polar plots, Radial distribution function(RDF), Radial distribution plots, electron density plots.

Spin orbitals: The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), representation of spin functions - explanation of spin based on space quantisation - construction of spin orbitals from atomic orbitals and spin functions

Reference

1. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books, 2003).
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition,* Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
5. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.
6. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
7. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
9. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
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1994.
11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
14. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.

SEMESTER I
Theory Course II
DCHE1B02T - INORGANIC CHEMISTRY- I
(3 Credits, 54hrs)

Unit 1: Molecular Structure and Bonding (9hrs)
The Lewis structure – Octet rule- Resonance – Formal charge –hyper valence electro neutrality principle- Iso electronic molecules. VSEPR theory, Walsh diagrams, dπ – pπ bonds. Bent rule and energetics of hybridization. The hydrogen bond and its consequences-van der Waal`s forces-Determination of molecular structure by X-Ray diffraction.

Unit 2: Concepts of Acids and Bases (9hrs)
Major acid-base concepts, Arrhenius, Bronsted-Lowry, Solvent system, Lux-Flood, Lewis and Usanovich concepts. Classification of acids and bases as hard and soft. HSAB principle.- Theoretical basis of hardness and softness. The Drago-Wayland equation, E and C parameters- Symbiosis. Applications of HSAB concept. Chemistry of non aqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Non aqueous solvents and acid-base strength. Super acids –surface acidity.

Unit 3: Chemistry of Main Group Elements-I (9hrs)
Chemical periodicity-First and Second raw anomalies-The diagonal relationship- Periodic anomalies of the non metals and post-transition metals. Allotropes of C, S, P. As, Sb, Bi, O and Se. Electron deficient compounds-Boron hydrides-preparation, reactions, structure and bonding. Styx numbers-closo, nido, arachno polyhedral structures. Boron cluster compounds- Wade's rule. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines and borides.

Unit 4: Chemistry of Main Group Elements-II(9hrs)
Silicates and alumino silicates-Structure, molecular sieves-Zeolite. Silicones-Synthesis, structure and uses. Carbides and silicides. Synthesis, structure, bonding and uses of Phosphorous-Nitrogen, Phosphorous -Sulphur and Sulphur-Nitrogen compounds.

Unit 5: Chemistry of Transition and Inner Transition Elements (9hrs)
Heteropoly and isopoly anions of W, Mo, V. Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram. Differences between 4f and 5f orbitals. Magnetic and spectroscopic properties.

Uranyl compounds. Trans-actinide elements. Super heavy elements –production and chemistry.

Unit 6: Nuclear and Radiation Chemistry (9hrs)

Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models.

Nuclear reaction: Bethe`s notation of nuclear process- Types-reaction cross section photonuclear and thermonuclear reactions.

Nuclear fission: Theory of fission- neutron capture cross section and critical size.

Nuclear fusion: Neutron activation analysis

Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water- radiation hazards radiation dosimetry.

References

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2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi. *Inorganic Chemistry, principles of structure and reactivity*, Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,* Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,* Oxford University Press, 2002
5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press,2005.
6. Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.
7. James E House, *Inorganic Chemistry,* Academic Press, 2008.
8. H.J.Arnikar, *Essentials of Nuclear chemistry,* New Age International, 2005.
9. Friedlander and J.W.Kennedy, *Introduction to Radiochemistry,* John Wiley and Sons, 1981.
10. S.Glastone, *Source Book on Atomic Energy, 3rd* edn., Affiliated East-West Press Pvt.Ltd., 1967.

SEMESTER I

Theory Course III

DCHE1B03T- ORGANIC CHEMISTRY – 1

(4 Credits, 72 h)

UNIT I. Aromaticity and Reactions (9 h)

Aromaticity: Qualitative application of Huckel MO theory and perturbation theory (PMO approach) to systems containing delocalized electrons. Concept of aromaticity, delocalization of electrons – Huckel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems – annulenes – anti- and homo- aromatic systems.

Aromatic Electrophilic Substitution: Arenium ion mechanism, orientation and reactivity (ortho, meta and para directing groups), ortho/para ratio, ipso attack. Typical reactions – Diazonium coupling, Vilsmeier-Haack reaction, Gattermann-Koch reaction, Pechman reaction and Houben-Hoesch reaction.

Aromatic Nucleophilic Substitution: Addition-elimination (S_NAr), elimination-addition (benzyne), S_N1 (reaction of diazonium salts without copper salts) and $S_{RN}1$ (reaction of diazonium salts with copper salts) mechanisms.

UNIT II. Reaction Mechanism: Structure and Reactivity (9 h)

Types of reaction, types of mechanisms, thermodynamic and kinetic requirement, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, kinetic isotope effects, methods of determining mechanisms.

Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatment. Linear free energy relationships, Hammet and Taft equations, σ and ρ parameters; Applications of acid-base concept-HSAB theory.

UNIT III. Reaction Intermediates (9 h)

Generation, structure, stability and characteristic reactions of carbocations, carbanions, free radicals, carbenes and nitrenes. Carbocations - Classical and non-classical carbocations. C-X bond (X = C, O, N) formations through the intermediary of carbocations, Wagner-Meerwin rearrangement. Carbenes: cyclopropanation - spin dependence and stereochemistry, carbene insertion to C-H bonds, Arndt Eistert synthesis. Nitrenes - spin states of nitrenes; C-H bond insertions and aziridine formation.

UNIT IV: Conformational Analysis – I (9 h)

Difference between configuration and conformation. Internal factors affecting the stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformational analysis of acyclic compounds: ethane, propane, *n*-butane and 1,2–disubstituted ethanes. Conformations of carboxylic rings of different sizes three to seven. Conformations of monosubstituted cyclo cyclohexanes (monomethyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes (dialkyl, dihalo, diols). Conformations of fused and bridged ring systems. Conformational analysis of glucose, ribose and galactose. The role of anomeric effect in the conformation of cyclic compounds. Chemical consequence of conformational equilibrium – Curtin Hammett principle.

UNIT V: Conformational Analysis – II (9 h):

Effect of conformation on the course and rate of reactions: (a) Debromination of vicinal dibromides using KI, (b) Semipinacolic deamination of α-amino alcohols, (c) Dehydrohalogination of vicinal dihalides. Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent in flexible and rigid systems. (b) E1, E2 eliminations in substituted halocyclohexanes and cyclohexyl tosylate. (c) Pyrolytic elimination of cyclohexyl esters. (d) Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol (e) Oxidation of secondary axial and equatorial hydroxyl group to ketones by chronic acid. Conformational analysis and trans-annular reactions of medium rings: Hydrolysis of epoxides and bromination of C_8 – C_{10} cyclic dienes. Polar substituent effects in the reduction of cyclohexanones and norbornan-7-ones. Percent axial and equatorial approach in reduction of 2-substituted 4-*t*- butyl cyclohexanones.

UNIT VI. Stereochemistry – I (9 h)

Stereoisomerism: Fischer, Newman and Sawhorse projection formulae and their inter conversion. Introduction to molecular symmetry and chirality: Examples from common objects to molecules. Axis, plane, center and alternating axis of symmetry. Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with more than one center of chirality, definition of diastereoisomers, erythro, threo nomenclature.

Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes. Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to folding of helical structures.
Optical activity in *cis-trans* conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes. Mixtures of stereoisomers: Optical purity, enantiomeric excess and diastereomeric excess and their determination.
Racemisation and resolution: Mechanism of racemisation, methods of resolution: chemical, kinetic and equilibrium asymmetric transformation, chiral chromatography and through inclusion compounds.

UNIT VII. Stereochemistry – II (9 h)

Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers. Stereochemistry of aldoximes and ketoximes.
Stereoselective and stereospecific reactions: (i) Bromination of *E*-and *Z*-2-butene-a stereospecific *anti* addition, (ii) Epoxidation of E-and Z-2 butene-a stereospecific reaction, (iii) Bromination of cyclohexene- a stereoselective reaction, (iv) Hydroboration-Oxidation hydration of alkenes- a stereospecific *anti*-markovnikov hydration (v) Addition of carbenes to alkenes.
Topicity and prostereoisomerism, prochiral centre, enantiotopic, homotopic, diastereotopic hydrogen atoms, topicity of ligands and faces as well as their nomenclature-Pro-R, Pro-S, Re and Si.

Unit VIII: Asymmetric Synthesis (9 h)

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity. Strategies in Asymmetric Synthesis:

1. Chiral pool: Amino acids in the synthesis of benzodiazepines- conversion of L-tyrosine into L-Dopa; synthesis of beetle pheromone component (*S*)- (–)-ipsenol from (S)-(–)-leucine, Carbohydrates – (*R*) Sulcatol from 2-deoxy-D-ribose.
2. Substrate controlled: Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule, Felkin-Anh model and Crams chelation control.
3. Chiral auxiliary controlled: Oxazolidinone controlled Diels-Alder reaction and alkylation of chiral enolates.
4. Chiral reagent controlled: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Sharpless asymmetric epoxidations.
5. Chiral catalyst controlled: Rhodium and Ruthenium catalysts with chiral phosphine ligands like BINAP and DIOP. Preparation and use of CBS asymmetric reducing agent, baker's yeast reduction.

References:

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8. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 3/e, New Age Pub., 2010.
9. P. S. Kalsi, *Stereochemistry*, 4/e, New Age International Ltd.
10. P.S. Kalsi, *Organic reactions & their mechanisms*, 3/e revised, New Age International Ltd.
11. G. L. D. Krupadanam, *Fundamentals of Asymmetric Synthesis*, Universities Press, 2013.

SEMESTER I

Theory Course IV

DCHE1B04T – PHYSICAL CHEMISTRY - I

(4 Credits, 72 hrs)

Unit 1: Thermodynamics –I (9 hrs)

Review of First and Second law of thermodynamics, Third law of thermodynamics, Need for third law, Nernst heat theorem, Apparent exceptions to third law, Applications of Third law, Determination of Absolute entropies, Residual entropy. Thermodynamics of Solutions: Partial molar quantities, Chemical potential, Variation of chemical potential with temperature and pressure, Partial molar volume and its determination, Gibbs-Duhem equation, Thermodynamics of ideal and real gases and gaseous mixtures

Unit 2: Thermodynamics –II (9hrs)

Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents)-ionic strength, variation of activity coefficients with concentration; Duhem-Margules equation and its applications. Thermodynamics of ideal solutions, Deduction of the laws of Raoult's ebullioscopy, cryoscopy, and osmotic pressure. Non ideal solutions, Deviations from Raoult's law, Excess functions- excess free energy, excess entropy, excess enthalpy, excess volume.

Unit 3: Thermodynamics of Irreversible Processes (9 hrs).

Simple examples of irreversible processes, general theory of non-equilibrium processes, entropy production, the phenomenological relations, Onsager reciprocal relations, application to the theory of diffusion, thermal diffusion, thermo-osmosis and thermo molecular pressure difference, electro-kinetic effects, the Glansdorf - Pregogine equation.

Unit 4: Statistical Thermodynamics- I (9 hrs)

Fundamentals – concept of distribution, thermodynamic probability and most probable distribution, ensembles, statistical mechanics for systems of independent particles and its importance in chemistry, thermodynamic probability & entropy, idea of microstates and macro states, statistical weight factor (g), Sterling approximation, Maxwell- Boltzman statistics. The molecular partition function and its relation to the thermodynamic properties, derivation of third law of thermodynamics.

Unit 5: Statistical Thermodynamics- II (9 hrs)

Equilibrium constant & equi-partition principle in terms of partition functions, relation between molecular & molar partition functions, factorisation of the molecular partition function into translational, rotational, vibrational and electronic parts, the corresponding contributions to the thermodynamic properties; Evaluation of partition functions and thermodynamic properties for ideal mono-atomic and diatomic gases. Heat capacities of solids - classical and quantum theories, Einstein's theory of atomic crystals and Debye's modification. Quantum Statistics: Bose - Einstein distribution law, Bose-Einstein condensation, application to liquid helium; Fermi - Dirac distribution law, application to electrons in metals; Relationship between Maxwell-Boltzman, Bose-Einstein, and Fermi-Dirac statistics.

Unit 6: Chemical Kinetics –I (9 hrs)

Reaction rates and order of reactions, Determination of order of reactions, Complex reactions, Reversible, Consecutive and Concurrent reactions, Reactions of variable order-Steady State treatment, Reaction mechanism and molecularity. Kinetics of reactions involving reactive atoms and free radicals - Rice – Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions (acetaldehyde & ethane);

Unit 7: Chemical Kinetics – II (9 hrs)

Kinetics of chain reactions – branching chain and explosion limits (H_2-O_2 reaction as an example); Kinetics of fast reactions: relaxation methods, molecular beams, flash photolysis; Solution kinetics: Factors affecting reaction rates in solution, Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects. Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies

Unit 8: Molecular Reaction Dynamics (9 hrs)

Reactive encounters: Collision theory, diffusion controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories; The dynamics of molecular collisions – Molecular beams, principle of crossed-molecular beams; Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger and Kassel (RRK) model.

References:

1. P. Atkins & J. De Paula*, Atkins's Physical Chemistry, 10/e, OUP, 2014*.
2. Margaret Robsom Wright*, "An Introduction to Chemical Kinetics,"*John wiley & Sons, 200
3. Keith J. Laidler, *Chemical Kinetics 3rd edn*., Pearson Education, 1987(Indian reprint 2008).
4. Steinfeld, Francisco and Hase, *Chemical Kinetics and Dynamics, 2nd edition,* Prentice Hall International . Inc.
5. Santhosh K. Upadhyay, *Chemical Kinetics and Reaction Dynamics,* Springer, 2006.
6. S. Glasstone, *Thermodynamics for chemists,* East-West 1973.
7. Rajaram and Kuriocose, *Thermodynamics: Classical, Statistical and Irreversible;,* East-West 1986
6. Pigoggine, *An introduction to Thermodynamics of irreversible processes*, Interscience
7. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn, Prentice Hall of India

For Units 4 & 5

8. G.S. Rush Brooke, *Statistical mechanics,* Oxford University Press.
9. T.L. Hill, *Introduction to statistical thermodynamics,* Addison Wesley.
10. K. Huary, *Statistical mechanics, Thermodynamics and Kinetics* , John Wiley.
11. O.K.Rice, *Statistical mechanics, Thermodynamics and Kinetics,* Freeman and Co.

12. F.C. Andrews, *Equilibrium statistical mechanics*, John Wiley and sons, 1963.
13. M.C. Guptha, *Statistical Thermodynamics* , Wiley eastern Ltd., 1993.

SEMESTER II
Theory Course V
DCHE2B05T – THEORETICAL CHEMISTRY - II
(4 Credits, 72hrs)

Unit 1: Foundations of Group Theory & Molecular Symmetry (12hrs)

Molecular Symmetry: symmetry elements and symmetry operations in molecules - relations between symmetry operations such as squires and combinations – independent operations of $\hat{S}_3 \wedge \hat{S}_6 -$¿ complete set of symmetry operations of a molecule avoiding repetations

Basic principles of group theory : The four rules governing a mathematical group - finite and infinite groups - Abelian and cyclic groups – system integers as an example of group

Group multiplication tables (GMT): Group multiplication tables of abstract groups - Group multiplication tables C_{2v}, C_{3v} and C_{2h} - sub groups

Similarity transformation: classes in a group – classes in C_{3v} point group – effect of removing reflection from a point group; eg. C_{3v}

Symmetry point groups: Schoenflies notation of point groups - systematic identification of point groups, rules for grouping elements of point groups in to classes

Mathematical preliminaries: matrix algebra, addition and multiplication of matrices - square matrix - adjoint of a matrix – Determinants – minors and co factors - inverse of a matrix – special method to determine inverse of a 2 X 2 matrix - solving linear equations by the method of matrices

Bloc diagonalised matrices - character of a square matrix – bloc diagonalistion or bloc factorisation - diagonal matrix - direct product and direct sum of square matrices

Matrix representation of symmetry operations: Matrix representation of $\hat{E}$, $\hat{C}_n$, $\hat{S}_n$, $\hat{i}$, and $\hat{\sigma}$ - Matrix representation clockwise and anti clockwise rotation.

UNIT 2: Representations of Point Groups & Corresponding Theorems (12hrs)

Representations of point groups: basis for a representation - atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H2O as example) as bases, atomic orbitals of butadiene as basis

Reducible representations and irreducible representations of point groups: construction of irreducible representations by bloc diagonalistion (qualitative demonstration only)

The Great Orthogonality Theorem (GOT) (no derivation) : Five consequent rules of GOT - derivation of characters of IR using GOT, construction of character tables of point groups (C2V, C3V, C2h and C4V and C3 as examples)

Nomenclature of IR: Mulliken symbols - symmetry species - irreducible representations using vectors (translation and rotation)
Reduction formula - derivation of reduction formula using GOT- reduction of reducible representations using the reduction formula

Unit 3: Applications of Group Theory to Molecular Spectroscopy (18hrs)

Relation between group theory and quantum mechanics: wave functions (orbitals) as bases for IR of point groups (eg.NH_3).

Direct products: Direct product rule -Direct product –direct product of irreducible representations – vanishing and non vanishing integrals – use of direct products in determining vanishing and non – vanishing nature of integrals - transition moment integral and spectral transition probabilities - overlap integrals and conditions for overlap

Molecular vibrations: symmetry species of normal modes of vibration - construction of $\Gamma_{cart} \wedge$ *obtaining irreducible representations of normal modes using reduction formula* $-$ ¿ nor

mal coordinates and drawings of normal modes (e.g., H_2O and NH_3),

Selection rules: Selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules using character tables(e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra. Spectral transition probabilities Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

Unit 4: Applications of Group Theory to Chemical Bonding (12hrs)

Hybridisation: construction of Γ_{cart} and identification of orbitals involved in hybridisation of BF_3 and CH_4

SALC: Treatment of hybridization in BF_3 and CH_4 – inverse transformation - projection operator and construction of SALC - use of projection operator in constructing SALCs for the π MOs in cyclopropenyl ($C_3H_3{}^+$) cation. Molecular orbital theory

SAGO: HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, construction of group orbitals taking HCHO and H_2O as examples

Unit 5: Approximation Methods in Quantum Mechanics (18hrs)

Many electron atoms: $\hat{H}$ of helium atom - Schrodinger wave equation of helium atom- the problem term and need of approximation

Independent particle model: Schrodinger wave equation of helium atom according to Independent particle model – calculation of energy – accuracy of the method – auf bau principle (mention only)

Perturbation method: the time-independent perturbation method (non-degenerate case only), perturbation term in the $\hat{H}$ - correction terms to wave function and energy (Solution of perturbation equations not expected) - perturbation treatment of the ground state of the helium atom- illustration by application to particle in a ID-box with slanted bottom,

Variation method: variation theorem with proof - setting up of trial functions – linear and non linear trial functions - calculation of energy using trial function – secular equations and secular determinant – application to ground state of He atom - illustration of variation theorem using a trial function [e.g., x (a-x)] for particle in a 1D-box and using the trial function $e^{-\alpha r^2}$ for the hydrogen atom

References; Chapters 1-4

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2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* John Wiley &Sons Inc., 1965.
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10.A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.

Chapter 5

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12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
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14. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003

SEMESTER II
Theory Course VI
DCHE2B06T - INORGANIC CHEMISTRY- II
(4 Credits, 72 hrs)

Unit 1: Stability of Co-ordination Compounds (9hrs)

Stereochemistry of coordination compounds. Stepwise and overall formation constants and the relationship between them. Trends in stepwise formation constants. Determination of binary formation constants by pH-metry and spectro photometry. Stabilisation of unusual oxidation states. Ambidentate and macrocyclic ligands. Chelate effect and its thermodynamic origin. Macrocyclic and template effects.

Unit 2: Theories of Bonding in Coordination Compounds (9hrs)
Sidgwick`s electronic interpretation of coordination. The valence bond theory and its limitations. The crystal field and ligand field theories. Splitting of d-orbitals in octahedral, tetrahedral and square planar fields. Factors affecting crystal field splitting. Spectrochemical and nephelauxetic series. Racah parameters. Jahn-Teller effect. Molecular orbital theory-composition of ligand group orbitals. MO diagram of octahedral, tetrahedral and square planar complexes. π-bonding and molecular orbital theory.

Unit 3: Electronic Spectra Complexes and Magnetic Properties of Complexes (9hrs)
Spectroscopic ground state. Terms of d^n configurations. Selection rules for d-d transitions. Effect of ligand fields on RS terms in octahedral and tetrahedral complexes. Orgel diagrams. Calculation of Dq, B and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra. Spectra of f- block complexes.

Unit 4: Magnetic Properties of Complexes (9hrs)
Types of magnetic properties-Para magnetism and diamagnetism. Curie and Curie-Weiss laws. The μ_J , μ_{L+S} , and μ_S expressions. Orbital contribution to magnetic moment and its quenching. Spin-orbit coupling. Temperature independent para magnetism. Spin cross over in coordination complexes, magnetic properties of f- block elements. Anti ferro magnetism-types and exchange pathways. Determination of magnetic moment by Gouy method.

Unit 5: Characterization of Coordination Complexes- I (9hrs)
Infrared and Raman spectra of simple inorganic compounds and metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Application in coordination complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling.

Unit 6: Characterization of Coordination Complexes- II (9hrs)
ESR spectra of metal complexes- hyperfine splitting and A parameter, g value, zero field splitting and Kramers degeneracy. Application to simple copper complexes.
Mossbauer spectroscopy- the Mossbauer effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.
Application of NQR spectroscopy and mass spectrometry in the characterization of inorganic compounds.

Unit 7: Reaction Mechanism of Metal Complexes (9hrs)
Ligand substitution reactions. Labile and inert complexes. Rate laws. Classification of mechanisms-D, A and I mechanisms. Substitution reactions in octahedral complexes. The Eigen-Wilkins Mechanism. Fuoss-Eigen equation. Aquation and base hydrolysis mechanism.

Substitution reactions in square planar complexes. The trans effect-Applications and theories of trans effect. The cis effect.

Unit 8: Redox Reactions of Complexes (9hrs)

Electron transfer reactions. Outer sphere mechanism. Electron transfer and MO symmetry-Cross reactions: Marcus- Hush equation. Inner sphere mechanism. Influence of the bridging ligand on inner sphere electron transfer.

Two electron transfer. Non- complementary electron transfer reactions. Examples of electron transfer reactions in biological systems.

References:

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11. A.Earnshaw, *Introduction to Magnetochemistry, Academic Press, 1968.*
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13. A.E. Martell, *Coordination Chemistry, Vol. I*
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SEMESTER II

Theory Course VI

DCHE2B07T -ORGANIC CHEMISTRY – II

(3 Credits, 54 h)

UNIT I: Pericyclic reactions (9 h)
Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3 butadiene, 1,3,5-hexatriene and allyl system. Definition, types and classification of pericyclic reactions. Theoretical models of pericyclic reactions - Orbital correlation method, Transition state aromaticity method, Frontier molecular orbital method. Electrocyclic reactions – conrotatory and disrotatory motions: 4n, 4n+2 and allyl systems. Cycloaddition –antarafacial and suprafacial additions, [2+2] additions of ketenes, substituent effects on reactivity, regioselectivity and stereochemistry of Diels-Alder reactions. Catalysis of Diels-Alder reactions by lewis acids. Scope and synthetic applications of the Diels-Alder reaction. 1,3-dipolar cycloadditions, and cheleotropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, *ene* reaction. Sigmatropic shifts involving carbon moieties: [3,3]- and [5,5]- sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangements.
UNIT II: Photochemistry (9 hr):

Principles of photochemistry: Electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), quantum yield. Electronic energy transfer: photosensitization and quenching process.

Photochemistry of carbonyl compounds: π-π*, n-π* transitions, Norrish-I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, photochemistry of enones, photochemical rearrangements of α, β unsaturated ketones and cyclohexadienones. Photo Fries rearrangement.
Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π- methane rearrangement including oxa-di- π -methane. Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions.
Singlet oxygen and photooxygenation reactions. Barton and Hoffmann-Loeffler reaction.
UNIT III: Electronic & Vibrational Spectroscopy in Organic Chemistry (9 h)
UV-Visible spectroscopy: Different types of transition noticed in UV spectrum of organic functional groups and their relative energies. Chromophores and auxochromes. Factors affecting the position of UV bands: Conjugation, steric hindrance on coplanarity and solvent effects. Applications of UV-Visible spectroscopy: Structure determination, qualitative and quantitative analysis, determination of strength of hydrogen bonding, study of charge transfer complexes and study of isomerism.
Infrared Spectroscopy: Functional group and finger print regions. Factors affecting vibrational frequency: Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. Important absorption frequencies of different class of organic compounds- hydrocarbons, alcohols, thiols, carbonyl compounds, amines, nitriles.
Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, circular dichroism, ORD, CD curves and Cotton effect. Octant rule and Axial haloketone rule for the determination of conformation and configuration of 3-methyl cyclo hexanone and *cis*- and *trans*-decalones.
UNIT IV: Mass Spectrometry (9 h)
Mass Spectrometry: Basic concept of ionization techniques. Base peak, m/z ratio, molecular ion, fragment ions, metastable ions and isotopic clusters. General modes of fragmentation,

single and multiple bond cleavage, ortho effect and rearrangements - McLafferty rearrangement. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, carbonyl compounds, amines and amides. Index of hydrogen deficiency, nitrogen rule and rule of thirteen. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT V: NMR Spectroscopy in Organic Chemistry (9 h)

^{1}H NMR: Origin of NMR spectrum, Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic, and aromatic compounds) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides). Chemical, magnetic and stereochemical equivalence. Enantiotopic, daisteriotopic and homotopic protons. Quadrapole broadening. Spin –spin coupling, coupling constants, factors influencing coupling constant. Spin system notations: AB, AX, AMX and ABX spin systems with suitable examples. First order and non first order splitting. Heteronuclear couplings: coupling between ^{1}H and ^{13}C, ^{1}H and ^{14}N, ^{1}H and ^{19}F, ^{1}H and ^{31}P nmr spectra. Simplification of complex spectra: chemical shift reagents, deuterium labelling and exchange, high field NMR, spin decoupling. Nuclear Overhauser effect (NOE).

UNIT VI: ^{13}C-NMR and 2-D NMR spectroscopy (9 h)

^{13}C-NMR: Introduction, ^{13}C-chemical shifts (aliphatic, olefinic, alkyne, aromatic, and carbonyl) and structure correlation. Proton coupled ^{13}C spectra, proton decoupled ^{13}C spectra, Off-resonance decoupling, DEPT ^{13}C spectra and INADEQUATE.

2D NMR Techniques: Principles of 2D NMR, Classification of 2D-experiments - Homonuclear and Heteronuclear 2D-J-resolved spectroscopy. Correlation spectroscopy (COSY), HOMO COSY (^{1}H-^{1}H COSY), Hetero COSY (^{1}H-^{13}C HETCOR), HMBC and HMQC.

Structural determination of organic compounds based on the data from IR, Mass and NMR spectroscopy (Problem solving approach).

References:

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SEMESTER II
Theory Course VIII
DCHE2B08T – Physical Chemistry II
(4 Credits, 72hrs)

Unit1: Basic Aspects and Microwave Spectroscopy (12hrs)
Electromagnetic radiation & it's different regions, Interaction of matter with radiation and its effect on the energy of a molecule, Factors affecting the width and Intensity of spectral lines-

Microwave spectroscopy **-** Rotation spectra of diatomic and poly atomic molecules - rigid and non-rigid rotator models, asymmetric, symmetric and spherical tops, isotope effect on rotation spectra, Stark effect, nuclear and electron spin interactions, rotational transitions and election rules, determination of bond length using microwave spectral data.

Unit 2: Infrared, Raman and Electronic Spectroscopy (12hrs)

Vibrational spectroscopy -Normal modes of vibration of a molecule; Vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands; Vibrational spectra of polyatomic molecules; Vibration rotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & R branches.

Raman spectroscopy –Classical and Quantum theory of Raman effect Pure rotational & purevibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle; Introduction to Resonance Raman spectroscopy (basics only).

Electronic Spectroscopy- Beer-Lambert's law, characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions; Dissociation and pre-dissociation; Ground and excited electronic states of diatomic molecules; Electronic spectra of polyatomic molecules; Electronic spectra of conjugated molecules.

Unit 3: Magnetic Resonance Spectroscopy (12hrs)

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities using ladder operators-Nuclear shielding- Chemical shift- Spin-Spin coupling and splitting of NMR signals- Quantum mechanical Description- AX and AB NMR pattern-Effect of Relative magnitudes of J (Spin-Spin coupling) and Chemical Shift on the spectrum of AB type molecule. Karplus relationship.- Nuclear Overhauser Effect- FT NMR- Pulse sequence for T1and T2 (Relaxation) measurements. 2D NMR COSY

Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field- Energy levels-Population- Transition probabilities using Ladder operators- g factor-hyperfine interaction-Mc Connell Relation-Equivalent and non equivalent nucleus- g anisotropy- Zero field splitting -Kramer's theorem.

Mossbauer Spectroscopy: The Mossbauer effect, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions.

Unit 4: Quantum Mechanics of Many-electron Atoms (12hrs)

Approximate orbital for multi electron atoms: Slater type orbitals (STO): approximation adopted in STO - Slater rules – quantum defect – screening constant

Gaussian type orbitals (GTO): approximation adopted in GTO – primitive Gaussian – contracted Gaussian

Comparison of efficiency of AO, STO and GTO

Hartree Self-Consistent Field method for atoms: $\hat{H}$ for many electron atoms – coulomb operator - Fock operator – Hatree field – Guess set or basis set – improved sets - self consistent field orbitals - Roothan's concept of basis functions

Pauli's anti symmetry principle: Spin orbitals for many electron atoms - symmetric and anti symmetric wave functions - Slater determinants - Pauli's anti symmetry or exclusion principle – Slater determinant – one electron spin orbitals – Slater determinants of helium atom ground and exited state, lithium atom.

Hund's Rule: spin-orbital interactions - Spectroscopic term symbols of atoms – term symbols of carbon atom – equivalent and non equivalent electrons – relative stability of terms and Hund's rule.

Unit 5: Quantum Mechanics of Molecules I: The Chemical Bonding in diatomic molecule (12hrs)

Schrödinger equation for molecule: Born – Oppenheimer approximation _ electronic $\hat{H}$ -nuclear frame work – Equilibrium inter nuclear distance – bond dissociation energy – potential energy diagram for nuclear movement.

Molecular Orbital (MO) theory: MO theory of H_2^{+} ion - LCAO - Secular equations – secular determinants – Bonding and anti- Bonding MO – singlet and triplet state functions (spin orbitals) of H_2 – bond order - MO energy level diagram.

MO theory of H_2 molecule: The orbital approximation.

MO treatment of homo nuclear diatomic molecules: Li_2, Be_2, C_2, N_2, O_2 & F_2 – bond order and magnetic nature.

MO treatment of hetero nuclear diatomic molecules: LiH, CO, NO & HF - bond order .

Valence Bond (VB) theory: VB theory of H_2 molecule - Secular equations – secular determinants – Heitler- London Orbitals.

Comparison of MO and VB theories.

Unit 6: Quantum Mechanics of Molecules II: The Chemical Bonding in polyatomic molecules (12hrs)

Shapes of molecules and the principle of Hybridization: Quantum mechanical treatment of sp, sp^2 & sp^3 hybridisation – ortho normal nature of hybridised orbitals.

Semi empirical MO treatment of planar conjugated molecules: Hückel Molecular Orbital (HMO) theory – HMO approximations – Huckel determinant – formula for the roots of the Hückel determinantal equation - evaluation of HMO coefficients.

Application Hückel Molecular Orbital treatment to ethylene, butadiene & allylic system - π bond energy and delocalisation energy - charge distributions and bond orders from the coefficients of HMO - Calculation of free valence - HMO theory of aromatic hydrocarbons (benzene).

References: Chapters 1,2 & 3

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Chapters 4,5 &6

1. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books, 2003).
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition,* Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
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6. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
7. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
9. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
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11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
14. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.

SEMESTER I & II

Practical Course I

DCHE2B09P – INORGANIC CHEMISTRY PRACTICALS– I & II

(4 Credits)

UNIT 1: Inorganic Cation Mixture Analysis

Separation and identification of four metal ions of which two are less familiar elements like W, Se Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present). Confirmation by spot tests.

UNIT 2: Volumetric Analysis

Volumetric Determinations using:
(a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)
(b) Cerimetry (Fe^{2+}, nitrite)
(c) Potassium Iodate (Iodide, Sn^{2+})

UNIT 3: Colorimetric Analysis

Colorimetric Determinations of metal ions Fe, Cr, Ni, Mn and Ti.

References

1. G.H. Jeffery, J. Basseett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.
2. D.A. Skoog and D.M. West, *Analytical Chemistry, An Introduction*, 4th Edition, CBS Publishing Japan Ltd., 1986.
3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, *Quantitative Chemical Analysis*, 4th Edition, The Macmillan Company, 1969.
4. R.A. Day (Jr.) and A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall of India, 1993.

SEMESTER I & II

Practical Course II

DCHE2B10P – ORGANIC CHEMISTRY PRACTICALS– I & II

(4 Credits)

PART I: Separation and identification of the components of organic mixtures using micro-scale technique

(i) Separation of components of binary mixtures based upon differences in the physical and the chemical properties of the components.
(ii) Purification of the components and determination of their physical constants.
(iii) Separation and identification of a few ternary mixtures.

PART II: Organic preparations

(i) Preparations involving two step / multistep synthetic sequences.
(ii) Enzyme/coenzyme catalyzed reactions.
(iii) Preparations involving green alternatives of chemical methods.

Students are expected to know

(i) the planning of synthesis, effect of reaction parameters such as stoichiometry and safety aspects including MSDS.
(ii) the purification techniques (recrystalization / column chromatography), use of rotary evaporator, use of TLC for monitoring/establishing purity, determine physical constants and calculate percentage yield.
(iii) the possible mechanism, expected spectral data (IR/NMR/UV) of the starting material and final product.
(iv) to draw the structures of organic molecules and reaction schemes by ChemDraw/ Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products.

References:

1. A. I.Vogel, *A textbook of practical organic chemistry compounds*, Vol I & II.
2. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5/e, Pearson, 1989.
3. N. K. Vishnoi, *Advanced Practical Organic Chemistry*, Vikas Publishing.
4. Pavia, Kriz, Lampman, and Engel, *A Microscale Approach to Organic Laboratory Techniques,* 5/e, Cengage, 2013.
5. P.R. Singh, D.C. Gupta and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II, 1980.
6. Mohrig, Hammond and Schatz, *Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale,* 3/e, W. H. Freeman and

Co., 2010.

SEMESTER I & II
Practical Course III (Physical)
DCHE2B11P – PHYSICAL CHEMISTRY – I & II
(4 Credits)

SECTION A

Unit 1: Solubility and Heat of solution (minimum 2 experiments)

1. Determination of molar heat of solution of a substance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method

Unit 2: Phase Equilibria (minimum 3 experiments)

1. (a) Determination of phase diagram of a simple eutectic system (e.g., Biphenyl, naphthalene-Diphenyl amine) (b) Determination of the composition of a binary solid mixture.
2. Determination of phase diagram of a binary solid system forming a compound (e.g.,Naphthalene – m-dinitrobenzene).

Unit 3: Viscosity (minimum 2 experiments)

1. Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene - nitrobenzene, water-alcohol).
2. Determination of molecular weight of a polymer (e.g., polystyrene in Benzene)

Unit 4: Distribution Law (minimum 3 experiments)

1. Determination of distribution coefficient of I_2 between CCl_4 and H_2O.
2. Determination of equilibrium constant of $KI + I_2 = KI_3$
3. Determination of concentration of KI solution

SECTION B

Unit 5: Refractometry (minimum 3 experiments)

1. Determination of molar refractions of pure liquids (e.g., water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol)
2. Determination of composition of liquid mixtures (e.g., alcohol -water, glycerol-water)
3. Determination of molar refraction and refractive index of a solid

Unit 6: Conductivity (minimum 4 experiments)

1. Determination of equivalent conductance of a weak electrolyte (e.g.,acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
2. Determination of solubility product of a sparingly soluble salt (e.g., AgCl, BaSO4)

3. Conductometric titrations
(a) HCl vs NaOH
(b) (HCl + CH_3-COOH) vs NaOH
4. Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (minimum 3 experiments)
1. Potentiometric titration: HCl vs NaOH, CH_3-COOH vs NaOH
2. Redox titration: KI vs $KMnO_4$, $FeSO_4$ vs $K_2Cr_2O_7$
3. Determination of dissociation constant of acetic acid by potentiometric titration
4. Determination of pH of weak acid using Potentiometry
5. Determination of pH of acids and bases using pH meter

References:

1. A. Finlay, *Practical Physical Chemistry*, Longman's Green & Co.
2. J.B. Firth, *Practical Physical Chemistry*, Read Books (Reprint 2008).
3. A.M. James, *Practical Physical Chemistry*, Longman, 1974.
4. F. Daniel, J.W. Williams, P. Bender, R.A. Alberty, C.D. Cornwell and J.E. Harriman, *Experimental Physical Chemistry* , McGraw Hill, 1970.
5. W.G. Palmer, *Experimental Physical Chemistry*, 2nd Edition, Cambridge University Press, 1962.
6. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry*, McGraw Hill.
7. J. B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications,* 1989.
8. B. Viswanathan & R.S. Raghavan, *Practical Physical Chemistry*, Viva Books, 2009

SEMESTER III
Theory Course IX
DCHE3B13T - INORGANIC CHEMISTRY-III
(4 Credits, 72h)

Unit 1: Introduction to Organometallic Chemistry (9hrs)
Historical background. Classification and nomenclature. Alkyls and aryls of main group metals. Organometallic compounds of transition metals. The 18-electron rule-electron counting by neutral atom method and oxidation state method. The 16-electron rule. Metal

carbonyls- Synthesis, structure, bonding and reactions. Nytrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbynes.

Unit 2: Organometallic Compounds of Linear and Cyclic π-Systems (9hrs)
Transition metal complexes with linear π- systems-Hapticity. Sythesis , structure, bonding and properties of complexes with ethylene, allyl, butadiene and acetylene. Complexes of cyclic π- systems-Synthesis, structure, bonding and properties of complexes with cyclo butadiene, $C_5H_5^-$ C_6H_6, $C_7H_7^+$ and $C_8H_8^{2-}$.

Unit 3: Reactions of Organometallic Compounds (9hrs)
Organometallic reactions- ligand dissociation and substitution- Oxidative addition and reductive elimination. Insertion reactions involving CO and alkenes. Carbonylation by Collman`s reagent. Electrophilic and Nucleophilic attack on coordinated ligand.

Unit 4: Catalysis by Organometallic Compounds (9hrs)
Homogeneous and heterogeneous catalysts. Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydro formylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis. Heterogeneous catalysis by organometallic compounds: Ziegler-Natta polymerizations, Fischer- Tropsch process and water gas shift reaction.

Unit 5: Metal Clusters (9hrs)
Metal-Metal bond and metal clusters. Bonding in metal-metal single, double, triple and quadruple bonded non-carbonyl clusters. Carbonyl clusters-electron count and structure of clusters. Wade- Mingos-Lauher rules. Structure and isolobal analogies. Carbide clusters. Polyatomic Zintl anions and cations. Chevrel phases.

Unit 6: Bioinorganic Chemistry-I (9hrs)
Occurrence of inorganic elements in biological systems- bulk and trace metal ions. Emergence of bioinorganic chemistry. Coordination sites in biologically important ligands. Bioenergetics and ATP cycle**.** Ion transport across membranes- ionophores and passive transport. Role of alkali metal ions in biological systems. The sodium/potassium pump. Structural role of calcium.

Unit 7: Bioinorganic Chemistry-II (9hrs)
Storage and transport of metal ions- ferritin, transferrin and siderophores. Oxygen transport by heme proteins-hemoglobin and myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin.

Unit 8: Bioinorganic Chemistry-III (9hrs)
Metallo enzymes and electron carrier metallo proteins. Iron enzymes: Cytochrome P-450, catalase and peroxidase.Copper enzymes: Oxidase, superoxide dismutase and tyrosinase. Lewis acid. Role of Zn(II) and Mn(II) containing enzymes.Vitamin B12 and coenzymes. Chlorophyll- Photosystem I and II. Nitrogen fixation-Nitrogenases.

References:

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements,* 2/e, Elsevier Butterworth-Heinemann, 2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi, *Inorganic Chemistry, principles of structure and reactivity*, Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,* Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,* Oxford University Press, 2002
5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press, 2005.
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7. James E House, *Inorganic Chemistry,* Academic Press, 2008.
8. B.Douglas, D.McDaniel, J.Alexander, *Concepts and Models of Inorganic Chemistry,* Wiley Student Edition, 2006.
9. F.A.Cotton and G.Wilkinson, *Advanced Inorganic Chemistry,* Wiley.
10. R.C.Mehrothra and A.Singh, *Organometallic Chemistry, A Unified Approach, W*iley eastern.
11. P.Powell, *Principles of Organometallic Chemistry, ELBS.*
12. B.D.Gupta and A.J.Elias, *Basic Organometallic Chemistry, Concepts, Synthesis andApplications,* Universities Press, 2010.
13. Piet W.N. M.van Leeuwen, *Homogeneous Catalysis*, Springer, 2010.
14. S.J. Lippard and J.M.Berg, *Principles of Bioinorganic Chemistry*, University Science Books.
15. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, *Bioinorganic Chemistry, Viva Books*

SEMESTER III

Theory Course X
DCHE3B14T - ORGANIC CHEMISTRY – III

(4 Credits, 72 h)

Unit I: Aliphatic Substitution Reactions (9 h)

Mechanism and stereochemistry of nucleophilic (S_N1, S_N2, S_Ni) substitutions at aliphatic carbon with suitable examples. Neighbouring group participation - participation of O, S, N, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, pi bond participation in acylic and bicyclic systems (Non- classic carbocations). Substitution at allylic and vinylic carbon atoms. Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity and regioselectivity.

Aliphatic Electrophilic substitutions: S_E1 S_E2 and S_Ei mechanisms with suitable examples. Effect of substrates, leaving group and solvent polarity on the reactivity.

Unit II: Addition and Elimination Reactions (9 h)

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of reactions involving electrophiles, nucleophiles and free radicals. Electrophilic addition-Markovnikov's and anti-Markovnikov's addition, Hydroboration. Nucleophilic addition-Michael addition. Addition to cyclopropane ring.

Elimination Reaction: Mechanistic and stereochemical aspects of E1, E2 and E1cB eliminations. Orientation of the double bond: (i) Zaitsev's Rule, (ii) Hofmann Rule, (iii) Bredt's Rule. *Anti* elimination and *Syn* elimination. Effects of substrate structures, attacking base, the leaving group and reaction medium on elimination reactions. Mechanism and orientation in Hofmann degradation, Pyrolytic eliminations and Corey-Winter reaction.

Unit III: Chemistry of Carbanions (9 h)

Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates − lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates. Named reactions under carbanion chemistry- Aldol, Claisen, Reformatsky, Perkin, Stobbe, Darzen, Knoevenagel, Dieckmann and Thorpe condensations.

Unit IV: Free Radical Reactions (9 h)

Generation of radical intermediates and its reactions. Formation of carbon-halogen bonds - substitution in saturated compounds, substitution in allylic and benzylic compounds by NBS and decarboxylative bromination (Hunsdiecker reaction). C−C bond formation − Addition to alkenes, alkynes (inter and intra molecular), coupling of alkynes, McMurry coupling. C−N bond formation – Hofmann-Loffler-Freytag reaction, Barton reaction. C-O bond formation – Autooxidation.

Unit V: Molecular Rearrangements (18 h)

Unifying principles and mechanisms of rearrangements taking place at an electron deficient and electron rich substrates.

Rearrangements taking place at electron deficient carbon

(1) Arndt Eistert synthesis (2) Wagner Meerwein (3) Benzil-benzilic acid (4) Pinacol (5) Dienone phenol

Rearrangements at electron deficient nitrogen

(1) Hofmann (2) Curtius (3) Lossen (4) Schmidt (5) Beckmann

Rearrangements at electron deficient oxygen

(1) Baeyer Villiger (2) Dakin's reaction

Rearrangements at electron rich carbon

(1) Wittig (2) Favorskii (3) Stevens

Aromatic rearrangements

(1) Benzidine (2) Fries (3) Von Richter (4) Sommelet-Hauser

Unit VI: Natural Products (9 h)

Chemical classification of natural products. Classification of alkaloids based on ring structure. Isolation and general methods of structure elucidation based on degradative reactions. Structure elucidation of atropine. Terpenoids- Isolation and classification of terpenoids. Synthesis of Juvabione. Structure of steroids. Classification of steroids. Conversion of Cholesterol to testosterone. Chemistry and stereochemical features involved in the total synthesis of Reserpine and Cephalosporine C.

Unit VII: Chemistry of Heterocyclic Compounds (9 h)

Principles of heterocyclic synthesis involving cyclisation reactions and cycloadditions. *(i) Three-membered and four-membered heterocycles:* Synthesis and reactions of aziridines, oxiranes, thiranes, azetidine, oxetanes and thietanes. *(ii) Five-membered heterocycles containing one hetero atom:* Synthesis and reactions of pyrroles, furans, thiophens, reduced pyrroles, reduced furans and reduced thiophens. *(iii) Five-membered heterocycles containing two heteroatoms:* Synthesis of pyrazole, imidazole, oxazole, isoxazole and thiazole. *(iv) Five-membered heterocycles containing three heteroatoms***:** Synthesis of 1,2,3-triazole and 1,2,4-tetrazole. Five-membered heterocycles containing four hetero atoms: Synthesis of Tetrazoles.

References:

1. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press, 2002.
2. F.A. Carey, R.A. Sundberg, *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5/e., Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2004.
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6. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*, 7/e, Pearson, 2011.
7. P.S.Kalsi,*Organic reactions & their mechanisms*, 3/e revised, New Age International Publishers.
8. Bradford P. Mundy, Michael G. Ellard and Frank Favoloro, Jr. *Name reactions and reagents in organic synthesis*, 2/e, Wiley-Interscience.
9. Jie Jack Li, *Name reactions*, 3/e, Springer.
10. Thomas L. Gilchrist, *Heterocyclic chemistry*, 3/ e, Pearson Education, 2007.
11. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry Vol. 1-3,* Springer Velag.
12. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.
13. A. R. Kartritzky and C. W. Rees, *Comprehensive Heterocyclic Chemistry, Vol-1-7*, Pergamon press.
14. I. L. Finar, *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*, *Vol 2,* 5/e, Pearson, 2006.

15. N. R. Krishnaswamy, *Chemistry of Natural Products: A Laboratory Hand Book*, 2/e, Universities Press.
16. O. P. Agarwal, *Organic Chemistry: Natural Products Volume-II*, Krishna Prakashan, 2011.
17. V.K. Ahluwalia*, Chemistry of natural products*, Vishal Publishing Co. 2008.
18. Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, *Natural products chemistry and Applications*, Narosa Publishing House, 2011.

SEMESTER III

Theory Course XI

DCHE3B15T - PHYSICAL CHEMISTRY III

(4 Credits, 72hrs)

Unit 1: Electrochemistry - I (9hrs)

The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential and thermodynamic functions. The Debye-Hückel equation, Limiting and extended forms of the Debye- Hückel equation, Applications of the Debye-Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution Origin of electrode potentials-half cell potential-standard hydrogen electrode, reference electrodes- electrochemical series, applications- cell potential, Nernst equation for electrode and cell potentials, Nernst equation for potential of hydrogen electrode and oxygen electrode.

Unit 2: Electrochemistry – II (9 hrs)

Anomalous behaviour of strong electrolytes, theory of strong electrolytes, ionic atmosphere, variation of ionic speeds, relaxation time, mechanism of electrolytic conductance, relaxation and electrophoretic effects, derivation of Debye-Huckel-Onsager equation, Determination of Degree of Dissociation, Conductance ratio, Debye-Falkenhagen effect, Wein effect.
Derivation of Debye-Huckel limiting law and its various forms, qualitative and quantitative of the verification Debye-Huckel limiting law.

Unit 3: Non-Equilibrium Electrochemistry (9 hrs)

Electrical double layer-electrode kinetics of electrode processes, the Butler-Volmer equation- The relationship between current density and overvoltage, the Tafel equation. Polarization - electrolytic polarization, dissolution and deposition potentials, concentration polarization; Overvoltage: hydrogen overvoltage and oxygen overvoltage: decomposition potential and overvoltage, individual electrode over voltages and its determination-metal deposition over voltage and its determination- theories of hydrogen overvoltage, the catalytic theory, the slow discharge theory, the electrochemical theory. Principles of polarography -dropping mercury electrode, the half wave potential.

Unit 4: Solid State – I (9 hrs)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.

Unit 5: Solid State –II (9 hrs)
Bragg's law and applications, lattice planes and miller indices, *d*-spacing formulae, crystal densities and unit cell contents, Imperfections in solids - point, line and plane defects, non-stoichiometry. Electronic structure of solids – free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties - electrical conductivity,

Unit 6: Solid State – II (9 hrs)
Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity; Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity; Optical properties - photo conductivity, luminescence, colour centers, lasers, refraction & birefringence; Magnetic properties - diamagnetism, para magnetism, ferromagnetism, anti ferromagnetism & ferri magnetism; Thermal properties - thermal conductivity & specific heat

Unit 7: Colloids and Surface Chemistry (9 hrs)
Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium. **Adsorption**: Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination; Experimental methods for studying surfaces – SEM, TEM, and ESCA

Unit 8: Catalysis (9 hrs)
Homogeneous catalysis–mechanism -Arrhenius intermediates and van't Hoff intermediates - acid base catalysis – specific and general acid catalysis – enzyme catalysis- Michaelis-Menten Mechanism- Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko -Volterra, brusselator and oregonator) Heterogenous catalysis –adsorption and catalysis- unimolecular surface reactions – bimolecular surface reaction –Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2 \longrightarrow 2CO_2$

References:
For Units 1-3

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall, London, 1979.
2. J.O.M. Bockris and A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers, 2000.
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8. R. Stephen Berry, Stuart A Rice, John Ross, *Physical Chemistry*, 2nd Edn., Oxford University Press, 2000.

For Units 4-6

9. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1960.
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11. A.R. West, *Solid State Chemistry & its Applications,* John Wiley & Sons, 2003 (Reprint 2007).
12. Charles Kittel, *Introduction to Solid State Physics, 7th Edn*, John Wiley & Sons, 2004 (Reprint 2009).
13. Mark Ladd, *Crystal Structures: Lattices & Solids in Stereo view*, Horwood, 1999.
14. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.
15. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd Edn.*, Oxford Uty. Press, 2002.
16.Hans H Jaffe and Milton Orchin, "*Symmetry in Chemistry*", Dover Publications Inc., 2002.
17. Werner Massa, "*Crystal Structure Determination*" 2nd Edn., Springer 2004.
18. N.B. Hanna, *Solid state Chemistry,* Prentice Hall

For Units 7 & 8

19. Richard I. Masel, *Chemical Kinetics and Catalysis*, Wiley Interscience, 2001.
20. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
21. A.W. Adamson, *Physical Chemistry of Surfaces*, 4th edition, Interscience, New York, 1982.
22. G. K. Vemulapalli, *Physical Chemistry*, Prentice Hall of India.
23. M.K. Adam, *The Physics and Chemistry of surfaces*, Dover Publications
24. Robert G. Mortimer, *Physical Chemistry*, 3rd Edition, Academic Press, Elsevier Inc., 2008.

SEMESTER III

Theory Course XII

Elective I

DCHE3E01T - SYNTHETIC ORGANIC CHEMISTRY

(3 Credits, 54 h)

Unit I: Reagents for Oxidation (9 h)

Metal based and non-metal based oxidations of (a) alcohols to carbonyls using Chromium, Manganese and Aluminium metal based reagents, DMSO and other reagents like IBX, DMP, TEMPO and TPAP. (b) alkenes to epoxides (peroxides/per acids based) (c) alkenes to diols (Manganese and Osmium based)-Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage hydroboration- oxidation, Wacker oxidation, selenium/chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation, (g) Oxidation of allylic and benzylic C-H bonds: DDQ and SeO_2.

Unit II: Reagents for Reduction (9 h)

(a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic hydrogenation of alkenes. (b) Hydride transfer reagents from Group III and Group IV in reductions – $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkylstannane. (c) Reduction with hydrazine & derivatives: Reduction of carbonyl group with hydrazine; *p*-tosylhydrazine, diimide and semicarbazide. (d) Dissolving metal reductions: Liquid ammonia reduction with alkali metals, Birch reduction of arenes, Acyloin condensation and related reactions.

Unit III: Synthetic Reagents (9 h)

*Organometallic Reagents***:** (a) Preparation and application of the following in organic synthesis - Grignard, Organo lithium and Organo copper reagents. (b) Organo boranes in C-C bond formation. (c) Organosilicon reagents: Important features of silicon governing the reactivity of C-Si compounds: preparation and important bond forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations as intermediates. Utility of trimethyl silyl halides, cyanides and triflates. (d) Organo chromium reagents: Benzene Tricarbonyl Chromium.

Unit IV. Coupling Reactions (9 h)

Coupling Reactions: Palladium catalysts for C−C, C−N and C−O bond formation, Palladium catalyzed amine arylation (mechanism and synthetic applications). Sonogashira cross coupling reaction (mechanism and synthetic applications in Cyclic peptides), Stille carbonylative cross coupling reaction (mechanism and synthetic applications). Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling reactions. Buchwald-Hartwig coupling reaction.

Unit V: The Ylids in Organic Synthesis (9 h)

Phosphorus Ylids: Nomenclature and Preparation. Wittig olefination: mechanism, stereoselctivity, *cis* and *trans* selective reactions, Wittig reagents derived from α-halo carbonyl compounds, Horner – Wadsworth – Emons modification with achiral and chiral substrates. Controlling the geometry of double bonds: Peterson reaction and the Julia Olifination.

Sulfur Ylids: sulfonium and sulfoxonium ylids in synthesis, diphenylcyclopropyl sulfonium ylids and their reactions with carbonyl compounds / Michael acceptors.

Nitrogen Ylids: Formation, the synthetic utility of Stevens and the Sommelet rearrangement.

Unit VI: Synthetic Strategies (9 h)

Retrosynthetic analysis: target, synthon, synthetic equivalent, disconnection approach, functional group inter-conversion (FGI), functional group addition, functional group elimination. Protection and deprotection of the following functional groups: hydroxyl, carbonyl, amino and carboxyl with applications. Importance of order of events in organic synthesis, one group and two group C−X disconnections, chemo selectivity, reversal of polarity, cyclisation reactions.

One group C−C disconnections−alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two group C−C disconnections – Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Mannich bases as intermediates in organic synthesis. Michael addition and Robinson annulations. Synthetic routes based on retrosynthetic analysis for Juvabione.

References:

1. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
2. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
3. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis,* 3/e, CRC Press, 1998.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
5. A. Molnar, *Palladium-Catalyzed Coupling Reactions: Practical Aspects and Future Developments*, Wiely-VCH, 2013.
6. H. O. House, *Modern Synthetic Reactions*, W. A. Benjamin.
7. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, Wiley.
8. P. Wyatt and S. Warren, *Organic Synthesis: Strategy and Control,* Wiley.
9. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
10. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
11. T. W. Greene and P. G. M. Wuts: *Protecting Groups in Organic Synthesis*, 2nd ed., Wiley
12. E. J. Corey and Xue-Min Cheng, *The Logic of Chemical Synthesis*, Wiley Interscience.
13. K. C. Nicolaou and E. J. Sorensen, *Classics in Total Synthesis*, Weinhem: VCH, 1996.

SEMESTER III
Theory Course XII
Elective II

DCHE3E02T - COMPUTATIONAL CHEMISTRY (ELECTIVE)
(3credits, 54 hrs)

Unit 1: Introduction to Computational Chemistry (9 hrs)

Theory, computation & modeling – Definition of terms; Need of approximate methods in quantum mechanics; Computable Quantities – structure, potential energy surfaces and chemical properties; Cost & Efficiency – relative CPU time, software & hardware; Classification of computational methods.

Unit 2: Computer Simulation Methods- I (9 hrs)

Introduction – molecular dynamics and Monte Carlo methods, calculation of simple thermodynamic properties - energy, heat capacity, pressure and temperature, phase space,practical aspects of computer simulation, periodic boundary conditions, Monitoring the equilibration, analyzing the results of a simulation, error estimation.

Unit 3: Computer Simulation Methods- II (9 hrs)
Molecular dynamics (MD) method – molecular dynamics using simple models – MD with continuous potentials, finite difference methods, choosing the time step, setting up and running a MD simulation; Monte Carlo (MC) method - calculating properties by integration, Metropolis method, random number generators, MC simulation of rigid molecules.

UNIT 4: ab intio Methods in Computational Chemistry (9hrs)
Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post -HF) methods.

UNIT 5: Density Functional Methods (9 hrs)
Introduction to density matrices, N-reprentability & V-represetability problems, Hohenberg – Kohn theorems, Kohn-Sham orbitals; Exchange correlation functional Thomas-Fermi-Dirac model, Local density approximation, generalised gradient approximation, hybrid functionals; Comparison between DFT and HF methods.

UNIT 6: Basis Set Approximation (9 hrs)
Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered & well tempered basis sets, contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on cpu time.

References:
1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models,* John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry,* John Wiley & Sons LTD 1999.
3. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems"*, Wiley -Interscience, 2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics,* 2 nd edn., Springer 2011.
6. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.

8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.

SEMESTER III
Theory Course XII
Elective III
DCHE3E03T - GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE)
(3credits, 54 hrs)

Unit I: Introduction to green chemistry (9hrs)
Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

UNIT-2: Microwave mediated organic synthesis (MAOS) (9hrs)
Microwave activation –advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions _ Functional group transformations – condensations reactions – oxidations – reductions reactions – multi-component reactions.

Unit 3: Alternative synthesis, reagents and reaction conditions (9hrs)
Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – expoxidations – synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications. A photochemical alternative to Friedel-crafts reactions - Dimethyl carbonate as amethylating agent – the design and applications of green oxidants – super critical carbon dioxide for synthetic chemistry.

Unit 4: Nanomaterials – An Introduction & Synthetic Methods (9hrs)
Definition of nano dimensional materials - Historical milestones - unique properties due to nanosize, Quantum dots, Classification of Nano materials .General methods of synthesis of nano materials – Hydrothermal synthesis, Solvothermal synthesis, Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis, Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated Synthesis of Nano materials using micro organisms and other biological agents, Sono chemical Synthesis, Hydrodynamic Cavitation. Inorganic nano materials – Typical examples –nano TiO_2 / ZnO/CdO/CdS , Organic nano materials – examples – Rotaxanes and Catenanes

Unit 5: Techniques for Characterization of nanoscale materials (9hrs)
Principles of Atomic force microscopy (AFM)- Transmission electron microscopy (TEM)-Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM),Scanning ion

conductance microscope, scanning thermal microscope, scanning probe microscopes and surface Plasmon spectroscopy.

Unit 6: Carbon Clusters and Nanostructures (9hrs)

Nature of carbon bond - New carbon structures - Carbon clusters: Discovery of C60 – Alkali doped C60 -Superconductivity in C60 - Larger and smaller fullerenes. Carbon nanotubes: Synthesis - Single walled carbon nanotubes - Structure and characterization - Mechanism of formation - Chemically modified carbon nanotubes - Doping - Functionalizing nanotubes - Application of carbon nanotubes. Nanowires -Synthetic strategies - Gas phase and solution phase growth - Growth control - Properties.

References:

For Units 1, 2 & 3

1. V. K. Ahluwalia, *Green Chemistry – Environmentally benign reactions,* Ane Books India (Publisher), (2006).
2. V. K. Ahluwalia, *Green Chemistry : A Textbook*, Narosa Publishing House, 2013.
3. *Green Chemistry – Designing Chemistry for the Environment* – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
4. *Green Chemistry – Frontiers in benign chemical synthesis and processes*- edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
5. *Green Chemistry – Environment friendly alternatives*- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

For Units 4, 5 & 6

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), *The Chemistry of Nanomaterials*, Vol.1, 2, Wiley –VCH, Weinheim, 2004.
2. C.P. Poole, Jr: F.J. Owens, *Introduction to Nanotechnology* Wiley Interscience, New jersey, 2003
3. Kenneth J. Klabunde (Ed), *Nanoscale materials in Chemistry*, Wiley- Interscience, New York, 2001.
4. T. Pradeep, *Nano: The Essentials in understanding nanoscience and nanotechnology*, Tata McGraw Hill, New Delhi, 2007.
5. H. Fujita (Ed.), *Micromachines as tools in nanotechnology*, Springer- Verlag, Berlin, 2003.
6. Bengt Nolting, *Methods in modern biophysics*, Springer-Verlarg, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II and 147 – 163 for Unit V)
7. H. Gleiter, *Nanostructured Materials: Basic Concepts, Microstructure and Properties*
8. W. Kain and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life,* John-Wiley R Sons, New York.
9. T. Tang and p. Sheng (Eds), *Nano Science and Technology Novel Structures and Phenomena,*Taylor & Francis, New York, 2004.
10. A. Nabok, *Organic and Inorganic Nanostructures*, Artech House, Boston, 2005.
11. Edward A. Rietman, *Molecular engineering of Nanosystems*, Springer- Verlag, New York, 2001.
12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/

13. Nano letters - http://pubs.acs.org/journals/nalefd/index.html Nanotation - http://www.acsnanotation.org/

SEMESTER III
Theory Course XII
Elective IV
DCHE3E04T - INDUSTRIAL CATALYSIS (ELECTIVE)
(3 Credits, 54hrs)

Unit 1: Introduction to Adsorption process (9hrs)
Intermolecular interactions, physisorption – the forces of adsorption – dispersion and repulsive
forces – classical electrostatic interactions – adsorbate-adsorbate interactions, chemisorption, potential energy curves, thermodynamics of adsorption – isothermal and adiabatic heats of adsorption – variation of heats of adsorption with coverage, adsorption isotherms, Langmuir, BET and Freundlich, kinetics of chemisorption – activated and non-activated chemisorption – absolute rate theory – electronic theories, hysteresis and shapes of capillaries.

Unit 2: Kinetics and Catalysis (9hrs)
Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption equilibrium and catalysis, kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism, kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

References:
1. A. Clark, *"Theory of adsorption and catalysis",* Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, *"Introduction to principles of heterogeneous catalysis",* Academic Press, New York, 1967.
3. R.H.P. Gasser, *"An introduction to chemisorption and catalysis by metals",* Oxford, 1985.
4. D.K Chakraborthy, *"Adsorption and catalysis by solids",* Wiley Eastern Ltd. 1990.

Unit 3: Catalyst - Praparative Methods(9hrs)
Surface area and porosity measurement – measurement of acidity of surfaces; Support materials – preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process. General methods of synthesis of zeolites, mechanism of nuclear formation and crystal

growth, structuresof some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9hrs)

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

References:

1. J.R. Anderson and M. Boudart (Eds), *"Catalysis, Science and Technology",* Vol 6, Springer-
Verlag, Berlin Heildberg, 1984.
2. R.B. Anderson, *"Experimental methods in catalysis research",* Vol I, II, Academic press, NY, 1981.
3. R. Szostak, *"Molecular sieves: principles of synthesis and identification*", Van Nostrand, NY,1989.
4. R. Hughes*, "Deactivation of catalysts",* Academic press, London, 1984.

UNIT 5: Phase Transfer Catalysis (9hrs)

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts. Use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds –use of dual phase transfer catalyst or co-catalyst in phase transfer systems –separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT 6: Biocatalysis (9hrs)

Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes.

References:

1. C.M. Starks, C.L. Liotta And M. Halpern, *"Phase Transfer Catalysis – Fundamentals, Applications And Industrial Perspectives"*, Chapman & Hall, New York, 1994.
2. A.L. Lehninger, *"Principles of Biochemistry",* Worth Publishers, USA, 1987.

SEMESTER IV

Theory Course XIV

DCHE4B16T- ADVANCED INORGANIC CHEMISTRY
(4Credits, 72hrs)

Unit 1: Nanomaterials (9hrs)

History of nanomaterials- Classification. Size- dependence of properties. Electronic structure theory of metals and semiconductors. Quantum size effects. Synthesis of nanostructures: bottom-up-approach, top- down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis. Nanocomposites.

Unit 2: Characterisation and Applications of Nanomaterials (9hrs)

Methods of characterization: Electron microscopies- SEM, TEM. Scaning probe microscopies- STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD).

Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofilteration, diagnostic and therapeutic applications and targeted drug delivery. Introduction to graphenes and fullerenes.

Unit 3: Heterogeneous catalysts (9hrs)

Structure and chemical nature of surfaces. Physisorption and chemisorptions. Energy exchange at surface. Homogeneous and heterogeneous catalysts. Preparative methods for heterogeneous catalysts- precipitation and coprecipitaion methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Determination of surface area and pore structure of catalysts - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorptions methods. Determination of surface acidity-TPD method. Catalyst selectivity, effect of pore size on selectivity. Mesoporous materials.

Unit 4: Industrial Heterogeneous Catalysis (9hrs)

Introduction to Phase transfer catalysis, bio catalysis, nano catalysis and polymer supported catalysis. Application of heterogeneous catalysts in ammonia synthesis, SO_2 oxidation and catalytic cracking. Zeolite based heterogeneous catalysis. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

Unit 5: Inorganic Medicinal Compounds (9 hrs)

Cisplatin and related complexes, auranofin and arthritis treatment, vanadium complexes in medicine, lithium and mental health.

Diagnostic agents- Technetium Imaging Agents and Gadolinium MRI Imaging Agents.

Metal deficiency and diseases, toxic effect of heavy metals (As, Pb, Hg,Cd and Cu) and their detoxification.

Unit 6: Photoinorganic Chemistry(9hrs)

Photochemical reactions of metal complexes- Prompt and delayed reactions. Exited states of metal complexes- Inter ligand, ligand field, charge transfer and delocalized states. Properties of ligand field excited states. Photo substitution-Prediction of substitution lability by Adamson`s rules. Photo aquation. Photo isomerisation and photo recimization. Illustration of reducing and oxidizing character of $[Ru(bipy)_3]^{2+}$ in the excited state. Metal complex sensitizers- water photolysis.

Unit 7: Advanced organometallic chemistry (9 hrs)

Fullerene complexes. Fluxional organometallics. Dioxygen complexes, insertion reactions of CO_2, SO_2 and RNC, olefin metathesis, asymmetric hydrogenation using chiral catalyst, oxidative coupling, palladium catalysed C-C and C-N cross coupling.

Organometallic polymers. Organometallic compounds as drugs and sensors.

Unit 8: Environmental Chemistry (9 hrs)

The chemistry of processes in atmosphere: Composition of the atmosphere: Automobile pollutants. Photochemical smog. Chemistry of the stratosphere. Catalytic destruction of ozone. Depletion of the protective ozone layer. Effects of air pollutants on the human health.

The Chemistry of processes in hydrosphere: The hydrologic cycle. Cycling and purification. The unique properties of water. Acid base properties. CO_2 in water. Alkalinity. O_2 consuming waste.

The chemistry of processes in Lithosphere: Redox status in soil. pE pH predominance diagrams for redox sensitive elements. Acidity in soil materials.Acid neutralization capacity and the quantification of the soil acidity. Ion speciation in soil solution. Quantitative aspects of ion speciation. Cation exchange capacity and exchange phase composition.

References:

1. C.P.Poole(Jr.) and F.J. Owens, *Introduction to Nanotechnology*,Wiley India, 2007.
2. G.A.Ozin and A.C.Arsenault, *Nanochemistry*, RSC Publishing,2008.
3. T.Pradeep, *The essentials of Nanotechnology*, Tata McGra Hill, New Delhi, 2007.
4. K.J.Klabunde(Ed.), *Nanoscale Materials in Chemistry*, John Wiley&Sons, 2001.
5. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6 Edn., Wiley, 2011.
6. Jens Hajen, *Industrial Catalysis: A Practical Approach.* 2nd Edn., Wiley VCH, 2006.
7. Dipak Kumar Chakrabarty, *Adsorption and Catalysis by Solids,* New Age. 2007.
8. C.H. Bartholomew and R.J. Farrauto, *Fundamentals of Industrial Catalysis Process,* 2nd Edn.Wiley & Sons Inc. 2006.
9. Woodruff, D. P. and Delchar T. A., *Modern Techniques of Surface Science*, Cambridge Solid State Science Series, 1994.
10. Kurt K. Kolasinski, *Surface Science: Foundations of Catalysis and Nanoscience,* 3rd Edn.,Wiley U. K., 2012.
11. S.L. Lippard and J.M.Berry, *Principles of Bioinorganic Chemistry*, University Science Books, Californis, 1997.
12. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, *Bioinorganic Chemistry,* University Science Books, 1994.
13. D.E. Fenton, *Biocoordination Chemistry*, Oxford University Press, Oxford, 1995.
14. R.M. Roat- Malone, *Bioinorganic Chemistry: A Short Course*, John Wiley & Sons, 2002.
15. A.W.Adamson and P.D.Fleischauer, *Concepts of Inorganic Photochemistry,* Wiley.
16. V. Balzari, V. Carassiti*, Photochemistry of Coordination Compounds,* Academic Press
17. G.J. Ferraudi*, Elements of Inorganic Photochemistry,* Wiley.

18. R.C.Mehrothra and A.Singh, *Organometallic Chemistry, A Unified Approach, W*iley eastern.
19. P.Powell, *Principles of Organometallic Chemistry, ELBS.*
20. B.D.Gupta and A.J.Elias, *Basic Organometallic Chemistry, Concepts, Synthesis andApplications,* Universities Press, 2010.
21. James E. Girard, *Principles of Environmental Chemistry*, Jones & Bartlett Publishers, 2005
22. H.V. Jadhav, *Elements of Environmental Chemistry,* Himalaya Publishing House, 1992
23. Michael E. Essington, *Soil and Water Chemistry: An Integrative Approach*, 2nd edn., CRC Press, 2015
24. A.K. De, Environmental Chemistry, 7th edn., New Age International, 2015.

SEMESTER IV
Theory Course XIV
DCHE4B17T- ADVANCED ORGANIC CHEMISTRY
(4 Credits, 72 h)

Unit I: Supramolecular chemistry (9 h)
Definition and development of supramolecular chemistry, nature of supramolecular interactions - hydrogen bonding, dipole-dipole, charge transfer, van der Waals and π-π stacking interactions.
Concepts in supramolecular chemistry: Molecular self-assembly, Molecular recognition and complexation – factors and forces involved in molecular recognition, classification of molecular receptors (crown ethers, cryptands, spherands, cyclodextrins, calixarenes and cyclophanes), Mechanically-interlocked molecular architectures (catenanes and rotaxanes), Biomimetics and Molecular machinery. Supramolecular materials: Liquid crystals, gels and dendrimers. Applications of supramolecular chemistry – Molecular sensors, Materials technology, Catalysis, Medicine, Data storage and processing.
Unit II: Green Chemistry (9 h)
Principles of Green Chemistry: basic concepts, atom economy, twelve principles of green chemistry, comparison of traditional process versus green process in the synthesis of ibuprofen. Use of the following in green synthesis with suitable examples: (a) Green reagents: dimethylcarbonate, polymer supported reagents. (b) Green catalysts: Phase transfer catalysts [Tetra-n-butyl ammonium chloride, benzyltrimethyl ammonium chloride (TMBA), crown ethers, Aliquat 336], biocatalysts. (c) Green solvents: water, ionic liquids and supercritical fluids. (d) Solid state reactions: solid phase synthesis, solid supported synthesis. (e) Microwave assisted synthesis. (f) Ultrasound assisted reactions.
Unit III: New reactions in organic synthesis (9 h)
(a) *C=C Formation Reactions*: Bamford-Stevens reaction, Shapiro reaction, Julia olefination and Peterson olefination.

(b) *Ring Formation Reactions*: Pauson-Khand reaction, Bergman cyclisation and Nazerov cyclisation, Tiffeneau–Demjanov rearrangement.
(c) *Multicomponent Reactions*: Biginelli synthesis; multicomponent reactions using alkyl isocyanides−Passerini and Ugi-4-component synthesis.
(d) *Olefin metathesis* using Grubb's catalyst.
(e) *Other important synthetic reactions*: Mukaiyama esterification, Mitsunobu reaction and Baylis Hillman reaction.

Unit IV: New techniques and Concepts in organic synthesis (9 h)

Polymer Supported Reagents and Synthesis: Properties of polymer support, Advantages of polymer supported reagents. Applications – Synthesis of peptides (Merrifield solid-phase peptide synthesis), synthesis of oligonucleotide and oligosaccharide.
Combinatorial synthesis: Basic ideas and concepts of combinatorial chemistry.
Click Chemistry: Criteria for click reaction, Sharpless azides cycloadditions.
Domino/Cascade reactions: Introduction and applications in organic synthesis.
Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

Unit V: Medicinal Chemistry and Drug design (9 h)

Theories of drug activity: Occupancy theory, rate theory and induced fit theory, General Principles of dosage form design and drug administration, Pharmacokinetics, pharmacodynamics, metabolites and antimetabolites, Prodrugs and parmacophores, agonists and antagonists, Drug design, factors governing drug design, rational approach to drug design, the design of agonists, the design of antagonists, Concept of drug receptor, Elementary treatment of drugs receptor interaction, Quantitative structure activity relationship (QSAR), General methods of drug synthesis, Synthetic strategies, stereochemistry, combinatorial library synthesis.

Unit VI: Biomolecules (9 h)

Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure.
Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP,ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.

Unit VII: Six-membered Heterocyclic & Fused Ring Heterocyclic Compounds (9 h)

Six-membered Heterocyclic Compounds: (i) Six-membered heterocycles containing one heteroatom: Synthesis and reactions of pyridine. synthesis of pyrones and pyrylium salts.
(ii) Six-membered heterocycles containing two hetero atoms: Synthesis of pyridazines, pyrimidines (uracil, thymine and cytosine), pyrazines. Synthesis of purines- adenine and guanine. (iii) Six-membered heterocycles containing three hetero atoms: Synthesis of 1,3,5-triazines, 1,2,3-triazines and 1,2,4-triazines.

Fused ring hetero cyclic compounds: Synthesis and reactions of benzofuran, indole, isoindole, benzothiophene, quinoline, isoquinoline, benzoxazole, benzthiazole and benzimidazole. Structure and synthesis of azepines, oxepines, thiepins, diazepines and benzodiazepines. Structure and synthesis of uric and caffeine.

Unit VIII: Research methodology in Chemistry (9 h)

Science and scientific method. The choice and statement of a research problem. Searching the literature. Literature databases − Google scholar, SciFinder, Web of science, PubMed, INFLIBNET etc. Formulation of hypothesis. Research plans. Design of experiment. Design of apparatus. The execution of experiments. Analysis of the experimental data. Interpretation and generalization of the findings. Patenting and reporting the results of research. Scientific writing – research reports, journal articles, books and thesis. Type of journal publications− articles, communications, reviews. Organization of reports – general format, the title, authors, abstract, text (introduction, method, results, discussion, conclusions), acknowledgement, references. Abbreviations, foot notes, Tables, Figures, Proof reading. Important scientific and chemistry journals. Impact factor.

References:

1. K. Ariga and T. Kunitake, *Supramolecular Chemistry — Fundamentals and Applications*, Springer, 2006.
2. Jonathan W. Steed and Jerry L. Atwood, *Supramolecular Chemistry*, 2/e, Wiley, 2009.
3. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.
4. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993.
5. V. K. Ahluwalia, *Green Chemistry – Environmentally benign reactions,* Ane Books India (Publisher), (2006).
6. V. K. Ahluwalia, *Green Chemistry: A Textbook*, Narosa Publishing House, 2013.
7. *Green Chemistry – Designing Chemistry for the Environment* – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
8. V. K. Ahluwalia and R. Aggarwal, *Organic synthesis – Special Techniques*, 2/e, Narosa.
9. W. Carruthers*, Some modern methods of organic synthesis*, Cambridge University Press.
10. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
11. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis,* 3/e, CRC Press, 1998.
12. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
13. N. K. Terret: *Combinatorial Chemistry*, Oxford University Press, 1998.
14. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
15. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
16. Gringuaz Alex, *Introduction to medicinal chemistry*, New York: Wiley-VCH, 1996.
17. S. N. Pandeya and J. R. Dimmock, *An introduction to drug design*. New Age International.
18. *Richard B. Silverman and Mark W. Holladay, The organic chemistry of drug design and drug action*, 3/e, Elsevier.
19. Lednicer Daniel, *Strategies for organic drug synthesis and design*, 2/e, John Wiley, 2008.

20. Patrick Graham, *Instant notes in medicinal chemistry*, Taylor & Francis.
21. G. R. Chatwal, *Medicinal Chemistry*, Himalaya, 2002.
22. J. Richard Smith and Michael L, *Analysis of Drug Impurities*, John Wiley & Sons, 2007.
23. G. L. Patrick, *An Introduction to Medicinal Chemistry*, 3/e, Oxford University Press, 2005.
24. David L. Nelson and Michael M. Cox, *Lehninger, Principles of Biochemistry*,6/e WH-Freeman.
25. Jeremy M Berg, John L Tymoczko and Lubert Stryer, *Biochemistry*, 5/e, WH-Freeman.
26. U. Satyanarayana and U. Chakrapani, *Essentials of Biochemistry*, 2/e, 2012.
27. Thomas L. Gilchrist, *Heterocyclic chemistry*, 3/ e, Pearson Education, 2007.
28. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry Vol. 1-3,* Springer Velag.
29. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.
30. A. R. Kartritzky and C. W. Rees, *Comprehensive Heterocyclic Chemistry, Vol-1-7*, Pergamon press.
31. R. L. Dominoswki, *Research Methods*, Prentice Hall, 1981.
32. J.W. Best, J.V. Kahn, *Research in Education*, 10^{th} Edn., Pearson/Allyn&Bacon, 2006.
33. H. F. Ebel, C. Bliefert, W.E. Russey, *The Art of Scientific Writing*, Wiley-VCH, 2004.

SEMESTER IV

Theory Paper XV

DCHE4B18T - ADVANCED PHYSICAL CHEMISTRY

(4 Credits, 72 h)

Unit 1: Photochemistry (9hrs)

Photochemical reactions-Dimerisation of Anthracene, H_2-Br_2 reactions and H_2-Cl_2 reactions, Photopolymerization, Principles of utilizations of solar energy –Solar cells and their working, Photochemical processes- Radiative and non-radiative transitions- Jablonski Diagram, Chemiluminiscence, Photoluminiscence, Bioluminiscence, Thermoluminiscence, Cathodoluminiscence. Fluoroscence, Theory of Fluoroscence, Stokes, Anti-Stokes and Resonance Fluorescence, Photosensitisation, Sensitised Fluoroscence, Quenching of Fluoroscence, Stern-Volmer equation (derivation)

References for Unit 1:

1. K.J. Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
2. Gurdeep Raj and H Misra, *Photochemistry*, Goel Publishing House
3. KK Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International Publishers, 2006.

Unit 2: **Polymerization Processes I (9 hrs)**
Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Mayo-walling equation of the steady state. Molecular weight distribution and molecular weight control. Radical Atom Transfer and Fragmentation – Addition mechanism. Free radical living polymers. Cationic and anionic polymerization. Kinetics and mechanism, Polymerization without termination.

Unit 3: Polymerization Processes II (9 hrs)

Step Growth polymerization. Kinetics and mechanism. Molecular weight distribution. Linear Vs cyclic polymerization, other modes of polymerization. Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking.

Unit 4 : Speciality Polymers (9 hrs)
Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers. Polymers with high bandwidth. Poly anilines, poly pyrrols, poly thiophines, poly (vinylene phenylene). Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photo resists. Electrical properties of Polymers, Polymers with NLO properties, second and third harmonic generation, wave guide devises.

References for Unit 2, 3 & 4
1. F.W. Billmayer. *Textbook of Polymer* Science. 3rd Edn, Wiley. N.Y. 1991.
2. G. Odiyan*, Principles of Polymerisation*, 4/e, Wiley, 2004.
3. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
4. J.M.G Cowie. *Polymers: Physics and Chemistry of Modern Materials*. Blackie. London, 1992.
5. R.J.Young, *Principles of Polymer Science*, 3rd Edn. , Chapman and Hall. N.Y. 1991.
6. P.J. Flory. *A Text Book of Polymer Science.* Cornell University Press. Ithacka, 1953.
7. F. Ullrich, *Industrial Polymers*, Kluwer, N.Y. 1993.
8. H.G.Elias, *Macromolecules,* Vol. I & II, Academic, N.Y. 1991

Unit 5: Electroanalytical Techniques-I (9 hrs)

Voltametry and polarography: Voltametry - cyclic voltametry, ion selective electrodes, anodic stripping voltametry. Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves. The dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition methods, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.

Unit 6: Electroanalytical Techniques-II (9 hrs)

Amperometric titrations: general principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, titration procedure, merits and demerits of amperometric titrations. **Coulometry**: coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations. Advantages of coulometry.

References for Units 5 & 6

1.A.I. Vogel, A Text Book of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.
2. H.H. Willard, J.A .Dean, L.L. Merritt, Instrumental Methods of Analysis, Van Nostrand, 1965.
3. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

4. J.M. Mermet, M. Otto, R. Kellner, *Analytical Chemistry*, Wiley-VCH, 2004.

5. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry,* 9th Edn., Cengage Learning., 2014.
6. J.G. Dick, *Analytical Chemistry*, R.E. Krieger Pub.,1978.50
7. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub., 1990.
8. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley& sons,1989.
9. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier, 1982.
10. G.D. Christian, J.E. O'Reilly, *Instrumental Analysis*, Allyn & Bacon, 1986.
11. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.

Unit 7: Advanced Electrochemistry (9 hrs)

Thermodynamics of electrochemical cells, efficiency of electrochemical cells and comparison with heat engines-primary cells (Zn, MnO_2) and secondary cells (lead acid, Ni-Cd and Ni-MH cells), electrode reactions, potentials and cell voltages, advantages and limitations three types of secondary cells. fuel cells; polymer electrolyte fuel cell (PEMFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), direct methanol fuel cells, electrode reactions and potentials, cell reactions and cell voltages, advantages and limitations of four types of fuel cells

References for Unit 7

1. Praveen Tyagi, *Electrochemistry,* Discovery Publishing House, 2006.
2. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications, 1961.
3. B. Viswanathan & M.Aulice Scibioh, "*Fuel Cells: Principles and Applications*," Taylor & Francis Group, 2007.
4. Era Levine, *Physical Chemistry*, Tata Mc-GrawHill

Unit 8: Introduction to Computational Quantum Chemistry (9hrs)

Electronic structure of molecules-Review of Hartee-Fock SCF method. Basis sets STOs and GTOs . Nomenclature of Basis sets. Semi empirical and ab initio methods. Calculations using Gaussian programme . Spesification of molecular geometry using a) Cartisian coordinates and b) Internal coordinates. The Z-matrix. Z- matrices of some simple molecules like H_2, H_2O,formaldehyde ammonia and methanol.

References:

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons, 2002.
2. Frank Jensen*, Introduction to Computational Chemistry*, John Wiley & Sons,1999.
3. Errol G Lewars *Computational Chemistry*: *Introduction to the theory and applications of molecular quantum mechanics,* Springer,2001.
4. David Young, *Computational Chemistry,* Wiley –Interscience, 2001.

SEMESTER IV

Theory Course XVI

Elective V

DCHE4E05T - ANALYTICAL CHEMISTRY

(3 Credits, 54 hrs)

Unit 1: **Errors in Chemical Analysis (9hrs)**

Treatment of analytical data, accuracy and precision, absolute and relative errors, classification and minimization of errors, significant figures, Statistical treatment- mean and standard deviation, variance, confidence limits, student-t and f tests, detection of gross errors, rejection of a result-Q test. Least square method, linear regression; covariance and correlation coefficient

Unit 2: **Conventional Analytical Procedures (9hrs)**

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents:

NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-lnaphthol, dithiocarbamates, Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in non-aqueous media. Indicators for non-aqueous titrations. Redox titrations: Permanganometry, dichcrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators. Precipitation titrations, adsorption indicators Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

Unit 3: Spectroscopic methods (9hrs)
Techniques and instrumentation of IR spectroscopy – single beam and double beam spectrometer, radiation sources, detectors, sample handling. FTIR spectrophotometer Techniques and instrumentation of Raman spectroscopy-radiation sources, detectors, sample handling and illumination.
Techniques and instrumentation of UV-Visible spectroscopy- radiation sources, filters & monochromators, cells and sampling devices, detectors. Instrumentation of NMR spectroscopy – continuous wave NMR spectrometers-the magnet, the probe unit, pulsed FTNMR spectrometer.

Unit 4: Optical Methods (9 hrs)
Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glue discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications. X-ray methods,: X-ray absorption and X-ray diffraction

Unit 5: **Thermal and Radiochemical Methods (9hrs)**
Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) and their instrumentation. Thermometric Titrations. Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods

Unit 6: Chromatography (9 hrs)
Classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography. Gas chromatography – basic instrumental set up. Carriers and columns (mention only). Brief discussion of detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC. Theory and applications of GC-MS and LC-MS.

References

1. H. H Willard, L. L Merritt, Jr., J. A Dean & F. A. Settle. Jr., *Instrumental methods of analysis*, 7th Ed. , CBS Publishers 1986
2. D.A. Skoog, F.J. Holler, S.R. Crouch, *Principles of Instrumental analysis*, Thomson and Brooks, 2007
3. J.M. Mermet, M. Otto, R. Kellner, *Analytical Chemistry*, Wiley-VCH, 2004.
4. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry,* 9th Edn., Cengage Learning., 2014.
5. J.G. Dick, *Analytical Chemistry*, R.E. Krieger Pub.,1978.50
6. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub., 1990.
7. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley& sons,1989.
8. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier, 1982.
9. G.D. Christian, J.E. O'Reilly, *Instrumental Analysis*, Allyn & Bacon, 1986.
10. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
11. A.I. Vogel, *A Textbook of Practical Organic Chemistry*, 5/e Pearson, 1989.
12. . H.A. Laitinen, W.E. Harris, *Chemical Analysis*, McGraw Hill,1975.
13. V.K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, CRC, 2008.
14. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry,* Blackwell Science, 2000.
15. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, *Vogel's Text Book of Quantitative Chemical Analysis*, 6th Edn., Pearson Education, Ltd.,2000.
16. B. K. Sharma, *Instrumental methods of chemical analysis* Goel publications 1998.

SEMESTER IV

Theory Course XVI

Elective VII

DCHE4E06T - PETROCHEMICALS AND COSMETICS (ELECTIVE)

(3Credits, 54hrs)

Unit 1: Introduction to Petrochemistry (9hrs)

Introduction – Petroleum – Refining of crude oil – Fuels for internal combustion engines. Knocking, Octane number. Unleaded petrol. Diesel Engine and Cetane number. Cracking – Thermal, Catalytic. Mechanism of cracking process. Reforming Activation Gasoline. Petrochemicals.

Unit 2: Hydrocarbons from Petroleum (9hrs)

Introduction. Raw materials. Saturated hydrocarbons from natural gas. Uses of saturated hydrocarbons. Unsaturated hydrocarbons – Acetylene, Ethylene, Propylene, Butylenes. Aromatic hydrocarbons - Benzene. Toluene. Xylenes. Chemical processing of paraffin hydrocarbons. Chemical processing of ethylene hydrocarbons. Chemical processing of acetylene. Chemical processing of aromatic hydrocarbons.

Unit 3: Industrial Organic Synthesis (9hrs)
Introduction. The raw materials and basic processes. Chemical process used in industrial organic synthesis. Petrochemicals- Methanol. Important points. Ethanol. Important points. Rectified spirit from beer. Methylated spirit. Proof spirit. Preparation of the absolute alcohol from rectified spirit. Acetaldehyde. Aceti acid. Isopropanol. Ethylene glycol. Glycerine. Acetone. Phenol. Formaldehyde. Important points. Ethyl acetate. Important points.

Unit 4: Composition of Petroleum Crude (9hrs)
Composition of petroleum crude. Composition of the petroleum products. Isomeric compounds. Classification of petroleum crude. A survey of the world crude. Sulphur compounds in petroleum.Physical Properties and Test Methods **1**. Viscosity: Other methods for finding out viscosity. Viscosity of an oil blend. Use of the figure for finding out viscosity. Viscosities of hydrocarbons. **2**. Density, **3**. Surface and interfacial tensions. **4**. Refractive Index. **5**. Flash and fire points. **6.** Cloud and pour points. **7**. Aniline point. **8**. Diesel index. **9**. Cetane number. 10. Octane number andcharacteristics. **11**. Distillation curves. (a) ASTM (American Society for Testing Materials) distillation curve. (b). Hempel or semi fractionating distillation curve.

Unit 5: Distillation of Crude Petroleum (9hrs)
Preparation of petroleum for processing. Destruction of petroleum emulsion. Electric desalting plants. Fundamentals of preliminary distillation. Methods of petroleum distillation. Distillation of crude petroleum. Treatment of the residual liquid processing of liquid fuels such as petroleum andpetroleum products. Petroleum processing equipments. Storage tanks. Rectification columns. Captray or bubble tray columns. Heat exchange apparatus. Steam space heaters or boilers. Condensers.Pipe furnaces. Pipelines. Fitting Compressors and pumps.

Unit 6: Petroleum Products (9hrs)
Introduction. Classification of petroleum products. Liquefied hydrocarbons, gases and fuels. Fuel oils or boiler oils. Fuel for Jet engines and gas turbine engines. Lubricants, products of oil paraffin processing and other petroleum products. Lubricating and other oils. Paraffin, ceresins, petroleum. Miscellaneous petroleum products. Products of petrochemical and basic organic synthesis. Dye intermediates. Lacquers. Solvents. Thinners.

References:
1. B. K. Sharma, *Industrial Chemistry*, Goel Publication, Goa.
2. N. K. Sinha, *Petroleum Refining and petrochemicals,*
3. John W. Hill, *Chemistry for Changing times*, Surjeet Publication
4. Uttam Ray Chaudhuri, *"Fundamentals of Petroleum and Petrochemical Engineering",*
, Boca Raton London New York.
5. S ukumar Maiti, *"Introduction To Petrochemicals"* India Book House Pvt Ltd.
6. Gabriella Baki, Kenneth S. Alexander, *"Introduction to Cosmetic Formulation and Technology",* Wiley.

1. Tony Curtis, David Williams, *“Introduction to Perfumery”,* Micelle Press; 2nd edition

SEMESTER IV
Theory Course XVI
Elective VII
DCHE4E07T - NATURAL PRODUCTS & POLYMERS
(3Credits, 54 hrs)

UNIT 1: Basic aspects of Natural Products (9 hrs)
Classification of Natural Products**:** Classification of Natural products based on chemical structure, physiological activity, taxonomy and Biogenesis. Carbohydrates, Terpenoids, Carotenoids, alkaloids, steroids, anthocyanins etc. Methods of isolation of each class of compound Essential Oils: Isolation and study of important constituents of lemon grass oil, citronella oil, cinnamon oil, palmarosa oil, turpentine oil, clove oil, sandalwood oil, Essential oils of turmeric and ginger. Oleoresins of pepper, chilly, ginger and turmeric. Aromatherapy.

UNIT 2: Terpenoids and Steroids (9 hrs)
Terpenoids: classification, structure elucidation and synthesis of abietic acid. Steroids : Classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids and steroids. Steroids: Classification and structure elucidation of Cholesterol, Ergosterol, Oesterone ,Androsterone,Testosterone, Progestrone, Cortisone and Corticosterone.

UNIT 3: Alkaloids and Anthocyanins (9 hrs)
Alkaloids – classification of alkaloids, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine. Anthocyanins**:** Introduction, General Nature and Structure of Anthocyanidins. Flavone, Flavonol, Isoflavone and Chalcone

UNIT 4: Dyes, Pigments and Supramolecules (9 hrs)
Brief introduction to dyes and pigments (natural and synthetic): β -carotene, indigo, cyclic tetrapyrroles (porphyrins, chlorins, chlorophyll, heme), study of phthalocyanines, squarenes, cyanine dyes Introduction to Supramolecular chemistry and Molecular Recognition

References
1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. F. A. Carey and R. J. Sundberg*: Advanced Organic Chemistry (part B),* 3rd ed., Plenum Press.
3. T.W. G. Solomons: *Fundamentals of Organic Chemistry*, 5th ed., John Wiley
4. H. O. House: *Modern Synthetic Reactions*, W. A. Benjamin
5. W. Carruthers: *Some Modern Methods of Organic Synthesis*, 4/e, CambridgeUniversity Press.
6. I. L. Finar: *Organic Chemistry* Volumes 1 (6th ed.) and 2 (5th ed.), Pearson.

7. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2/e, OxfordUniversity Press
8. N. R. Krishnaswamy: *Chemistry of Natural Products*; A Unified Approach, Universities Press
9. R. J. Simmonds: *Chemistry of Biomolecules: An Introduction*, RSC
10. R. O. C. Norman: *Principles of Organic Synthesis*, 3nd ed., CRC Press, 1998.
11. J. M. Lehn, *Supramolecular Chemistry*

UNIT 5: **Polymerization Processes (9 hrs)**

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Mayo-walling equation of the steady state. Molecular weight distribution and molecular weight control. Radical Atom Transfer and Fragmentation – Addition mechanism. Free radical living polymers. Cationic and anionic polymerization. Kinetics and mechanism, Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Molecular weight distribution. Linear Vs cyclic polymerization, other modes of polymerization. Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking. Copolymer composition drift Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques

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UNIT 6: Characterization and Stereochemistry of Polymers (9 hrs)

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts. Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. Static and dynamic methods, Light scattering and GPC. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellac. Degree of Crystallinity, X-ray diffraction

References:

1. F.W. Billmayer. *Textbook of Polymer* Science. 3rd Edn, Wiley. N.Y. 1991.
2. G. Odiyan*, Principles of Polymerisation*, 4/e, Wiley, 2004.
3. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
4. J.M.G Cowie. *Polymers: Physics and Chemistry of Modern Materials*. Blackie. London, 1992.
5. R.J.Young, *Principles of Polymer Science*, 3rd Edn. , Chapman and Hall. N.Y. 1991.
6. P.J. Flory. *A Text Book of Polymer Science.* Cornell University Press. Ithacka, 1953.
7. F. Ullrich, *Industrial Polymers*, Kluwer, N.Y. 1993.
8. H.G.Elias, *Macromolecules,* Vol. I & II, Academic, N.Y. 1991

SEMESTER IV
Theory Course XVI
Elective VIII
DCHE4E08T - MATERIAL SCIENCE (ELECTIVE)
(3 credits, 54hrs)

Unit 1: Introduction to Material Science (9hrs)
Introduction, classification of materials, functional classification, classification based on structure, environmental and other effects, material design and selection; Mechanical properties – significance and terminology, the tensile test, true stress and true strain, bend test, hardness of materials.

Unit 2: Ceramic Materials (9hrs)
Definition of ceramics, traditional and new ceramics, structure of ceramics, atomic interactions and types of bonds, phase equilibriums in ceramic systems, one component and multi component systems, use of phase diagrams in predicting material behaviour, electrical, magnetic, and optical properties of ceramic materials.

Unit 3: Nano materials and Nanotechnology (9hrs)
Nano materials, nanostructures, self-assembly, Nano particles- methods of synthesis, sol-gel process, hydrolysis of salts and alkoxides, precipitation, condensation reactions, electro kinetic potential and peptization reactions; Gelatin network- xerogels, aerogels, drying of gels; Chemical modifications of nano surfaces, applications of sol-gel process, sol-gel coating, porous solids, catalysts, dispersions and powders

Unit 4: Materials for Special Purposes – I (9hrs)
Production of ultra pure materials - zone refining, vacuum distillation and electro refining; Ferroelectric and piezoelectric materials - general properties, classification of ferroelectric materials, theory of ferro electricity, ferroelectric domains, applications, piezoelectric materials and applications; Metallic glasses - preparation, properties and applications.

Unit 5: Materials for Special Purposes – II (9hrs)
Magnetic materials, ferri and ferro magnetism, metallic magnets, soft, hard & supe rconducting magnets; Ceramic magnets, low conducting and superconducting magnets; Superconducting materials - metallic and ceramic superconducting materials, theories of super conductivity Meissner effect; High temperature superconductors - structure and applications.

Unit 6: Some Special Polymers (9hrs)
Functional polymers - photoconductive, electro conductive, piezoelectric and light sensitive polymers; Industrial polymers - production, properties, & compounding of industrial polymers; Commodity plastics such as PP, PE, PVC, & PS ; Engineering plastics such as poly

acetyl, polyamide (nylon 6 and nylon 66), poly acrylate, polycarbonate, polyester (PET, PBT), polyether ketones; Thermosetting plastics such as PF, UF & MF.

References:

1. W.D. Eingery, H.K. Dowen and R.D. Uhlman, *Introduction to Ceramics*, John Wiley.
2. A.G. Guy, *Essentials of Material Science*, McGraw Hill.
3. M.J. Starfield and Shrager, *Introductory Material Science*, McGraw Hill.
4. S.K. Hajra Choudhary, *Material Science and Engineering*, Indian Book Dist. Co., Calcutta.
5. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill, 1997.
6. M. Tinkham, *Introduction to Superconductivity*, McGraw Hill, 1975.
7. A.V. Narlikar and S.N.Edbote, *Superconductivity and Superconducting Materials*, South Asian Publishers, New Delhi, 1983.
8. S.V. Subramanyan and E.S. Rajagopal, *High Temperature Superconductors*, Wiley Eastern Ltd., 1988.
9. Azaroff and Brophy, *Electronic Processes in Materials*, McGraw Hill, 1985.
10. C.M. Srivastava and C. Srinivasan, Science of Engineering Materials, Wiley Eastern Ltd., 1987.
11. R.J. Young, *Introduction to Polymer Science*, John Wiley and Sons.
12. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
13. H. Ulrich, *Introduction to Industrial Polymers*, Hansen Publishers, 1982.
14. F.R. Jones, *Handbook of Polymer Fibre Composites*, Longman Scientific and Tech.
15. K.K. Chowla, *Composite Materials*, Springer-Verlag, NY, 1987.

SEMESTER III & IV
Practical Course IV

DCHE4B19P – INORGANIC CHEMISTRY PRACTICALS– III & IV
(4 Credits)

Unit 1: Estimation of ions in mixture

Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, Nl^{2+}, Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and $Cr_2O_7^{2-}$) by volumetric colorimetric or gravimetric methods only one of the components to be estimated.

Unit 2: Colorimetric Estimations

Colorimetric estimations of Ni, Cu, Fe and Mo, after separation from other ions in solution by solvent extraction. (Minimum two experiments.)

Unit 3: Ion Exchange Methods

Ion- exchange separation and estimation of binary mixtures (Co^{2+} & Ni^{2+}, Zn^{2+} & Mg^{2+}. Hardness of water).

Unit 4: Preparation of Inorganic Complexes. (5 Nos)
Preparation and characterization complexes using IR and electronic spectra.
1. Tris (thiourea)copper(I) complex
2. Potassium tris (oxalate) aluminate (III).
3. Hexammine cobalt (III) chloride.
4. Tetrammine copper (II) sulphate.
5. Schiff base complexes of various divalent metal ions.

References:

1. *Vogel's Text Book of Qualitative Inorganic Analysis*.
2. I.M. Kolthoff and E.A. Sanderson, *Quantitative Chemical Analysis.*
3. D.A. Adams and J.B. Rayner, *Advanced Practical Inorganic Chemistry*.
4. W.G.Palmer, *Experimental Inorganic Chemistry.*
5. G. Brauer, *Hand book of Preparative Inorganic Chemistry*

SEMESTER III & IV
Practical Course V

DCHE4B20P – ORGANIC CHEMISTRY PRACTICALS– III & IV
(4 Credits)

PART I: Laboratory Techniques

General methods of separation and purification of organic compounds by:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. Vacuum distillation
5. Steam distillation
6. TLC and Paper Chromatography
7. Column Chromatography

PART II: Quantitative Organic Analysis

(i) Estimation of saponification value of oil
(ii) Estimation of reducing sugars, Estimation of amino group, phenolic group and esters.
(iii) Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulpha guanidine), Antibiotics – Penicillin, Streptomycin.
(iv) Estimation of equivalent weight of acids by Silver Salt method
(v) Estimation of nitrogen by Kjeldahl method
(vi) Estimation of iodine value of oils.

PART III: Isolation of natural products

Extraction of Natural products and purification by column chromatography and TLC –

(i) Caffeine from Tea or Coffee
(ii) Extraction of nicotine dipicrate from tobacco
(iii) Extraction of oil of cloves by steam distillation

(iv) Flavonoids (Soxhlet extraction)
(v) Casein from milk.

PART IV: Chromatography
Practical application of column chromatography, paper chromatography and thin layer chromatography (TLC), preparation of TLC plates, identification of compounds (mixture of amino acids / commercial drug samples / food colourants etc.) using R_f values.

References:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5/e, Pearson, 1989.
2. Beebet, *Pharmacuetical Analysis*
3. E. Hoftmann, *Chromatography*, non Nostrand Reinhold Company, New York, 1975.
4. J. Sherma and G. Zwig, *TLC and LC analysis of pesticides of international importance*, Vol. VI & VII, Academic Press.
5. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., *Plant Drug Analysis*, Springer-Verlag, Tokyo, 1984.
6. Vishnoi, *Practical Organic Chemistry*.
7. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, ELBS/Longman, 1989.
8. Beebet, *Pharmaceutical Analysis*.

SEMESTER III & IV
Practical Course VI

DCHE4B21P – PHYSICAL CHEMISTRY PRACTICALS– III & IV
(4 Credits)

SECTION A

Unit 1: Chemical Kinetics (4 experiments)
1. Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.
2. Determination of Arrhenius parameters of acid hydrolysis of an ester
3. Determination of specific reaction rate of saponification of ethyl acetate
4. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

Unit 2: Adsorption (3 experiments)
1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system.
   Determination of the concentration of a given acetic acid solution using the isotherm
2. Verification of Langmuir adsorption isothem – charcoal-oxalic acid system.
   Determination of the concentration of a given acetic acid solution using the isothem.
3. Determination of surface area of adsorbent.

Unit 3: Phase Equilibria (2 experiments)

1. (a) Determination of phase diagram of a ternary liquid system (e .g., chloroform – acetic acid –water , Nitro benzene – acetic acid – water)

(b) Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, Nitro benzene-acetic acid)

2. (a) Determination of mutual miscibility curve of a binary liquid system (e.g., phenol – water) and critical solution temperature (CST).

(b) Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system

(c) Effect of a given impurity (e.g., KCl) on the CST of water –phenol system and determination of the concentration of the given solution of

Unit 4: Cryoscopy

Beckman Thermometer Method (3 experiments)

1. Determination of cyroscopic constant of a liquid (water, benzene)
2. Determination of molecular mass of a soute (urea, glucose, cane sugar,mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)
3. Determination of Van't Hoff factor and percentage of dissociation of NaCl.
4. Study of the reaction 2Kl + Hgl 2 .K2Hgl4 and determination of the concentration of the given Kl solution.

Unit 5: Polarimetry (3 experiments)

1. Determination of specific and molar optical rotations of glucose, fructose and sucrose.
2. Determination of specific rate of inversion of cane sugar in presence of HCl.
3. Determination of concentration of HCl

Unit 6: Spectrophotometry (3 experiments)

1. Determination of equilibrium constants of acid -base indicators.
2. Simultaneous of determination Mn and Cr in a solution of KMnO4 and K2Cr2O7
3. Investigation of complex formation between Fe (III) and thiocyanate.

References:

1. A. Finlay and J.A. Kitchener, *Practical Physical Chemistry,* Longman.
2. F. Daniels and J.H. Mathews, *Experimental Physical Chemistry,* Longman.
3. A.H. James, *Practical Physical Chemistry* , J.A. Churchil Ltd., 1961.
4. H.H. Willard, L.L. Merit and J.A. Dean, *Instrumental Methods of Analysis,* 4th Education, Affiliated East-West Press Pvt. Ltd., 1965.
5. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry,* McGraw Hill.
6. J.B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications,* 1989.

SECTION B

Use of Computational Chemistry software like pc GAMESS (firefly), Gaussian etc., to calculate molecular parameters.
Ref: http://classic.chem.msu.su/gran/gamess/index.html

FIRST SEMESTER M. Sc. DEGREE EXAMINATION
(CSS)
Chemistry
DCHE1B01T – Theoretical Chemistry I (2016 Admissions)

Time: 3 hours Maximum Marks: 80

Section A

(Answer all questions. Each question carries 2 marks)

1 Define well behaved wave function.
2 What do you mean by square integrable nature of the wave function
3 Find the commutator of x and d/dx
4 Write recursion formula. Explain its significance.
5 Express Lz in cartesian and spherical polar co-ordinates.
6 Define spherical harmonics. Write one example.
7 List out all the symmetry elements and operations associated with a Td molecule.
8 Explain with example degenerate and Non degenerate representation.
9 Define abelian and group and class.
10 Generate matrices for C_6 and S_6
11 In the C3v point group all the three reflection planes are in the same class. Why?
12 State and explain the rearrangement theorem.

(12 × 2 = 24 Marks)

Section B

(Answer any 8 questions. Each question carries 4 marks)

13 Define Hermitian operator. Show that Kinetic energy operator is hermitian.
14 Write Hamiltonian operator. Show that is a hermitian operator
15 Define spherical harmonics. Draw the polar plots for one of the spherical harmonics function and discuss.

16 For a rigid rotator $\hat{L}^2$ and $\hat{H}$ have the same set of eigen functions. Justify your answer.

17 An electron confined to a cubical box of length 20 A^0. Calculate the energy level spacing

between (110) and (200) electron mass in 9.1 X 10^{-31} kg.

18 Find the commutator of $\hat{L}_x$ and $\hat{L}_x$. (L = angular momentum operator)

19 Show that the 4 symmetry operations in the C2V point group form a mathematical group under multiplication

20 List the symmetry operations associated with D_{4h} point group and classify them into different classes. Justify your answer

21 Set up the group multiplication table for C_{3v} point group.

22 State "Great orthogonality theorem". What are the consequence of the theorem?

23 Derive C4v character table.

24 Find out E x E using the C_{3v} character table

C_{3v}	E	$2C_3$	$3\sigma_v$
A1	1	1	1
A2	1	1	-1
E	2	-1	0

(8 × 4 = 32 Marks)

Section C

(Answer any 2 questions. Each question carries 12 Marks)

25 Using "Great Orthogonality theorem" derive the C_{3V} character table

26 Apply Schrodinger equation for 1 D simple harmonic oscillator. Find the eigen functions and Eigen values.

27 Apply Schrodinger equation for H atom. Transform it into spherical polar co-ordinates and separate the variables. Solve the phi equation.

28 Prove that a) Eigen values of hermitian operators are real and b) Eigen functions of hermitian operators corresponding to two different eigen values are orthogonal

(2 x 12 = 24 Marks)

FIRST SEMESTER M. Sc. DEGREE EXAMINATION

(CSS)

Chemistry

DCHE1B02T - INORGANIC CHEMISTRY I

(2016 Admissions)

Time: 3 hours Maximum Marks: 80

Section A

(Answer all questions. Each question has 2 Marks)

1. Name the molecule which is iso electronic with NH_4^{+} and BF_4^{-}

2. What is the name of correlation diagram represents energy of molecular orbitals with change in bond angle?

3. Arrange the following in the increasing order of acidity H_2O, H_2Se, H_2S, H_2Te

4. Give one example for aprotic solvent

5. To which class of compounds the polyhedral skeletal electron pair theory applicable.

6. Which allotropic form of phosphorous is an insulator?

7. What are phosphazenes?

8. What is zeolite?

9. What are the hydrolysis products of uranyl ion in aqueous solution?

10. The contraction between consecutive actinide ions is greater than in the case of lanthanide ions. Why?

11. What is Dosimetry?

12. Give one example for photo nuclear reactions.

(12 × 2 = 24 Marks)

Section B

(Answer any 8 questions. Each question carries 4 Marks)

13. What is Bent rule of hybridization? Explain.

14. Explain electroneutrality principle with example.

15. Explain Bronsted-Lowry concept of acids and bases.

16. Write down Drago-Wayland equation and explain.

17. Explain the diagonal relationship of first and second group of elements.

18. What is meant by ‘styx’ numbers. Explain with an example.

19. Discuss the structure of S-N compounds. 20. What are silicones? Give any two uses.

21. Differentiate between 4f and 5f orbitals of inner transition elements.

22. What are super heavy elements? Give two examples.

23. Explain the Bethe’s notation of nuclear process with example.

24. Give the principles of neutron activation analysis.

(8 × 4 = 32 Marks)

Section C

(Answer any 2 questions. Each question carries 12 Marks)

25. Write an essay on the applications of VSEPR theory with suitable examples.
26. Explain the various methods used for the detection and measurements of radiation.
27. Explain the structure, bonding and preparation of B_2H_6.
28. Discuss the synthesis, structure and bonding of P-N and P-S compounds.

(2 × 12 = 24 Marks)

FIRST SEMESTER M. Sc. DEGREE EXAMINATION

(CSS)

Chemistry

DCHE1B03T - ORGANIC CHEMISTRY I

(2016 Admissions)

Time: 3 hours Maximum: 80 Marks

Section A

(Answer all questions. Each question has 2 Marks)

1. State Hammond's postulate.
2. Among the cis and trans isomers of 2-acetoxycyclohexyl p-toluenesulfonate, which one is more reactive and why?
3. Neomenthyl chloride readily undergoes HCl elimination than menthyl chloride. Why?
4. Using a Fischer projection of phenylacetaldehyde, identify its pro-R and pro-S hydrogens.
5. Construct a qualitative MO diagram for ethylene and 1,3-butadiene.
6. Among the following which one is more aromatic and why?
   a) [18] annulene b) [10] annulene
7. Identify the most stable conformation of methyl 4-t-butylcyclohexane-1-carboxylate and why?
8. What are chiral auxiliaries?
9. The Z- isomer of N-methylformamide is much more stable compared to E-isomer. Why?
10. Draw the chair conformation of cis and trans-decalins.
11. What are enantiotopic, homotopic and diastereotopic hydrogens?
12. Distinguish between stereoselectivity and stereospecificity.

(12 x 2 = 24 Marks)

Section B

(Answer any 8 questions. Each question carries 4 Marks)

13. On the basis of MO theory discuss the aromaticity of benzene and antiaromaticity of cyclobutadiene.
14. What are crown ethers? What are their important synthetic applications?
15. Explain Marcus equation.
16. Discuss the effect of conformation on S_N1 and S_N2 reactions of equatorial leaving groups

in flexible and rigid cyclohexanes.

17. Predict the different products formed by the reaction four diastereomeric 2-bromo-4-phenylcyclohexanols with base and Ag_2O.
18. Describe the conformers and their stability of a) n-butane and b) ethylene glycol
19. Discuss the optical activity of compounds without chiral carbons.
20. Discuss the various methods for the resolution of enantiomers.
21. Explain the stereochemistry involved in Sharpless' asymmetric epoxidation and dihydroxylation.
22. Discuss the Felkin-Ahn model of Cram's rule in predicting the stereochemistry of the reaction between Grignard reagent and chiral aldehydes.
23. What are alterant and nonalterant hydrocarbons?
24. Discuss the effect of semipinacolic deamination of cis- and trans-2-aminocyclohexanols.

(8 x 4 = 32 Marks)

Section C

(Answer any 2 questions. Each question carries 12 Marks)

25. Write brief notes on (a) electron donor-acceptor complexes; (b) cryptates; (c) inclusion compounds and (d) cyclodextrins
26. Write brief notes on (a) Curtin-Hammett principle; (b) neighbouring group participation; (c) electronic substituents effects in S_N1 and S_N2 reactions.
27. Discuss the different methods for the asymmetric synthesis.
28. Discuss the conformation and stability of disubstituted cyclohexanes, decalines and adamantanes.

(2 x 12 = 24 Marks)

FIRST SEMESTER M. Sc. DEGREE EXAMINATION

(CSS)

Chemistry

DCHE1B04T – PHYSICAL CHEMISTRY I

(2016 Admissions)

Time: 3 hours | Maximum: 80 Marks

Section A

(Answer all questions. Each question has 2 Marks)

1. State and explain third law of thermodynamics.
2. Explain Onsager reciprocal relations.
2. Define forces and fluxes with reference to irreversible processes.

3. Briefly explain secondary salt effect.
4. Explain residual entropy.
5. Using Jacobians prove that $\left(\frac{\partial T}{\partial V}\right)_s = -\left(\frac{\partial P}{\partial S}\right)_v$

6. Define auto catalysis. Give one example.
7. Distinguish between diffusion controlled and activation controlled reactions.
8. Write London equation for calculating activation energy. Explain the terms.
9. Write the expression for rate constant for a reaction between A and B under the combined influence of diffusion and electrostatic forces. Explain the terms involved.
10. Unimolecular gas phase reactions on solids follows first order kinetics at low pressures and zero order kinetics at high pressures. Illustrate.
11. Write down Glansdorf-Pregognine equation
12. What is BET equation and explain the terms?

(12 x 2 = 24 Marks)

Section B

(Answer any 8 questions. Each question carries 4 Marks)

13. Derive BET adsorption isotherm.
14. Define phenomenological coefficients. Show that direct coefficients always dominate indirect coefficients?
15. Using third law of thermodynamics show that absolute zero of temperature is unattainable.
16. With the help of Lindemann's theory discuss unimolecular reactions
17. Discus the role of bistability with respect to Oregonator mechanism.
18. Explain Arrhenius intermediates and Van't Hoff intermediates. How do they differ in their potential energy diagrams?
19. Discuss the applications of ESCA, SEM and TEM in the study of surfaces.
20. Discuss the kinetics of chain reactions taking H2-O2 reaction as an example.
21. Explain the term "reaction co-ordinate" with reference to potential energy surfaces.
22. Describe the effect of solvent and ionic strength on the rate constant of a reaction?
23. Derive the Eyring equation?
24. Explain Langmuir-Hinshelwood mechanism of the bimolecular surface reaction

(8 x 4 = 32 Marks)

Section C

(Answer any 2 questions. Each question carries 12 Marks)

25. (a) Explain the BET theory of adsorption.
(b) Discuss the use of Langmuir and BET isotherms for surface area determination.
26. Discuss briefly the Rice-Herzfeld mechanism of organic decomposition reaction.
27. Show that for a bimolecular reaction, Absolute rate theory agrees well with simple collision theory?
28. (a) Describe the essential features of Langmuir-Hinshelwood, Eley-Rideal mechanism for surface catalyzed reactions.
(b) If the reaction between CO and O_2 on Pt surface is obeying Langmuir-Hinshelwood rate equation, then show that if [CO] is held constant ($\theta_{CO} < 0.35$) and [O_2] is varied, the

maximum rate of the reaction is,

$$V_{max} = ¿ \; k_3K_{CO}[CO])/(4(1+K_{CO}[CO].$$

(2 x 12 = 24 Marks)