FAROOK COLLEGE
(Autonomous)

M.Sc. DEGREE PROGRAMME
IN
CHEMISTRY

CHOICE BASED CREDIT AND SEMESTER SYSTEM-PG
(FCCBCSSPG-2019)
SCHEME AND SYLLABI

2019 ADMISSION ONWARDS

CERTIFICATE

I hereby certify that the documents attached are the bona fide copies of the syllabus of M.Sc. Chemistry Programme to be effective from the academic year 2019-20 onwards.

Date:
Place: P R I N C I P A L

FAROOK COLLEGE (AUTONOMOUS)
MSc. CHEMISTRY (CSS PATTERN)
Regulations and Syllabus with effect from 2019 admission

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 College from time to time.
d. Details of the courses offered for the programme are given in Table 1.

The programme shall be conducted in accordance with the programme pattern, scheme of examination and syllabus prescribed.

Of the 25 hours per week, 13 hours shall be allotted for theory and 12 hours for practical; 1 theory hour per week during even semesters shall be allotted for seminar.

Theory Courses

In the first three semesters, there will be four theory courses; and in the fourth semester, three theory courses. All the theory courses in the first and second semesters are core courses. In the third semester there will be three core theory courses and one elective theory course. College can choose any one of the elective courses given in Table 1. In the fourth semester there will be one core theory course and two elective theory courses. College can select any two of the elective courses given in Table 1. However, a student may be permitted to choose any other elective course of his choice given in Table 1 in the third and fourth semesters, without having any lecture classes.

One elective course in the Third semester and Two elective courses in the Fourth semester chosen by the college will be considered for calculating the workload of teachers.

All the theory courses in the first, third, and fourth semesters (both core and elective) are of 4 credits while the theory courses (both core and elective) in the **second semester** are of 3 credits.

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. At the end of second semester, three practical examinations with the codes MCH1L01 & MCH2L04 (Inorganic chemistry practical I and II), MCH1L02 & MCH2L05(Organic chemistry practical I and II) and MCH1L03 & MCH2L06 (Physical chemistry practical I and II) will be conducted. Practical examinations for the codes MCH3L07 & MCH4L10 (Inorganic chemistry practical III and IV), MCH3L08 & MCH4L11 (Organic chemistry practical III and IV) and MCH3L09 & MCH4L12 (Physical chemistry practical III and IV) will be conducted at the end of fourth semester. Each practical examination will be of six hour duration and 3 credits. Three hours per week in the fourth semester are allotted for conducting individual project work by the students under the guidance of a faculty and it can be treated as practical hours while calculating the workload of teachers.

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 recognized research institutions. 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. A comprehensive viva voce examination (2credits), based on all the theory and practical courses, will be conducted at the end of the fourth semester, on a separate day.

Grading and Evaluation

1. Accumulated minimum credit required for successful completion of the programme shall be 80.
2. A project work of 4 credits is compulsory and it should be done during the programme.

Project evaluation should be conducted at the end of the fourth semester, by three external examiners: one each from inorganic chemistry, organic chemistry and physical chemistry area, on a separate day.

Also, a comprehensive Viva Voce Examination (carrying 2 credits) may be conducted by three external examiners: one each from inorganic chemistry, organic chemistry and physical chemistry area; at the end of the fourth semester on a separate day.

Evaluation and Grading should be done by direct grading system. All grading during the evaluation of courses and the semester is done on 6 point scale (A+, A, B, C, D, E). Grading in 6 point scale is as given below.

Grade	Grade Point
A+	5
A	4
B	3
C	2
D	1
E	0

The calculation of GPA, SGPA & CGPA Shall be based on the direct grading system using 10 point scale as detailed below.

Letter Grade	Grade Range	Range of Percentage (%)	Merit / Indicator
O	4.25 – 5.00	85.00 – 100.00	Outstanding
A+	3.75 – 4.24	75.00 – 84.99	Excellent
A	3.25 – 3.74	65.00 – 74.99	Very Good
B+	2.75 – 3.24	55.00 – 64.99	Good
B	2.50 – 2.74	50.00 – 54.99	Above Average
C	2.25 – 2.49	45.00 – 49.99	Average
P	2.00 -2.24	40.00 – 44.99	Pass
F	< 2.00	Below 40	Fail
I	0	-	Incomplete
Ab	0	-	Absent

Pass in a course

P grade and above (GPA 2.00 and above).

Pass in all courses in a semester is compulsory to calculate the SGPA.

GPA, SGPA and CGPA – between 0 to 5 and in two decimal points.

An overall letter grade (Cumulative Grade) for the whole programme shall be awarded to the student based on the value of CGPA using a 10-point scale given below.

CGPA	Overall Letter Grade
4.25 – 5.00	O
3.75 – 4.24	A+
3.25 – 3.74	A
2.75 – 3.24	B+
2.50 – 2.74	B
2.25 – 2.49	C
2.00 -2.24	P
< 2.00	F
0	I
0	Ab

(1) Weightage of Internal and External valuation:

The evaluation scheme for each course shall contain two parts

(a) Internal evaluation

(b) External evaluation.

Its weightages are as follows:

Evaluation	*Weightage*
Internal	1 (or 20%)
External	4 (or 80%)

Both internal and external evaluation will be carried out using Direct Grading System, in 6 point scale

Internal evaluation (must be transparent and fair):

a) Theory: 5 weightage

i. Internal Examinations*- weightage = 2 (2 internal exams, both should be considered)
ii. Assignments and Exercises- weightage =1
iii. Seminars/Viva Voce- weightage =1
iv. Attendance - weightage =1

Internal Exam: Mark distribution.

*4.5 to 5.0 = A+, 3.75 to 4.49 = A, 3.0 to 3.74 = B, 2.0 to 2.99 = C, below 2.0 = D, Absent = E.

b) Practical: 10 weightage

i. Attendance - weightage =2
ii. Lab skill/quality of their results- weightage =2
iii. Model practical test-weightage= 2 (Best one, out of two model exams
iv. is considered)
v. Record – weightage = 2
vi. Viva Voce- weightage =2

c) Project: 10 weightage

i. Literature survey and data collection -weightage=2
ii. Interpretation of data & Preparation of Project report - weightage =2
iii. Research attitude - weightage = 2
iv. Viva Voce- weightage =4

The internal evaluation of Project work of each student should be done by the supervising faculty assigned by the department.

d) **Viva Voce**:

No internal evaluation for viva voce examinations (at the end of 4th semester).

e) Attendance:

Percentage	**Letter Grade**	**Grade Point**
Above 90%	A+	5
85 – 89.99%	A	4
75 – 84.99%	B	3
75 -79.99%	C	2
70 - 74.99%	D	1
< 70%	E	0

External evaluation:

a. Theory:

In all semesters the theory courses have 30 weightage each. Pattern of question Papers for theory courses is as follows

Division	**Type**	**No. of Questions**	**Weightage**	**Total Weightage**
Section A	Short Answer	8 out of 12	1	8
Section B	Short Essay	4 out of 7	3	12
Section C	Essay	2 out of 4	5	10
Total weightage in a question paper				30

b) Practicals:

At the end of II and IV semesters. There will be three practical examinations at the end of second semester as well as at the end of fourth semester. Each examination has 30 weightage and 3 credits

c) Comprehensive Viva Voce:

At the end of IV semester on a separate day (2credits). Viva voce will be based on both the theory and practical courses during the programme.

Component	Weightage
Physical & Theoretical Chemistry – theory courses	5
Physical Chemistry – practical courses	5
Inorganic Chemistry – theory courses	5
Inorganic Chemistry – practical courses	5
Organic Chemistry – theory courses	5
Organic Chemistry – practical courses	5
Total weightage	**30**

d) Project Evaluation:

End of IV semester on a separate day. Evaluation is based on:

a) Significance and relevance of the project-weightage=5

b) Project report - weightage =8

c) Presentation- weightage = 5

c) Viva Voce- weightage =12

Total weightage 30 and credit for project is 4.

(Further details regarding the grading and evaluation are as per the Farook College PG regulations 2019)

Audit courses:

Ability Enhancement Courses (AEC):

This course aims to have hands on experience for the students in their respective field of study, both in the core and elective subject area. Also it is a platform for the student community to have basic concepts of research and publication.

AEC is 4 credit course and should be conducted during the first semester of the programme. Credit of the AE course will not be considered while calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements in this course, which is compulsory for overall pass in the programme

One particular AEC may be selected for all the students in a batch in the department or each student in a batch may choose one AEC, among the pool of courses suggested below. Either a single faculty from the department may be in charge of this course for a batch or each student may be assigned to a particular faculty in the department, in charge of this AEC, which will be decided by the department council/ HoD.

a) Industrial/Research institution visit/visits
b) Publication of a research article/articles in national/international journal
c) Presentation of research paper/papers in national level seminar/conference, which should be published in the seminar/conference proceedings
d) Review article/articles on research topics which is presented in a national level seminar/conference and published in the proceedings
e) Internships at any reputed research institutions/R&D centre/Industry

After conducting the AEC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the AEC conducted. The evaluation/ examination must be conducted jointly by the teacher in charge of the AEC and the head of the department. The result of the AEC, duly signed and sealed by both teacher in charge and head of the department, during the stipulated time period in the third semester of the programme. Evaluation/examination must be conducted by 30 weightage pattern, as in the theory courses. Evaluation/examination on AEC must contain the following components: MCQ type written examination, Report on AEC, Presentation of AEC, Viva voce on AEC. Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department.

TABLE 1

Courses offered for M.Sc. Chemistry Programme under CSS Patten in Affiliated Colleges (2019 onwards)

Semester	Course Code	Course Title	Instructions / Week	Credits	Internal	External
I	MCH1C01	Quantum Mechanics and Computational Chemistry	4	4	5	30
	MCH1C02	Chemistry of Elements	3	4	5	30
	MCH1C03	Structure and Reactivity of Organic Compounds	3	4	5	30
	MCH1C04	Thermodynamics, Kinetics and Catalysis	3	4	5	30
	MCH1L01	Inorganic Chemistry Practical I	4	–	–	–
	MCH1L02	Organic Chemistry Practical I	4	–	–	–
	MCH1L03	Physical Chemistry Practical I	4	–	–	–
	Total credits:	**Core**		**16**		
II	MCH2C05	Group Theory and Chemical Bonding	3	3	5	30
	MCH2C06	Coordination Chemistry	3	3	5	30
	MCH2C07	Organic Reaction Mechanisms	3	3	5	30
	MCH2C08	Electrochemistry, Solid State Chemistry and Statistical Thermodynamics	3	3	5	30
	MCH2L04	Inorganic Chemistry Practical II	4	3	10	30
	MCH2L05	Organic Chemistry Practical II	4	3	10	30
	MCH2L06	Physical Chemistry Practical II	4	3	10	30
	Total credits:	**Core**		**21**		
III	MCH3C09	Molecular Spectroscopy	4	4	5	30
	MCH3C10	Organometallic & Bioinorganic Chemistry	3	4	5	30
	MCH3C11	Reagents and Transformations in Organic Chemistry	3	4	5	30
	MCH3L07	Inorganic Chemistry Practical III	4	–	–	–
	MCH3L08	Organic Chemistry Practical III	4	–	–	–

	MCH3L09	Physical Chemistry Practical III	4	–	–	–
	MCH3E01	**Synthetic Organic Chemistry (Elective)**	**3**	**4**	5	30
	MCH3E02	Computational Chemistry (Elective)	3	4	5	30
	MCH3E03	Green and Nanochemistry (Elective)	3	4	5	30
	Total Credits:	Core		12		
		Elective		4		
		Total		**16**		
IV	MCH4C12	Instrumental Methods of Analysis	4	4	5	30
	MCH4L10	Inorganic Chemistry Practical IV	3	3	10	30
	MCH4L11	Organic Chemistry Practical IV	3	3	10	30
	MCH4L12	Physical Chemistry Practical IV	3	3	10	30
	MCH4E04	Petrochemicals and Cosmetics(Elective)	4	4	5	30
	MCH4E05	Industrial Catalysis(Elective)	4	4	5	30
	MCH4E06	**Natural Products & Polymers (Elective)**	**4**	**4**	5	30
	MCH4E07	Material Science (Elective)	4	4	5	30
	MCH4E08	**Organometallic Chemistry (Elective)**	**4**	**4**	5	30
	MCH 4 P 01	Research Project	3	4	10	30
	MCH 4 V 01	Viva Voce		2	–	30
	Total Credits:	Core		13		
		Elective		8		
		Project		4		
		Viva Voce		2		
		Total		**27**		
Total Credits of the Programme			Core	62		
			Elective	12		
			Project	4		
			Viva Voce	2		
			Total Credits	**80**		

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
MCH1C01 - QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
(4 Credits, 72 hours)

Unit 1: Introduction to Quantum Mechanics (9hrs)

Black body radiation and Planck's quantum postulate. Einstein's photoelectric equation, Schrodinger's wave mechanics, Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Non-commuting operators and the Heisenberg's Uncertainty principle, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, Expectation value postulate; Postulate of time- dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation. Stationary states.

Unit 2: Quantum Mechanics of Translational & Vibrational Motions (9hrs)

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem, Introduction to tunneling; Particle in a three dimensional box, Separation of variables, degeneracy, Symmetry breaking.

One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions and energies, important features of the problem, harmonic oscillator model and molecular vibrations.

Unit: 3 Quantum Mechanics of Rotational Motion (9hrs)

Co-ordinate systems: - Cartesian, and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation, One particle Rigid rotator (non-planar rigid rotator or particle on a sphere) (complete treatment): The wave equation in spherical polar coordinates, separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((L_x, L_y, L_z), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (9hrs)

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and spin functions.

Unit 5: Approximation Methods in Quantum Mechanics (9hrs)

Many body problem and the need of approximation methods; Independent particle model; Variation method – variation theorem with proof, illustration of variation theorem using a trial function [e.g., x (a-x)] for particle in a 1D-box, variation treatment for the ground state of helium atom; Perturbation method – time-independent perturbation method (non-degenerate case only), illustration by application to particle in a ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom.

Unit 6: Quantum Mechanics of Many-electron Atoms (9hrs)

Hartree's Self-Consistent Field method for atoms, Fock modification using spin orbitals & Hartree - Fock Self- Consistent Field (HF-SCF) method for atoms, the Fock operator; Pauli's antisymmetry principle - Slater determinants; Roothan's concept of basis functions – Slater type orbitals (STO) and Gaussian type orbitals (GTO).

Unit 7: Introduction to Computational Chemistry - I (9hrs)

Electronic structure of molecules – Basics of HF-SCF method of molecules (derivation not required). Classification of Computational Chemistry methods – Molecular mechanics methods (concept of force field) and Electronic structure methods, ab initio and semi-empirical methods (Basic idea only), Concept of electron correlation and post HF methods. (Elementary idea)

Unit 8: Introduction to Computational Chemistry – II (9hrs)

Basis set approximation in ab initio methods - classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, Pople-style basis sets and their nomenclature. Simple calculations using Gaussian programme – The structure of a Gaussian input file, Types of key words, Specification 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.

Reference (for units 1 to 6)

1. F.L. Pilar, Elementary Quantum Chemistry, McGraw-Hill, 1968.
2. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc.,
3. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, 2005.
4. M.W. Hanna, Quantum Mechanics in Chemistry, 2nd Edition, W.A. Benjamin Inc., 1969.
5. Donald, A. McQuarrie, Quantum Chemistry, University Science Books, 1983 (first Indian

edition, Viva books, 2003).

6. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
7. J.P. Lowe, Quantum Chemistry, 2nd Edition, Academic Press Inc., 1993.
8. Horia Metiu, Physical Chemistry – Quantum Mechanics, Taylor & Francis, 2006.
9. A.K. Chandra, Introduction to Quantum Chemistry, 4th Edition, Tata McGraw-Hill, 1994.
10. L. Pauling and E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935 (A good source book for many derivations).
11. R.L. Flurry, Jr., Quantum Chemistry, Prentice Hall, 1983.
12. R.K. Prasad, Quantum Chemistry, 3rd Edition, New Age International, 2006.
13. M.S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.
14. C.N. Datta, Lectures on Chemical Bonding and Quantum Chemistry, Prism Books Pvt. Ltd., 1998.
15. Jack Simons, An Introduction to Theoretical Chemistry, Cambridge University Press, 2003.

Reference (for units 7 & 8)

16. C. J. Cramer, Essentials of computational Chemistry: Theories and models, John Wiley & Sons 2002.
17. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons LTD 1999.
18. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
19. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems", Wiley -Interscience, 2001.
20. Errol G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd edn. Springer 2011.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
MCH1C02 – CHEMISTRY OF ELEMENTS
(4 Credits, 54hrs)

Unit 1: 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 nonaqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Nonaqueous solvents and acid-base strength. Super acids –surface acidity.

Unit 2: Chemistry of Main Group Elements-I (9hrs)

Chemical periodicity-First and Second raw anomalies-The diagonal relationship- Periodic anomalies of the nonmetals 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 3: 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 4: 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 5: 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.

Unit 6: Chemistry of Nanomaterials (9hrs)

History of nanomaterials - Classification. Size - dependence of properties. Synthesis of nanostructures: bottom-up-approach, top-down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis. Methods of characterization: Electron microscopies - SEM, TEM. Scaning prob 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

Reference (for units 1 to 5)

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.
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.

Reference (for unit 6):

11. C.P. Poole (Jr.) and F.J. Owens, *Introduction to Nanotechnology*, Wiley India, 2007.
12. G.A. Ozin and A.C. Arsenault, *Nanochemistry*, RSC Publishing, 2008.
13. T.Pradeep, *The essentials of Nanotechnology*, Tata McGra Hill, New Delhi, 2007.
14. K.J. Klabunde (Ed.), *Nanoscale Materials in Chemistry*, John Wiley&Sons, 2001.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
MCH1C03 - STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS
(4 Credits, 54hrs)

Unit 1: Structure and Bonding in Organic Molecules (9hrs)

Nature of Bonding in Organic Molecules: Localized and delocalized chemical bonding, bonding weaker than covalent bond, cross- conjugation, resonance, rules of resonance, resonance hybrid and resonance energy, tautomerism, hyperconjugation, π-π interactions, pπ-dπ bonding (ylides). Stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Hydrogen bonding: Inter and intra-molecular hydrogen bonding. Range of the energy of hydrogen bonding. Physical and chemical properties of organic compounds- volatility, acidity, basicity and stability, stabilization of hydrates of glyoxal, chloral, and ninhydrin, high acid strength of maleic acid compared to fumaric acid. Effect of hydrogen bond on conformation,

Electron donor-acceptor complexes, crown ether complexes, cryptates, inclusion compounds and cyclodextrins.

Hückel MO method. MO's of simple molecules, ethylene, allyl radical and 1,3-butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes and heptalenes.

Unit 2: Structure and Reactivity (9hrs)

Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi -bond. Classical and nonclassical carbocations

Basic concepts in the study of organic reaction mechanisms: Application of experimental criteria to mechanistic studies, kinetic versus thermodynamic control- Hammond postulate, Bell-Evans-Polanyi principle, Marcus equation, Curtin-Hammet principles,. Acidity constant, Hammet acidity function.

Isotope effect (labeling experiments), stereochemical correlations. Semiquantitative study of substituent effects on the acidity of carboxylic acids. Quantitative correlation of substituent effects on reactivity. Linear free energy relationships. Hammet and Taft equation for polar effects and Taft's steric substituent constant for steric effect. Solvent effects

Unit 3: Conformational Analysis – I (9hrs)

Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformation of acyclic compounds – Ethane, n- butane, alkene dihalides, glycols, chlorohydrines, tartaric acid, erythro and threo isomer.

Interconversion of axial and equatorial bonds in chair conformation of cylohexane– distance between the various H atoms and C atoms in chair and boat conformations. Monosubstituted cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclo hexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationaly biased molecules. Conformations of 1,4 -cis and -trans disubstituted cyclohexanes in which one of the substituent is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.

Unit 4: Conformational Analysis – II (9 hrs)

Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2,3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-amino ethanol. (c) dehydro halogination of stilbene dihalide (dl and meso) and erythreo threo- bromo-1,2-diphenyl propane.

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 illustrated by the following compounds. (i) 4-t-Butylcyclohexyl tosylate (cis and trans) (ii) 2- Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol). (f) Esterification of axial as well as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

Bredt's rule. Stereochemistry of fused, bridged and caged ring systems-decalins, norbornane, barrelene and adamantanes.

Unit 5: Stereochemistry (9hrs)

Conformation and configuration, Fischer, Newman and Sawhorse projection formulae and their interconversion. Concept of chirality, recognition of symmetry elements and chiral structures, conditions for optical activity, optical purity. Specific rotation and its variation in sign and magnitude under different conditions, relative and absolute configurations, Fisher projection formula, sequence rule – *R and S* notation in cyclic and acyclic compounds, Cahn-Ingold-Prelog (CIP) rule. Mixtures of stereoisomers; enantiomeric excess and diastereomeric excess and their determination. Methods of resolution diastereomers. Resolution of racemates after conversion into diastereomers; use of S-brucine, kinetic resolution of enantiomers, chiral chromatography.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, enantiotopic, homotopic, diastereotopic hydrogen atoms, prochiral centre. Pro-R, Pro-S, Re and Si.

Optical isomerism in biphenyls, allenes and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1,2-, 1,3- and 1,4-

dimethylcyclohexanes.

Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to folding of helical structures.

Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds-monocyclic, fused and bridged ring systems, inter conversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, stereochemistry of aldoximes and ketoximes

Unit 6: Asymmetric Synthesis (9 hrs)

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity. Chiral pool: chiral pool synthesis of beetle pheromone component (*S*)- (–)-ipsenol from (S)-(–)-leucine.

Classification of Asymmetric reactions into (1) Substrate controlled (2) Chiral auxiliary controlled (3) Chiral reagent controlled and (4) Chiral catalyst controlled.

Substrate controlled asymmetric synthesis: Nucleophillic addition to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulfoxides. 1,4-Asymmetric induction and Prelog's rule. Use of chiral auxiliary in Diels-Alder and Cope reactions.

Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL– H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation

Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann-*Traxler* model. Auxillary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol reactions

References:

1. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A,* Springer, 5/e, 2007.
2. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6/e, 2007.
3. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
5. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.
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12. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2/e, John Wiley & Sons, 2008.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
MCH1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS
(4 Credits, 54hrs)

Unit 1: Thermodynamics (9hrs)

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, Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents), 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 2: 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 3: Chemical Kinetics (9 hrs)

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); 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.

Unit 4: 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; Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies; Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger and Kassel (RRK) model.

Unit 5: Surface Chemistry (9 hrs)

Structure and chemical nature of surfaces, Adsorption at surfaces - Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation, Determination of surface area and pore structure of adsorbents - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorption methods. Determination of surface acidity - TPD method. Heat of adsorption and its determination.

Unit 6: Catalysis (9hrs)

Features of homogeneous catalysis – Enzyme catalysis - Michaelis-Menten Mechanism. Features of heterogeneous catalysis - Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2$ ---› $2CO_2$. Methods of preparation of heterogeneous catalysts - precipitation and co-precipitaion methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko -Volterra, brusselator and oregonator).

Reference:

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3. Steinfeld, Francisco and Hase, Chemical Kinetics and Dynamics, 2nd edition, Prentice Hall International. Inc
4. Santhosh K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer, 2006.
5. Richard I. Masel, Chemical Kinetics and Catalysis, Wiley Interscience, 2001.
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10. S. Glasstone, Thermodynamics for chemists, East-West 1973.
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12. Pigoggine, An introduction to Thermodynamics of irreversible processes, Interscience
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15. Jens Hajen, Industrial Catalysis: A Practical Approach. 2nd Edn., Wiley VCH, 2006.
16. Dipak Kumar Chakrabarty, Adsorption and Catalysis by Solids, New Age. 2007.
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18. Woodruff, D. P. and Delchar T. A., Modern Techniques of Surface Science, Cambridge Solid State Science Series, 1994.
19. Kurt K. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, 3rd Edn., Wiley U. K., 2012.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II
MCH2C05 - GROUP THEORY and CHEMICAL BONDING
(3 Credits, 54hrs)

Unit 1: Foundations of Group Theory & Molecular Symmetry (9hrs)

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group.

Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT of point groups;

Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices;

Matrix representation of symmetry operations.

UNIT 2: Representations of Point Groups & Corresponding Theorems (9hrs)

Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H_2O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only), Great Orthogonality Theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2V}, C_{3V}, C_{2h} and C_{4V} and C_3 as examples), nomenclature of IR - Mulliken symbols, symmetry species;

Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., Γ_{cart}) using the reduction formula;

Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

Unit 3: Applications of Group Theory to Molecular Spectroscopy (9hrs)

Molecular vibrations - symmetry species of normal modes of vibration, construction of

Γcart, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra.

Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non–vanishing integrals, transition moment integral and 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 (9hrs)

Hybridisation - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using proj ection operator, use of projection operator in constructing SALCs for the π MOs in cyclopropenyl ($C_3H_3^+$) cation.

Unit 5: Chemical bonding in diatomic molecule (9hrs)

Schrödinger equation for a molecule, Born – Oppenheimer approximation; Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2; Molecular Orbital (MO) theory – MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2 & F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

Unit 6: Chemical Bonding in polyatomic molecules (9hrs)

Hybridization – quantum mechanical treatment of sp, sp^2 & sp^3 hybridisation; Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion, charge distributions and bond orders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.

Reference (for Units 1 to 4)

1. F.A. Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc., 2003.
2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry*, John Wiley &Sons Inc., 1965.
3. L.H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill, 1969.
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Reference (for units 5 & 6)

11. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
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FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II
MCH2C06 – COORDINATION CHEMISTRY
(3Credits, 54hrs)

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 spectrophotometry. 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 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 D_q, B and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra.

Types of magnetic properties-Paramagnetism 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 paramagnetism. Antiferromagnetism- types and exchange pathways. Determination of magnetic moment by Gouy method.

Unit 4: Characterization of Coordination Complexes (9hrs)

Infrared spectra of metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Application in coordination complexes. ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling. Mossbauer spectroscopy- the Mossbauer Effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.

Unit 5: 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 6: Redox and Photochemical Reactions of Complexes (9hrs)

Classification of redox reaction mechanisms. Outer sphere and inner sphere mechanisms. Marcus equation. Effect of the bridging ligand. Methods for distinguishing outer- and inner-sphere redox reactions.

Photochemical reactions of metal complexes- Prompt and delayed reactions. Exited states of metal complexes- Interligand, ligand field, charge transfer and delocalized states. Properties of ligand field excited states. Photosubstitution-Prediction of substitution lability by Adamson`s rules. Photoaquation. 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.

References:

1. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, 2/e, Butterworth-Heinemann, 2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi, Inorganic Chemistry, principles of structure and reactivity, Pearson Education, 2006.
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10. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, Wiley.
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12. R.L.Dutta and A.Shyamal, Elements of Magnetochemistry, S.Chand and Co. 1982.
13. A.E. Martell, Coordination Chemistry, Vol. I
14. R.S. Drago, *Physical Methods in Inorganic Chemistry*, Affiliated East- West Press Pvt. Ltd., 1977.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II
MCH2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY
(3 Credits, 54hrs)

Unit 1: Aliphatic and Aromatic Substitutions (9 hrs)

Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions. S_Ni and neighboring group mechanism. SET mechanism. Allylic and bezylic substitutions. Ambident nucleophiles and substrates regioselectivity.

Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of S_E1, S_E2 (front), S_E2 (back) and S_Ei reactions. The effect of substrate structure, leaving group and reaction medium on S_E1 and S_E2 reactions.

Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Nucleophilic Aromatic substitution: Addition-elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, S_N1 and $S_{RN}1$ mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic nucleophilic substitution.

Unit 2: Addition & Elimination Reactions and Reactive Intermediates (9hrs)

Mechanistic and stereochemical aspects of addition to C=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.

Mechanistic and stereochemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev elimination, Hofmann elimination, α-elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions-extrusion of N_2, CO and CO_2.

Reactive Intermediates: Generation, geometry, stability and reactions of carbonium ions and carbanions, free radicals, carbenes, nitrenes and benzynes.

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

Reactions of Carbon-heteromultiple Bonds: Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration, addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium reagents- to carbonyl compounds. Aldol, Perkin, Claison, Dieckmann, Stobbe and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich and Prins reactions. MPV reduction and Oppenauer oxidation.

Addition to carbon-nitrogen multiple bond: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis and reduction of nitriles.

Esterification and Ester Hydrolysis: Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Unit 4: Pericyclic Reactions (9 hrs)

Phase and symmetry of molecular orbitals, FMOs of ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl and 1,3-pentadienyl systems. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar-Zimmerman approach), FMO method and Correlation diagram method (Woodward-Hoffmann approach). Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions. Stereochemistry of Diels-Alder reactions and regioselectivity. Cope and Claison rearrangements. Stereochemistry of cope rearrangement and valence tautomerism. 1,3-dipolar cycloaddition reactions and *ene* reactions.

Unit 5: Photochemistry of Organic Compounds (9 hrs)

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization and quenching. Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and β, γ-unsaturated carbonyl compounds, β- cleavage, γ- hydrogen abstraction: Norrish type-II cleavage, photo reduction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Büchi reaction, photodimerisation of α, β-unsaturated ketones, Photo rearrangemets: Photo –Fries, di-π- methane, lumiketone, oxa di-π-methane rearrangements. Barton and Hoffmann-Loeffler-Freytag reactions. Photo isomerisation and dimerisation of alkenes, photo isomerisation of benzene and substituted benzenes, photooxygenation.

Unit 6: Chemistry of 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 and quinine.

Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids. Woodward synthesis of cholesterol, conversion of cholesterol to testosterone. Total synthesis of Longifolene, Reserpine, Cephalosporin,

General structure of anthocyanins and flavonoids.

References:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A & B,* 5/e, Springer, 2007.
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FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II
MCH2C08 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS
(3 Credits, 54hrs)

Unit 1: Ionic Interaction & Equilibrium Electrochemistry (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- 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

Unit 2: Dynamic Electrochemistry (9hrs)

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 3: Solid State – I (9hrs)

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.

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.

UNIT 4: Solid State – II (9hrs)

Electronic structure of solids – free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties - electrical conductivity, 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, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism; Thermal properties - thermal conductivity & specific heat

Unit 5: Statistical Thermodynamics- I (9hrs)

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 macrostates, 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, 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.

Unit 6: Statistical Thermodynamics- II (9hrs)

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.

Reference:

For Units 1-4

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.
3. Carl. H. Hamann, A. Hamnett, W.Vielstich, *Electrochemistry 2nd edn*., Wiley- VCH, 2007.
4. Philip H Reiger, *Electrochemistry 2nd edn*., Chapman & Hall, 1994.
5. Praveen Tyagi, *Electrochemistry,* Discovery Publishing House, 2006.

6. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications, 1961.
7. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1960.
8. A.R. West, Basic Solid State Chemistry 2nd edn., John Wiley & Sons, 1999.
9. A.R. West, *Solid State Chemistry & its Applications,* John Wiley & Sons, 2003 (Reprint 2007).
10. Charles Kittel, *Introduction to Solid State Physics, 7th edn,* John Wiley & Sons, 2004 (Reprint 2009).
11. Mark Ladd, Crystal Structures: Lattices & Solids in Stereo view, Horwood, 1999.
12. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.
13. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd edn.*, Oxford Uty. Press, 2002.
14. Werner Massa, Crystal Structure Determination 2nd edn., Springer 2004.
15. N.B. Hanna, *Solid state Chemistry*, Prentice Hall

For Units 5 & 6

16. G.S. Rush Brooke, *Statistical mechanics*, Oxford University Press.
17. T.L. Hill, Introduction to statistical thermodynamics, Addison Wesley.
18. K. Huary, Statistical mechanics, Thermodynamics and Kinetics, John Wiley.
19. O.K.Rice, Statistical mechanics, Thermodynamics and Kinetics, Freeman and Co.
20. F.C. Andrews, *Equilibrium statistical mechanics,* John Wiley and sons, 1963.
21. M.C. Guptha, *Statistical Thermodynamics,* Wiley eastern Ltd., 1993.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY – SEMESTER I & II
MCH1L01 & MCH2L04 – INORGANIC CHEMISTRY PRACTICALS– I & II
(3 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: EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)

Cerimetry (Fe^{2+}, nitrite)

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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY – SEMESTER I & II
MCH1L02 & MCH2L05 – ORGANIC CHEMISTRY PRACTICALS– I & II
(3 Credits)

Unit 1: Laboratory Techniques

Methods of Separation and Purification of Organic Compounds – fractional, steam and low-pressure distillations, fractional crystallisation and sublimation.

Unit 2: Separation and identification of the components of organic binary mixtures.

Microscale analysis is preferred

Analysis of about ten binary mixtures, some of which containing compounds with more than one functional group. Separation and identification of a few ternary mixtures.

Unit 3: Organic preparations-double stage (minimum six) and three stage (minimum two)

References:

5. 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.
6. Shriner, Fuson and Cartin, Systematic Identification of Organic Compounds, 1964.
7. Fieser, Experiments in Organic Chemistry, 1957.
8. Dey, Sitaraman and Govindachari, *A Laboratory Manual of Organic Chemistry*, 3rd Edition, 1957.
9. P.R. Singh, D.C. Gupta and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II, 1980.
10. Vishnoi, Practical Organic Chemistry.
11. Pavia, Kriz, Lampman, and Engel, A Microscale Approach to Organic Laboratory Techniques, 5/e, Cengage, 2013.
12. Mohrig, Hammond and Schatz, Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale, 3/e, W. H. Freeman and Co., 2010.

FAROOK COLLEGE (AUTONOMOUS) M.Sc. CHEMISTRY – SEMESTER I & II
MCH1L03 & MCH2L06 – PHYSICAL CHEMISTRY – I & II
(3 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)

(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.

Determination of phase diagram of a binary solid system forming a compound (e.g., Naphthalene – m-dinitrobenzene).

Unit 3: Viscosity (minimum 2 experiments)

Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene - nitrobenzene, water-alcohol).

Determination of molecular weight of a polymer (e.g., polystyrene in

Unit 4: Distribution Law (minimum 3 experiments)

Determination of distribution coefficient of I_2 between CCl_4 and H_2O.

Determination of equilibrium constant of $KI + I_2 = KI_3$

Determination of concentration of KI solution

SECTION B

Unit 5: Refractometry (minimum 3 experiments)

Determination of molar refractions of pure liquids (e.g., water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol)

Determination of composition of liquid mixtures (e.g., alcohol-water, glycerol-water)

Determination of molar refraction and refractive index of a solid

Unit 6: Conductivity (minimum 4 experiments)

Determination of equivalent conductance of a weak electrolyte (e.g.,
acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.

Determination of solubility product of a sparingly soluble salt (e.g., AgCl, $BaSO_4$)

Conductometric titrations

HCl vs NaOH

($HCl + CH_3$-COOH) vs NaOH

Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (minimum 3 experiments)

Potentiometric titration: HCl vs NaOH, CH_3-COOH vs NaOH

Redox titration: KI vs $KMnO_4$, $FeSO_4$ vs $K_2Cr_2O_7$

Determination of dissociation constant of acetic acid by potentiometric titration

Determination of pH of weak acid using Potentiometry

Determination of pH of acids and bases using pH meter

Reference:

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

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III
MCH3C09 - MOLECULAR SPECTROSCOPY
(4 Credits, 72hrs)

Unit 1: Basic Aspects and Microwave Spectroscopy - *Theory only* (9hrs)

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 selection rules, determination of bond length using microwave spectral data.

Unit 2: Infrared, Raman and Electronic Spectroscopy - *Theory only* (9hrs)

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 & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle; Introduction to Resonance Raman spectroscopy (basics only).

Electronic Spectroscopy- 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 – I - *Theory only* (9hrs)

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 T1 and T2 (Relaxation) measurements. 2D NMR COSY

Unit 4: Magnetic Resonance Spectroscopy – II - *Theory only* (9hrs)

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 5: Electronic & Vibrational Spectroscopy in Organic Chemistry (9hrs)

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating λ_{max} of dienes, enones and benzene derivatives.

Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, elipticity and circular dichroism, ORD and Cotton effect. Octant rule and Axial haloketone rule for the determination of conformation and configuration of 3-methyl cyclohexanone and *cis*- and *trans*-decalones. CD curves.

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.

UNIT 6: NMR Spectroscopy in Organic Chemistry - I (9hrs)

^{1}HNMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, Chemical, magnetic and stereochemical equivalence. Enantiotopic, diasteriotopic and homotopic protons. Protons on oxygen and nitrogen. Quadrapole broadening. Spin – spin coupling, types of coupling. Coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectrum, First order and non first order nmr spectra,

UNIT 7: NMR Spectroscopy in Organic Chemistry - II (9hrs)

Simplification of NMR spectra: double resonance, shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra.

^{13}CNMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.

UNIT 8: Mass Spectrometry and Spectroscopy for Structure Elucidation (9hrs)

Mass Spectrometry: Basic concept of EIMS. Molecular ion and meta stable ion peaks, Isotopic peaks. Molecular weight and molecular formula. Single and multiple bond cleavage, rearrangements - McLafferty rearrangements. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, aldehydes and ketones, amines and amides. High resolution mass spectrometry, index of hydrogen deficiency, Nitrogen rule and Rule of Thirteen. Ionization techniques. FAB spectra.

Structural determination of organic compounds using spectroscopic techniques (Problem solving approach)

References:

For Units 1, 2, 3 & 4

1. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1962.
2. C.N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill,New Delhi, 1994.
3. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson education, 2006.
4. P. Atkins & J. De Paula, Atkins's Physical Chemistry, 8th Edition, W.H. Freeman & Co., 2006.
5. D.A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, University Science Books, 1997.
6. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, UniversityPress, 2000.
7. R.S. Drago, Physical methods for Chemists, Second edition, Saunders College Publishing 1977 (For NMR and EPR, Mossbauer)
8. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 2/e, John Wiley
9. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e, Academic Press, 2005.

For Units 5, 6, 7 & 8

10. Lambert, Organic Structural Spectroscopy, 2/e,—Pearson
11. Silverstein, Spectrometric Identification of Organic Compounds, 6/e,—John Wiley
12. Pavia, Spectroscopy, 4/e, – Cengage
13. Jag Mohan, Organic Spectroscopy: Principles and Applications, 2/e,—Narosa
14. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e, — McGraw-Hill
15. P S Kalsi, Spectroscopy of organic compounds, New Age International, 2007
16. William Kemp, Organic Spectroscopy**, 3e,** Palgrave, 2010

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III
MCH3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY
(4 Credits, 54h)

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 carbines.

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 cyclobutadiene, $C_5H_5^-$ $C_6H_6,$ $C_7H_7^+$ and $C_8H_8^{2-}$. Fullerene complexes. Fluxional organometallics.

Unit 3: Organometallic Reactions and Catalysis (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.

Homogeneous and heterogeneous catalysts.

Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydroformylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.

Heterogeneous catalysis by organometalic compounds: Ziegler-Natta polymerizations, Fischer-Tropsch process and water gas shift reaction.

Unit 4: 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 5: 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. Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump. Structural role of calcium. 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 6: Bioinorganic Chemistry-II (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. Carboxypeptidase. Vitamin B12 and coenzymes.Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases. Anticancer drugs.

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.
6. Keith F Purcell, John C Kotz, Inorganic Chemistry, Cengage Learning, 2010.
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, Wiley Eastern.
11. P.Powell, Principles of Organometallic Chemistry, ELBS.
12. B.D.Gupta and A.J.Elias, Basic Organometallic Chemistry, Concepts, Synthesis and Applications, Universities Press, 2010.
13. Piet W.N. M.van Leeuwen, Homogeneous Catalysis, Springer, 2010.S.J. Lippard and J.M.Berg, Principles of Bioinorganic Chemistry, University Science Books.
14. Ivano Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III
MCH3C11 - REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY
(4 Credits, 54hrs)

Unit 1: Oxidations (9hrs)

Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prévost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO_3-Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Baeyer-Villiger oxidation, Dess-Martin oxidation, Swern oxidation, hydroboration-oxidation.

Unit 2: Reductions (9hrs)

Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis. Liquid ammonia reduction with alkali metals. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide. Clemmensen reduction, Birch reduction. Wolff-Kishner reduction, Bouveault- Blanc reduction, MPV reduction, hydroboration, Pinacol coupling, McMurry coupling, Shapiro reaction.

Unit 3: Synthetic Reagents (9 hrs)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, $LiAlH_4$, $LiBH_4$, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman’s reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, $Pb(OAc)_4$, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.

Unit 4: Chemistry of Polymers (9 hrs)

Classification of polymers, chain, step, free-radical and ionic polymerizations. Plastics, rubbers and fibers, thermosets and thermoplastics, linear, branched, cross-linked and network polymers, block and graft copolymers.

Natural and synthetic rubbers.

Biopolymers: Primary, secondary and tertiary structure of proteins, Merrifield solid phase peptide synthesis, Protecting groups, sequence determination of peptides and proteins, Structure and synthesis of glutathione, structure of RNA and DNA, structure of cellulose and starch, conversion of cellulose to rayon.

Unit 5: Heterocyclic chemistry and supramolecular chemistry (9 hrs)

Aromatic and nonaromatic heterocyclics. Structure, synthesis and reactions of a few heterocyclics-aziridine, oxirane, indole, pyridine, quinolone, imidazole. Synthesis of uracil, thymine, adenine and guanine

Supramolecular Chemistry: Basic concepts and terminology. Molecular recognition: Molecular receptors for different types of cations, anions and neutral molecules, design of coreceptors and multiple recognition. Strong, weak and very weak Hydrogen bonds. Use of H bonds in in crystal-engineering and molecular recognition. Supramolecular reactivity and catalysis. Supramolecular photochemistry and examples for supramolecular devices

Unit 6: Molecular Rearrangements and Transformations (9hrs)

Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzil- benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Fries, Bayer- Villiger, Wittig, Orton, and Fries rearrangements. Peterson reaction, Woodward and Prevost hydroxylation reactions. Heck, Negishi, Sonogashira, Stille, and Suzuki coupling reactions (mechanism only)

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press, 1998.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
4. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
5. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
7. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
8. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, 2/e, Narosa Publishing House, 2006.
9. G. Odiyan, *Principles of Polymerisation*, 4/e, Wiley, 2004.
10. V.R. Gowariker and Others, *Polymer Science*, Wiley Eastern Ltd.
11. I.L. Finar, *Organic Chemistry*, Vol. II, 5/e, ELBS, 1975.
12. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.
13. T. L. Gilchrist, *Heterocyclic Chemistry*, 3/e, Pearson, 1997.
14. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.
15. F. Vogtle, *Supramolecular Chemistry*, John Wiley & Sons, Chichester, 1991.
16. J.M.Lehn, Supramolecular Chemistry, VCH.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER III
MCH3E01 - SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)
(4 Credits, 54hrs)

Unit 1: Reagents for Oxidation and Reduction (9hrs)

Reagents for oxidation and reduction: Oxone, IBX, PCC, osmium tetroxide, ruthenium tetroxide, selenium dioxide, molecular oxygen (singlet and triplet), peracids, hydrogen peroxide, aluminum isopropoxide, periodic acid, lead tetraacetate. Wacker oxidation, TEMPO oxidation, Swern oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation.

Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.

Unit 2: Organometallic and Organo-nonmetallic Reagents (9hrs)

Synthetic applications of organometallic and organo-nonmetallic reagents: Reagents based on chromium, nickel, palladium, silicon, and born, Gilman reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes. Gilman's reagent, Tri -n-butyl tin hydride, Benzene Tricarbonyl Chromium

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at α-carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfur ylides.

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit- 4. Coupling Reactions (9hrs)

Coupling Reactions: PalladiumCatalysts for C-N and C-O bond formation, Palladium catalyzed amine arylation (Mechanism and Synthetic applications). Sonogashira cross coupling reaction (Mechanism, 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.

Unit 5: Multi step Synthesis (9hrs)

Multi step Synthesis: Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis, Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone

Unit 6: Retro Synthetic Analysis and Heterocyclics (9hrs)

Retrosynthesis: General principles of retrosynthetic analysis - synthons and reagents, donor and acceptor synthons, umpolung, protecting group chemistry and functional group interconversions. One group and two group C - X and C - C disconnections, functional group transposition. Examples for a few retrosynthetic analyses - paracetamol from phenol, benzocain from toluene and propranolol from 1 - naphthol.

Structure, synthesis and reactions of fused ring heterocycles: Benzofuran, Indole, Benzothiophene, Quinoline, Benzoxazole, Benzthiazole, Benzimidazole, Triazoles , Oxadiazoles and Tetrazole.

Structure and synthesis of Azepines, Oxepines, Thiepins, Diazepines and Benzodiazepines Structure and synthesis (Reichstein process) of Vitamin C (Reichstein process).

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. S. Warren and P. Wyatt, Organic Synthesis: Strategy and Control, John Wiley
3. S. Warren: Organic Synthesis: The Disconnection Approach, John Wiley
4. H. O. House: *Modern Synthetic Reactions*, W. A. Benjamin
5. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
6. T. W. Greene and P. G. M. Wuts: *Protecting Groups in Organic Synthesis*, 2nd ed., John Wiley
7. M B Smith and J. March: Advanced Organic Chemistry-Reactions, Mechanisms and Structure, 6th ed., John Wiley
8. T. H. Lowry and K. S. Richardson: *Mechanism and Theory in Organic Chemistry*, 3rd ed.
9. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part A and B, 5/e, Springer, 2007
10. A. Pross: Theoretical and Physical Principles of Organic Chemistry, John Wiley
11. T.W. Graham Solomons: *Fundamentals of Organic Chemistry*, 5th ed., John Wiley
12. I. L. Finar: *Organic Chemistry* Volumes 1 (6th ed.), Pearson
13. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2/e, Oxford University Press
14. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
15. N. K. Terret: *Combinatorial Chemistry*, Oxford University Press, 1998.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III
MCH3E02 - COMPUTATIONAL CHEMISTRY (ELECTIVE)
(4 credits, 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 functionals
– 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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III
MCH3E03 - GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE)
(4 credits, 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 a methylating 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 nanodimensional materials - Historical milestones - unique properties due to nanosize,Quantum dots, Classification of Nanomaterials .General methods of synthesis of nanomaterials – 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 SynthesisSynthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation. Inorganic nanomaterials – Typical examples –nano TiO_2 / ZnO/CdO/CdS , Organic nanomaterials – examples – Rotaxanes and Catenanes

Unit 5: Techniques for Characterisation 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 ionconductance 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 C_{60} - 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
5. T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
6. *Green Chemistry – Environment friendly alternatives*- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

For Units 4, 5 & 6

7. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), *The Chemistry of Nanomaterials*, Vol.1, 2, Wiley –VCH, Weinheim, 2004.
8. C.P. Poole, Jr: F.J. Owens, *Introduction to Nanotechnology* Wiley Interscience, 2003
9. Kenneth J. Klabunde (Ed), *Nanoscale materials in Chemistry*, Wiley- Interscience, 2001.
10. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi, 2007.
11. H. Fujita (Ed.), *Micromachines as tools in nanotechnology*, Springer- Verlag, Berlin, 2003.
12. 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)
13. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties
14. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John-Wiley R Sons, New York.
15. T. Tang and p. Sheng (Eds), Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 2004.
16. A Nabok, *Organic and Inorganic Nanostructures*, Artech House, Boston, 2005.
17. Edward A. Rietman, *Molecular engineering of Nanosystems*, Springer- Verlag, New York, 2001.
18. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
19. Nano letters - http://pubs.acs.org/journals/nalefd/index.html Nanotation - http://www.acsnanotation.org/

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV M
MCH4C12- INSTRUMENTAL METHODS OF ANALYSIS
(4 Credits, 72 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: solubility 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 nonaqueous media. Different solvents and their selection for a titration. 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: Electro Analytical Methods- I (9hrs)

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Polarography micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

Unit 4 Electro Analytical Methods II (9hrs)

Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits.Voltammetric sensors. Organic polarography.

Unit 5 Optical Methods - I (9 hrs)

Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry. UV-visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. 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.

Unit 6 Optical Methods - II (9 hrs)

Theory, instrumentation and applications of: - Atomic fluorescence spectrometry, X-ray methods, X-ray absorption and X-ray diffraction, photoelectron spectroscopy, Auger, ESCA. SEM, TEM, AFM,

Unit 7: Thermal Methods (9hrs)

Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) Thermomechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA), and their instrumentation. Thermometric Titrations.

Unit 8: Chromatography (9 hrs)

Chromatography-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, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC

References:

1. J.M. Mermet, M. Otto, R. Kellner, *Analytical Chemistry*, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry,*
3. 9th Edn., Cengage Learning., 2014.
4. J.G. Dick, *Analytical Chemistry*, R.E. Krieger Pub., 1978, 50
5. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub., 1990.
6. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative*

Chemical Analysis, 5th Edn., John Wiley& sons,1989.

7. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier, 1982.
8. G.D. Christian, J.E. O’Reilly, *Instrumental Analysis*, Allyn & Bacon, 1986.
9. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
10. A.I. Vogel, A Textbook of Practical Organic Chemistry, 5/e Pearson, 1989.
11. H.A. Laitinen, W.E. Harris, *Chemical Analysis*, McGraw Hill,1975.
12. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, CRC, 2008.
13. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry*, Blackwell Science, 2000.
14. G.Gringauz, Introduction to Medical Chemistry, Wiley-VCH, 1997.
15. Harkishan Singh and V.K.Kapoor, *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, 2008.
16. W.Bannwarth and B.Hinzen, Combinatorial Chemistry-From Theory to Application, 2nd
17. Edition, Wiley-VCH, 2006.
18. A.W.Czarnik and S.H.DeWitt, *A Practical Guide to Combinatorial Chemistry*, 1st Edition, American Chemical Society, 1997.
19. Bansal N K, Kleeman M and Mells M, *Renewable Energy Sources and Conversion Technology*, Tata McGraw-Hill. (1990)
20. Kothari D.P., “Renewable energy resources and emerging technologies”, Prentice Hall of India Pvt. Ltd., 2008.
21. Rai G.D, "Non-Conventional energy Sources", Khanna Publishers, 2000.
22. Michael Grätzel, J. Photochemistry and Photobiology C: Photochemistry Reviews 4 (2003) 145–153, Solar Energy Conversion by Dye-Sensitized Photovoltaic Cells, Inorg. Chem., Vol. 44, No. 20, 2005 6841-6851.
23. Yoshihiro Hamakawa, Thin-Film Solar Cells-Next *Generation Photovoltaics and Its Applications*, Springer Series in Photonics 13, 2004.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
MCH4E04 - PETROCHEMICALS AND COSMETICS (ELECTIVE)
(4Credits, 72hrs)

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. Acetic 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

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 and knock characteristics. 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 and petroleum products. Petroleum processing equipments. Storage tanks. Rectification columns. Cap tray 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 paraffine processing and other petroleum products. Lubricating and other oils. Paraffins, ceresins, petroleum. Miscellaneous petroleum products. Products of petrochemical and basic organic synthesis. Dye intermediates. Lacquers. Solvents. Thinners.

Unit 7: Purification of Petroleum Products (9hrs)

Absorptive and adsorptive purification. Sulphuric acid purification. Alkaline purification. Hydrorefining. Purification in a DC electric field. New methods of purification. De mercaptanisation. Stabilisation.

Unit 8: Perfumes and Cosmetics (9hrs)

Perfumes: Introduction. Esters. Alcohols. Ketones. Ionones. Nitromusks. Aldehydes. Diphenyl compounds. Production of natural perfumes. Flower perfume. Fruit flavours. Artificial flavours.

Cosmetics: Introduction. Toothpaste. Ingradients. Preparation. Recipe for toothpaste. Shampoos. Ingradients. Recipe. Hair dyeing. Materials used. Colour and Curl of Hair. Creams and Lotions. Skin Chemicals. Their ingradients. Preparation and recipe. Lipsticks. Ingradients. Preparation and recipe. Perfumes, Colognes and after shave preparation.

Compounds with flowery and fruity odours used in perfumes with their structures. Compounds with unpleasant odours used to fix delicate odours in perfumes. Deodorants and Antiperspirants.

Cosmetics: Economics and Advertising.

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

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
MCH4E05 - INDUSTRIAL CATALYSIS (ELECTIVE)
(4 Credits, 72hrs)

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. AClark, "Theory of adsorption and catalysis", Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis",
3. Academic Press, New York, 1967.
4. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
5. 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, structures of 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.

UNIT 7: Industrial Catalysis-1 (9hrs)

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9hrs)

Hydroformylation of olefins, carbonylation of organic substrates, conversion of methanol to acetic acid, synthesis of vinyl acetate and acetic anhydride, palladium catalyzed oxidation of ethylene, acrylonitrile synthesis, Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

1. G. Ertl, H. Knozinger and J. Weitkamp, *"Handbook of Heterogeneous Catalysis*" Vol 1-5, Wiley-VCH, Weinheim, 1997.
2. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial Catalytic Processes", Blackie Academic and Professional – Chapman and Hall, 1997.
3. R. Pearce and W.R. Patterson, *"Catalysis and chemical processes*", Academic press, Leonard Hill, London, 1981.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
MCH4E06 - NATURAL PRODUCTS & POLYMER CHEMISTRY
(4 Credits, 72 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, Ergosterol, Oesterone, Androsterone, Testosterone, Progestrone, Cortisone and Corticosterone. Structural elucidation of Cholesterol. Conversion of cholesterol to progesterone, androsterone and testosterone.

Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids and steroids.

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):b-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,* 3rd 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.

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,

UNIT 7: Polymer Solutions, Industrial polymers and Copolymers (9 hrs)

Polymer Solutions. Treatment of dilute solution data. Thermodynamics. Flory-Huggins equation. Chain dimension-chain stiffness – End-to-end distance. Conformation-random coil, Solvation and Swelling. Flory-Reiner equation. Determination of degree of crosslinking and molecular weight between crosslinks.

Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. Homo and Copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PA. PMMA and related polymers.

Copolymers. EVA polymers. Flourine containing polymers. Polyacetals. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers.

UNIT 8: 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. Polyanilines, polypyrrols, polythiophines, poly(vinylene phenylene). Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photoresists. Electrical properties of Polymers, Polymers with NLO properties, second and third harmonic generation, wave guide devises.

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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
MCH4E07 - MATERIAL SCIENCE (ELECTIVE) (4 credits, 72hrs)

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 a nd types of bonds, phase equilibria 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: Nanomaterials and Nanotechnology (9hrs)

Nanomaterials, nanostructures, self-assembly, Nanoparticles- methods of synthesis, sol-gel process, hydrolysis of salts and alkoxides, precipitation, condensation reactions, electrokinetic potential and peptization reactions; Gelatin network- xerogels, aerogels, drying of gels; Chemical modifications of nanosurfaces, 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 ferroelectricity, 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 & superconducting magnets; Ceramic magnets, low conducting and superconducting magnets; Superconducting materials - metallic and ceramic superconducting materials, theories of superconductivity,

Meissner effect; High temperature superconductors - structure and applications.

Unit 6: Some Special Polymers (9hrs)

Functional polymers - photoconductive, electroconductive, 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 polyacetyl, polyamide (nylon 6 and nylon 66), polyacrylate, polycarbonate, polyester (PET, PBT), polyether ketones; Thermosetting plastics such as PF, UF & MF.

Unit 7: Composite Materials (9hrs)

Definition and classification of composites, fibres and matrices; Composites with metallic matrices – processing, solid and liquid state processing, deposition;

Ceramic matrix composite materials – processing, mixing & Pressing, liquid state processing, sol -gel processing & vapor deposition technique; Interfaces in composites - mechanical & microstructural characteristics; Applications of composites.

Unit 8: Fracture Mechanics (9hrs)

Importance of fracture mechanics, micro structural features of fracture in metals, ceramics, glasses & composites , Weibull statistics for failure, strength analysis; Fatigue, application of fatigue testing - creep, stress rupture & stress behavior, evaluation of creep behavior.

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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
MCH4E08 – ORGANOMETALLIC CHEMISTRY (ELECTIVE)
(4 credits, 72hrs)

UNIT I (9h)

Organometallic compounds, Classification and nomenclature, the 16 and 18 electron rules, electron counting-covalent and ionic models, Main group organometallics-alkyl and aryl, groups 1, 2, 12, 13, 14 and 15 synthesis structure and applications. Transition metal to carbon multiple bond-the metal carbenes and carbynes, Transition metal complexes with chain π ligands – synthesis, structure, bonding and reactions of complexes of ethylene, allyl, butadiene and acetylene.

UNIT II (9h)

Metal carbonyls- Bonding modes of CO, IR spectroscopy as a tool to study bonding and structure of metal carbonyls, Synthesis of Metal carbonyls Direct and reductive Carbonylation, Reactions of Metal carbonyls-Activation of metal carbonyls, Disproportion, Nucleophilic addition, electrophilic addition to the carbonyl oxygen, Carbonyl cation, anions and hydrides, Collmann's reagent, Migratory insertion of carbonyls, Oxidative decarbonylation, Photochemical substitution, Microwave assisted substitution.

UNIT III (9h)

General aspects of synthesis, structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H_2, CS, RNC and Phosphines. Metal-carbon multiple bonds - Metal carbenes and carbynes, bridging carbenes and carbynes, N-heterocyclic carbons, multiple bonds to hetero atoms.

UNIT IV (9h)

Organometallic π complexes – synthesis, structure, bonding (molecular orbital treatment) and reactions of C_5H_5, C_6H_6, C_7H_7 and $C_8H_8^{-2}$. Polyalkyls, polyhydrides and f-block organometallic complexes, Fluxional organometallics.

UNIT V (9h)

Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H_2, N_2, O_2, NO by transition metals. Catalytic steps, Oxidative addition, reductive elimination and insertion reactions Hydrozirconation of alkenes and alkynes. Homogeneous catalysis. Hydrogenation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis, hydroformylation of alkenes, Monsanto acetic acid process and Wacker process. Metal complexes in enantioselective synthesis

UNIT VI (9h)

Organometallic reactions. SN^2 Reactions, Radical Mechanisms, Ionic Mechanisms, σ-Bond Metathesis, Oxidative Coupling and Reductive decoupling, Reactions involving CO, Insertions

Involving Alkenes, Other Insertions, α, β, γ and δ Elimination, Deinsertion and Nucleophilic and electrophilic attack on coordinated ligand.

UNIT VII (9h)

Applications of organometallic reaction- Homogeneous catalysis- General features of catalysis, Types of catalyst, Catalytic steps. Water-gas shift reaction, Fisher-Tropsch reaction, Hydrosilation of alkenes, Hydrocyanation of alkenes.

UNIT VIII (9h)

Organometallic Polymers, Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, poly(ferrocenylsilane)s, applications of oly(ferrocenylsilane)s and related polymers, applications of rigid-rod polyynes, polygermanes and polystannanes, polymers prepared by ring opening polymerization, organometallic dendrimers.

References:

1. B. D. Gupta, A .J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, Second edition, University Press, 2013.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Fourth edn. 2005, Wiley Interscience.
3. J. E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson education, 1993.
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th edition, John and Wiley, 1999.
5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, Affiliated East West Press, 1993.
6. P. Powell, Principles of Organomettalic Chemistry, 2nd edition, Chapman and Hall, London, 1998.
7. S. F. A. Kettle, Concise co-ordination chemistry, Nelson, 1969.
8. S. F. A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.
9. Purcell and Kotz, Inorganic Chemistry.
10. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY – SEMESTER III & IV
MCH3L07 & MCH4L10 – INORGANIC CHEMISTRY PRACTICALS– III & IV
(3 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 $Cr2O1^{2-}$) 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 expts.)

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)

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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY – SEMESTER III & IV
MCH3L08 & MCH4L11 – ORGANIC CHEMISTRY PRACTICALS– III & IV
(3 Credits)

Unit 1: Quantitative Organic Analysis

Estimation of equivalent weight of acids by Silver Salt method, Estimation of nitrogen by Kjeldahl method, Determination of Acid value, iodine value and saponification value of oils and fats (at least one each), Estimation of reducing sugars, Estimation of amino group, phenolic group and esters. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulphaguanidine), Antibiotics – Pencillin, Stroptomycin.

References:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, ELBS/Longman, 1989.
2. Beebet, Pharmacuetical Analysis.

Unit 2: Extractions

Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophill Steroids, Flavonoid (Soxhlet extraction), citral from lemon grass (steam distillation). Casein from milk.

Unit 3: Chromatograhy

Practical application of PC and TLC, Preparation of TLC plates, Activation, Identification of the following classes of compounds using one- and two-dimensional techniques. Identification by using spray reagents and co-chromatography by authentic samples and also from Rf values.

Food additives and Dyes, Artificial sweeteners: Saccharine, cyclamates, Dulcin. Flavour adulterants – piperonal, Benzalacetate, ethyl acetate antioxidants: Butylated hydroxytoluene (BHT) Butylated hydroxy anisole (BHA), Hydroquinone.

Food colours: Permitted – Amaranth, Erythrosine, Tatrazine, susnet yellow, Fast green, Brilliant Blue, Nonpermitted colours: Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red.

Amino acids (Protein hydrolysates), Sugars, Terpinoids, Alkaloids, Flavonoids, Steroids. Pesticides and herbicides: Oragonochlorine pesticides organo phosphates and carbamate pesticides, Herbicides. Plant growth stimulants: Indole acetic acid.

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.

FAROOK COLLEGE (AUTONOMOUS)
M.Sc. CHEMISTRY – SEMESTER III & IV
MCH3L09 & MCH4L12 – PHYSICAL CHEMISTRY PRACTICALS– III & IV
(3 Credits)

SECTION A

Unit 1: Chemical Kinetics (4 experiments)

Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.

Determination of Arrhenius parameters of acid hydrolysis of an

Determination of specific reaction rate of saponification of ethyl

Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

Unit 2: Adsorption (3 experiments)

Verification of Langmuir adsorption isotherm – charcoal-acetic acid system. Determination of the concentration of a given acetic acid solution using the isotherm

Verification of Langmuir adsorption isotherm – charcoal-oxalic acid system. Determination of the concentration of a given acetic acid solution using the isotherm.

Determination of surface area of adsorbent.

Unit 3: Phase Equilibria (2 experiments)

(a) Determination of phase diagram of a ternary liquid system (e .g. chloroform – acetic acid – water – Benzene – acetic acid – water)

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

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

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

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)

Determination of cyroscopic constant of a liquid (water, benzene)

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)

Determination of Van't Hoff factor and percentage of dissociation of NaCl.

Study of the reaction 2Kl + Hgl 2 .K2Hgl4 and determination of the concentration of the given Kl solution.

Unit 5: Polarimetry (3 experiments)

Determination of specific and molar optical rotations of glucose, fructose and sucrose.

Determination of specific rate of inversion of cane sugar in presence of HCl.

Determination of concentration of HCl

Unit 6: Spectrophotometry (3 experiments)

Determination of equilibrium constants of acid -base indicators.

Simultaneous of determination Mn and Cr in a solution of KMnO4 and K2Cr2O7

Investigation of complex formation between Fe (III) and thiocyanate.

References:

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

SECTION B

Use of Computational Chemistry softwares like pc GAMESS (firefly), Gaussian etc., to calculate molecular parameters.

Unit 7: Computational Chemistry Calculations

1) Single point energy calculations of simple molecules like H_2O and NH_3 at the HF/3-21G level of theory.
2) The effect of basis set on the single point energy of H_2O and NH_3 using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
3) Geometry optimization of molecules like H_2O, NH_3, HCHO & C_2H_4 at the HF/6-31G level of theory.
4) Computation of dipole and quadrupole moments of HCHO & C_2H_4 at the HF/6-31G level of theory.
5) Effect of basis set on the computation of H-O-H bond angle in H_2O using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
6) Computation of the energy of HOMO and LUMO of formaldehyde and ethylene at the HF/6-31G level of theory.
7) Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene

at the HF/6-31G level of theory.

8) Comparison of stability of cis-planar and trans-planar conformers of H_2O_2 at the HF/6-31G level of theory.
9) Comparison of stability of cis- and trans- isomers of difluoroethylene at the HF/6-31G* level of theory.
10) Computation of the frequencies of normal modes of vibration of molecules like H_2O, NH_3 and CO_2 at the HF/6-31+G* level of theory.
11) Determination of hydrogen bond strength of H_2O dimer and H_2O trimer at the HF/6-31+G* level of theory.
12) Determination of hydrogen bond strength of HF dimer and HF trimer at the HF/6-31+G* level of theory.

Reference:

1. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems", Wiley -Interscience, 2001.
3. http://classic.chem.msu.su/gran/gamess/index.html

Model Question Papers

FAROOK COLLEGE (AUTONOMOUS)

First Semester MSc Degree Examination

MCH1C01 – Quantum Mechanics and Computational Chemistry

Time: 3hours Max. Weightage 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

1) Explain Born interpretation of wave function

2) Differentiate time-dependent and time independent Schrodinger equation.

3) Explain tunnelling

4) What do you mean by symmetry breaking?

5) Determine the commutator of the operator d/dx and 1/x

6) Draw the radial distribution functions of 2s, and 2p

7) What are Cartesian and spherical polar coordinates?

8) Differentiate Slater type orbitals and Gaussian type orbitals.

9) Explain Fock operator.

10) Explain Pauli's anti-symmetry principle.

11) Differentiate ab initio and semi-empirical methods.

12) Give the Z-matrix for H_2O molecule.

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

13) Explain the postulates of quantum mechanics.

14) Explain the system particle in three-dimensional box.

15) A hydrogen molecule is confined in c cubic box with sides 1 meter. (i) What is the value of quantum number n at a temperature of 300K? (ii) What is the energy level separation between the levels n and n+1? (iii) What is its de Broglie wavelength?

16) Discuss Variation method for the helium atom in the ground state.

17) Explain Hartree's Self consistent field method for atoms.

18) Explain Spin orbitals and their construction.

19) Explain the structure of Gaussian input file. Explain any two key words.

Section B Essay

Answer 2 Questions out of 4.
Each question carries a weightage of 5 (2 X 5 = 10)

20) Derive wave functions and energies of hydrogen-like systems

21) Discuss the harmonic oscillator model and molecular vibrations

22) Explain Perturbation theory. Discuss the perturbation treatment of ground state of helium.

23) Discuss the basis set classification

FAROOK COLLEGE (AUTONOMOUS)

First Semester MSc Degree Examination

MCH1C02 – Chemistry of Elements

Time: 3hours Max. Weightage 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

24) Explain symbiosis

25) Calculate the styx number of B_5H_9.

26) Discuss Wade's rule as applied to boranes.

27) Discuss first and second row anomalies in transition metals.

28) What are silicides?

29) Distinguish heteropoly and isopoly anions.

30) How is 4f orbital different from 5f?

31) What are super heavy elements?

32) Explain the principle of radiation dosimetry.

33) Explain critical size as applied to nuclear reaction.

34) With suitable examples, differentiate photo nuclear and thermos nuclear reactions

35) What are graphenes?

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

36) Illustrate the use of SO_2 as a non-aqueous solvent.

37) Discuss the classification of borides.

38) Explain different types of reactions of boranes.

39) Illustrate the structure, bonding and use of SN_x.

40) Compare and contrast the spectral properties of lanthanide and actinides.

41) Discuss the characteristics of Ellingham diagram.

42) Explain template assisted synthesis of nano materials

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

43) Discuss different theories of acids and bases.

44) Explain the structure, bonding and uses of Phosphorous-Nitrogen compound.

45) Illustrate theory of nuclear fusion reaction.

46) Write short note on the following characterization techniques

    (a) SEM

    (b) TEM

    (c) AFM

    (d) XPS

    (e) XRD

FAROOK COLLEGE (AUTONOMOUS)

First Semester MSc Degree Examination

MCH1C03 - Structure and Reactivity of Organic Compounds

Time: 3hours Max. Weightage 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

1) What is homo aromaticity
2) Explain Hammet acidity function
3) What are classical and non classical carbocations?
4) Explain neighbouring group participation with carboxylate ion as an example.
5) What are the factors affecting conformational stability of a molecule?
6) Discuss kinetic control versus thermodynamic control.
7) Explain the effect of conformation on the course of E2 elimination (i) 4-t-Butylcyclohexyl tosylate.
8) Draw the configurations of decalin.
9) Explain Cahn-Ingold-Prelog rule.
10) What is the catalyst used in Sharpless asymmetric epoxidation. Explain the mechanism.
11) Distinguish , stereoselectivity and stereospecificity

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

12) What is criteria for aromaticity and antiaromaticity ? Explain the molecular orbital description of aromaticity and antiaromaticity
13) Effect of conformation on the course and rate of reactions in the dehydro halogination of stilbene dihalide.
14) Explain the conformations of cyclohexane, and methyl cyclohexane.
15) Compare the rate of esterification of menthol, isomenthol, neomenthol and neoisomenthol.
16) Explain Bredt’s rule.
17) Discuss the stereochemistry of aldoximes and ketoximes.

18) What is chiral auxiliary controlled asymmetric synthesis? Explain the use of chiral auxiliary in Diels-Alder reaction.

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

19) Discuss the effect of hydrogen bonding on the physiochemical properties and conformations of organic compounds

20) Illustarte the conformations of alkene dihalides, glycols, chlorohydrins, and tartaric acid.

21) Explain the different methods of resolution

22) Discuss Cram’s rule and Felkin-Anh model.

FAROOK COLLEGE (AUTONOMOUS)

First Semester MSc Degree Examination

MCH1C04 - Thermodynamics, Kinetics and Catalysis

Time: 3hours Max. Weightage 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

1) Explain residual entropy

2) Explain Nernst heat theorem

3) Define fugacity

4) What is Thermo osmosis?

5) Explain Electrokinetic effect.

6) What is steady state approximation?

7) Explain explosion limit with H_2 – O_2 reaction as example.

8) Compare collision theory and activation complex theory.

9) Explain Langmuir theory of adsorption.

10) How is surface acidity determined?

11) What is TDP method?

12) Discuss with an example auto catalysis.

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

13) Explain chemical potential. Deduce the relation between chemical potential with temperature and pressure

14) Explain entropy production

15) Discuss Onsager reciprocal relations

16) Explain Potential energy surface

17) Discuss the kinetics of decomposition of acetaldehyde.

18) Discuss the factors affecting the reaction rates in solution.

19) Explain the Michaelis – menton mechanism of enzyme catalysis. Michaelis constant of an enzyme catalised reaction at 298K iss 0.073 mol/L. At a substrate concentration of 0.8

mol/L, the rate of the reaction is found to be 4.19 mol/L/S. Calculate the maximum velocity

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

20) Explain Excess functions. Illustrate the determination of Excess volume.

21) Discuss the theories of unimolecular reactions

22) Illustrate the determination of surface area and pore structure of adsorbents

23) What are oscillation reactions? Explain their mechanism.