CURRICULUM AND SYLLABI

CHOICE BASED CREDIT SYSTEM

(CBCS-PG)

M. Sc. CHEMISTRY PROGRAMME

INTRODUCED FROM 2016 ADMISSION ONWARDS

BOARD OF STUDIES IN CHEMISTRY

Sacred Heart College, Thevara, Kochi, Kerala

SACRED HEART COLLEGE (AUTONOMOUS) – THEVARA, KOCHI -13.

1. SCOPE

1.1. These regulations provided herein shall apply to all post-graduate programmes, conducted by Sacred Heart College (S.H. College), Thevara with effect from the academic year 2016-2017 admission onwards.

2. DEFINITIONS

2.1 'Academic **Committee'** means the Committee constituted by the principal under this regulation to monitor the running of the Post-Graduate programmes under the Choice Based Credit System (CBCS-PG).

2.2 'Programme' means the entire course of study and examinations.

2.3 'Duration **of Programme'** means the period of time required for the conduct of the programme. The duration of post-graduate programme shall be of 4 semesters.

2.4 **'Semester'** means a term consisting of a minimum of 90 working days, inclusive of examination, distributed over a minimum of 18 weeks of 5 working days, each with 5 contact hours of one hour duration

2.5 'Course' means a segment of subject matter to be covered in a semester. Each Course is to be designed variously under lectures / tutorials / laboratory or fieldwork / study tour /seminar / project / practical training / assignments/evaluation etc., to meet effective teaching and learning needs.

2.6 'Credit' (Cr) of a course is the numerical value assigned to a paper according to the relative importance of the content of the syllabus of the programme.

2.7 '**Programme Credit'** means the total credit of the PG Programmes, ie; **80 credits**.

2.8 '**Programme Core course'** Programme Core course means a course that the student admitted to a particular programme must successfully complete to receive the Degree and which cannot be substituted by any other course.

2.9 'Programme Elective course' Programme Elective course means a course, which can be chosen from a list of electives and a minimum number of courses is required to complete the programme.

2.10 '**Programme Project'** Programme Project means a regular project work with stated credits on which the student undergo a project under the supervision of a teacher in the parent department / any appropriate Institute in order to submit a dissertation on the project work as specified.

2.11 '**Plagiarism**' Plagiarism is the unreferenced use of other authors' material in dissertations and is a serious academic offence.

2.12 '**Tutorial'** Tutorial means a class to provide an opportunity to interact with students at their individual level to identify the strength and weakness of individual students.

2.13 '**Seminar'** seminar means a lecture expected to train the student in self-study, collection of relevant matter from the books and Internet resources, editing, document writing, typing and presentation.

2.14 '**Evaluation'** means every course shall be evaluated by 25% internal assessment and 75% external assessment.

2.15 '**Repeat course'** is a course that is repeated by a student for having failed in that course in an earlier registration.

2.16 **'Audit Course'** is a course for which no credits are awarded.

2.17 '**Department'** means any teaching Department offering a course of study approved by the college / Institute as per the Act or Statute of the University.

2.18 '**Parent Department'** means the Department which offers a particular Post graduate programme.

2.19 '**Department Council'** means the body of all teachers of a Department in a College.

2.20 **'Faculty Advisor'** is a teacher nominated by a Department Council to coordinate the continuous evaluation and other academic activities undertaken in the Department.

2.21 '**College Co-ordinator** means a teacher from the college nominated by the College Council to look into the matters relating to CBCS-PG System

2.22 **'Letter Grade'** or simply '**Grade**' in a course is a letter symbol (S, A, B, C, D, etc.) which indicates the broad level of performance of a student in a course.

2.23 Each letter grade is assigned a **'Grade point'** (GP) which is an integer indicating the numerical equivalent of the broad level of performance of a student in a course.

2.24 **'Credit point'** (CP) of a course is the value obtained by multiplying the grade point (GP) by the Credit (Cr) of the course CP=GP x Cr.

2.25 **'Extra credits'** are additional credits awarded to a student over and above the minimum credits required for a programme for achievements in co-curricular activities carried out outside the regular class hours as directed by the College/ department.

2.26 '**Semester Grade point average'** (SGPA) is the value obtained by dividing the sum of credit points (CP) obtained by a student in the various courses taken in a semester by the total number of credits taken by him/her in that semester . The grade points shall be rounded off to two decimal places. SGPA determines the overall performance of a student at the end of a semester.

2.27 **Cumulative Grade point average'** (CGPA) is the value obtained by dividing the sum of credit points in all the courses taken by the student for the entire programme by the total number of credits and shall be rounded off to two decimal places.

2.28 '**Grace Marks'** means marks awarded to course/s, as per the orders issued by the college from time to time, in recognition of meritorious achievements in NCC/NSS/Sports/Arts and cultural activities.

2.29 'Words **and expressions'** used and not defined in this regulation but defined in the Mahatma Gandhi University Act and Statutes shall have the meaning assigned to them in the Act and Statute.

3. **ACADEMIC COMMITTEE**

3.1 There shall be an Academic Committee constituted by the principal to manage and monitor the working of (CBCS-PG) 2016.

3.2 The Committee consists of

(a) The principal

(b) The vice principal

(c) Deans of the faculties of science, arts and commerce

(d) The Controller of Examinations

(e) IQAC –Co-ordinator

(f) The superintendent of the college

4. PROGRAMME STRUCTURE

4.1 Students shall be admitted into post graduate programmes under the various faculties.

4.2 The programme shall include two types of courses, Program Core (C) courses and Program Elective (E) Courses. There shall be a Program Project (D) with dissertation to be undertaken by all students. The Programme will also include assignments, seminars, practical (P), viva (V), study tour etc., if they are specified in the Curriculum

4.3 There shall be various groups of four Programme Elective courses for a programme such as Group A, Group B etc. for the choice of students subject to the availability of faculty and infrastructure in the institution and the selected group shall be the subject of specialization of the programme.

4.4 Project work

4.4.1 Project work shall be completed by working outside the regular teaching hours.

4.4.2 Project work shall be carried out under the supervision of a teacher in the concerned department.

4.4.3. A candidate may, however, in certain cases be permitted to work on the project in an industrial / Research Organization/ Institute on the recommendation of the Supervisor.

4.4.4 There should be an internal assessment and external assessment for the project work in the ratio 1:3

4.4.5 The external evaluation of the Project work is followed by presentation of work including dissertation and Viva-Voce.

4.4.6 The mark and credit with grade awarded for the program project should be entered in the grade card issued by the college.

4.5. **Assignments**: Every student shall submit one assignment as an internal component for every course.

4.6 Seminar Lecture: Every PG student may deliver one seminar lecture as an internal component for every course. The seminar lecture is expected to train the student in self-study, collection of relevant matter from the books and Internet resources, editing, document writing, typing and presentation.

4.7 Every student shall undergo **two class tests** as an internal component for every course.

4.8 The attendance of students for each course shall be another component of internal assessment.

4.9 Comprehensive Viva-voce shall be conducted at the end of the programme which covers questions from all courses in the programme as per the syllabus.

5. ATTENDANCE

5.1 The minimum requirement of aggregate attendance during a semester for appearing the end semester examination shall be 75%. Condonation of shortage of attendance to a maximum of 10 days in a semester subject to a maximum of two times during the whole period of Post Graduate programme may be granted by the College as forwarded on the recommendation by the class teacher/HOD.

5.2 If a student represents the college in University, State or Nation in Sports, NCC, NSS or Cultural or any other officially sponsored activities such as College union / University union activities, he/she shall be eligible to claim the attendance for the actual number of days participated subject to a maximum of 10 days in a Semester based on the specific recommendations of the Head of the concerned Department and Principal of the College.

5.3 A student who does not satisfy the requirements of attendance shall not be permitted to take the end Semester examinations.

5.4 Those students who are not eligible even with condonation of shortage of attendance shall repeat the course along with the next batch

6. **BOARD OF STUDIES AND COURSES.**

6.1 The Board of Studies concerned shall design all the courses offered in the PG programme. The Boards shall design and introduce new courses, modify or re-design existing courses and replace any existing courses with new/modified courses to facilitate better exposures and training for the students.

6.2 The syllabus of a course shall include the title of the course, contact hours, the number of credits and reference materials.

6.3 Each course shall have an alpha numeric code number which includes abbreviation of the subject in two letters, the semester number, the code of the course and the serial number of the course (‘C’ for Program Core course, ‘E’ for Program Elective course, ‘O’ for Open Elective course, ‘P’ for Practical and ‘D’ for

Project/ Dissertation and 'V' for Comprehensive Viva voce).

6.4 Every Programme conducted under Choice Based Credit System shall be monitored by Academic committee and the College Council.

7. **REGISTRATION**.

7.1 A student shall be permitted to register for the programme at the time of admission. The duration of the PG Programme shall be 4 semesters.

7.2 A student who registered for the course shall complete the course within a period of 8 continuous semesters from the date of commencement of the programme.

8. **ADMISSION**

8.1 The admission to all PG programmes shall be as per the rules and regulations of the college.

8.2 The eligibility criteria for admission shall be as announced by the college from time to time.

8.3 There shall be provision for inter collegiate and inter University transfer within a period of two weeks from the date of commencement of the semester.

8.4 There shall be provision for credit transfer subject to the conditions specified by the Board of Studies concerned.

9. ADMISSION REQUIREMENTS

9.1 Candidates for admission to the first semester of the PG programme through CBCS shall be required to have passed an appropriate Degree Examination of Mahatma Gandhi University as specified or any other examination of any recognized University or authority accepted by the Academic council of the college as equivalent thereto.

9.2 The candidate must forward the enrolment form to the Controller of Examinations of the college through the Head of the Department.

9.3 The candidate has to register all the courses prescribed for the particular semester. Cancellation of registration is applicable only when the request is made within two weeks from the time of admission.

9.4 Students admitted under this programme are governed by the Regulations in force.

10. .**PROMOTION**: A student who registers for the end semester examination shall be promoted to the next semester

11. EXAMINATIONS

11.1 There shall be an external examination at the end of each semester.

11.2 The answers must be written in **English** except for those coming under Faculty of languages.

11.3 Practical examinations shall be conducted by the college at the end of the semesters as per the syllabus.

11.4 Project evaluation and Comprehensive Viva -Voce shall be conducted as per the syllabus. Practical examination, Project evaluation and Comprehensive Viva-Voce shall be conducted by two external examiners.(For professional courses, one examiner can be opted from the same college itself)

11.5 There shall be one end-semester examination of 3 hours duration in each lecture based course (Theory).

11.6 A question paper may contain multiple choice /objective type , short answer type/annotation, short essay type questions/problems and long essay type questions. Different types of questions shall have different marks, but a general pattern may be followed by the Board of Studies.

12 **EVALUATION AND GRADING**

12.1 Evaluation: The evaluation scheme for each course shall contain two parts; (a) internal evaluation (ISA) and (b) end semester evaluation (ESA). 25 marks shall be given to internal evaluation and 75 marks to external evaluation so that the ratio between internal and external mark is 1:3. Both internal and external evaluation shall be carried out in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

12.2 Internal evaluation: The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars/viva/field survey and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for internal evaluation is a follows.

12.3 Components of Internal Evaluation

All the components of the internal evaluation are mandatory

a) For Theory

	Components	Marks
i.	Assignment	5
ii	Seminar/Quiz/Field survey /Viva etc.	5
iii	Attendance	5
iv	Two Test papers(2x5)	10
	Total	25

b) For Practical

Components	Marks
Attendance	5
Written/Lab test	5
Laboratory Involvement/ Record*	10
Viva	5
Total	**25**

*Marks awarded for Record should be related to number of experiments recorded

c) For Project

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	5
Punctuality	3
Compilation	5
Content	5

Presentation	5
Total	**25**

12.4 Evaluation of

Attendance

% of attendance	Mark
Above 90%	5
Between 85 and < 90	4
Between 80 and below 85	3
Between 76 and below 80	2
75	1

Assignment

Components	**Marks**
Punctuality	1
Content	2
Conclusion	1
Reference/Review	1
Total	**5**

Seminar

Components	**Marks**
Content	2
Presentation	2
Reference/Review	1
Total	**5**

12.5 To ensure transparency of the evaluation process, the internal assessment marks awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of external examination. There shall not be any chance for improvement for internal mark.

12.6 The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course which shall be forwarded to the controller of examinations through the Principal and a copy should be kept in the college for at least two years for verification.

12.7 **External Evaluation:** The external examination in theory courses shall be conducted by the college with question papers set by external experts/ question bank. The evaluation of the answer scripts shall be done by the examiners based on a well defined scheme of evaluation given by the question paper setters. The external evaluation shall be done immediately after the examination preferably through the centralised valuation.

12.8 The question paper should be strictly on the basis of model question paper set by BoS with due weightage for each module of the course and there shall be a combined meeting of the question paper setters and experts for scrutiny for finalisation of question paper. Each set of question should be accompanied by its scheme of valuation.

12.9 For all courses (theory & practical), Letter grades and grade point are given on a 10-point scale based on the total percentage of marks, (ISA+ESA) as given below:-

Percentage of Marks	Grade	Grade Point (GP)
95 and above	O Outstanding	10
85 to below 95	A^+ Excellent	9
75 to below 85	A Very Good	8
65 to below 75	B^+ Good	7
55 to below 65	B Above Average	6
45 to below 55	C Average	5
40 to below 45	D Pass	4
Below 40	F Fail	0
	Ab Absent	0

Grades for the different semesters and overall programme are given based on the corresponding GPA as shown below:

GPA	Grade
Equal to 9.5 and above	***O Outstanding***
Equal to 8.5 and below 9.5	***A+ Excellent***
Equal to 7.5 and below 8.5	***A Very Good***
Equal to 6.5 and below 7.5	***B+ Good***
Equal to 5.5 and below 6.5	***B Above Average***
Equal to 4.5 and below 5.5	***C Average***
Equal to 4.0 and below 4.5	***D Pass***
Below 4.0	***F Failure***

12.10 A **separate minimum of 40% marks** (D grade) required for a pass for both internal evaluation and external evaluation for every course.

12.11 A candidate who has not secured minimum marks/credits in internal examinations can re-do the same registering along with the end semester examination for the same semester, subsequently.

12.12 A student who fails to secure a minimum marks/grade for a pass in a course will be permitted to write the examination along with the next batch.

There will be no improvement examinations

12.13 After the successful completion of a semester, Semester Grade Point Average (SGPA) of a student in that semester is calculated using the formula given below. For the successful completion of semester, a student should pass all courses and score a minimum SGPA of 4.0 However, a student is permitted to move to the next semester irrespective of her/his SGPA.

Credit Point (CP) of a course is calculated using the formula

CP = Cr x GP, where Cr = Credit; GP = Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula

SGPA = TCP/TCr, where

TCP = Total Credit Point of that semester $= \sum_1^n \mathrm{CPi}$***;***

TCr = Total Credit of that semester $= \sum_1^n \mathrm{Cri}$

Where n is the number of courses in that semester

Cumulative Grade Point Average (CGPA) of a Programme is calculated using the formula

$$\textbf{CGPA} = \sum(TCP \times TCr) \Big/ \sum TCr \quad GPA \text{ shall be round off to two decimal places}$$

12.14 PATTERN OF QUESTIONS

Questions shall be set to assess knowledge acquired, standard, application of knowledge, application of knowledge in new situations, critical evaluation of knowledge and the ability to synthesize knowledge. The question setter shall ensure that questions covering all skills are set. He/She shall also submit a detailed scheme of evaluation along with the question paper.

A question paper shall be a judicious mix of, multiple /objective ,short answer type, short essay type /problem solving type and long essay type questions.

Pattern of questions for external examination for theory paper

Type of Questions	Total no. of questions	Number of questions to be answered	Marks of each question	Total marks
Section A – Short Answer	12	8	2	16
Section B- Short essay/ Problems	10	7	5	35
Section C- Long essay	4	2	12	24
	26	**17**		**75**

Pattern of questions for external examination of practical papers will decided by Practical exam board chairman as per the guidelines of Board of Studies.

13. GRADE CARD

The colleges under its seal shall issue to the students, a grade card on completion of each semester, which shall contain the following information.

a) Name of the College

b) Title of the Postgraduate Programme

- **c)** Name of the Semester
- **d)** Name and Register Number of the student
- **e)** Code, Title, Credits and Max. Marks (Internal, External & Total) of each course(theory& Practical) in the semester.
- **f)** Internal, External and Total Marks awarded, Grade, Grade point and Credit point in each course in the semester
- **g)** The total credits, total marks (Max. & Awarded) and total credit points in the semester
- **h)** Semester Grade Point Average (SGPA) and corresponding Grade.
- **i)** Cumulative Grade Point Average (CGPA)
- **j)** The final Mark cum Grade Card issued at the end of the final semester shall contain the details of all courses(theory & practical) taken during the final semester examination and shall include the final grade/marks scored by the candidate from 1st to 3rd semester, and the overall grade/marks for the total programme.

14. **AWARD OF DEGREE**

The successful completion of all the courses with 'D' grade (40%) shall be the minimum requirement for the award of the degree

15**. MONITORING COMMITTEE**

There shall be a Monitoring Committee constituted by the principal consisting of faculty advisors ,HOD, a member from teacher learning evaluation committee (TLE) and college coordinator to monitor the internal evaluations conducted by college. The Course teacher, Faculty Advisor, and the College Coordinator should keep all the records of the internal evaluation, for at least a period of two years, for verification.

16. GRIEVENCE REDRESSAL MECHANISM

In order to address the grievance of students regarding Continuous internal assessment (CIA) a three-level Grievance Redressal mechanism is envisaged. A student can approach the upper level only if grievance is not addressed at the lower level.

Level 1: At the level of the concerned course teacher

Level 2: At the level of a department committee consisting of the Head of the Department, a coordinator of internal assessment for each programme nominated by the HoD and the course teacher concerned.

Level 3: A committee with the Principal as Chairman, Dean of the concerned Faculty, HOD of concerned department and one member of the Academic council nominated by the principal every year as members.

17. **TRANSITORY PROVISION**

Notwithstanding anything contained in these regulations, the Principal shall, for a period of three year from the date of coming into force of these regulations, have the power to provide by order that these regulations shall be applied to any programme with such modifications as may be necessary

18. **REPEAL**

The Regulations now in force in so far as they are applicable to programmes offered by the college and to the extent they are inconsistent with these regulations are hereby repealed. In the case of any inconsistency between the existing regulations and these regulations relating to the Choice Based Credit System in their application to any course offered in the College, the latter shall prevail.

FOREWORD........

I am greatly privileged in presenting the revised curricula and syllabi of M.Sc. Chemistry and MSc Pharmaceutical Chemistry for the approval of Faculty, Board of Studies and Academic Council of Sacred heart College (Autonomous)Thevara.

Chemistry is beyond the science of mere observation and understanding of nature. In the words of James Watson, a 1962 Nobel Laureate in Physiology or Medicine, put it well: “Life is simply a matter of chemistry”. It is with this vision we revised the syllabi for the PG courses, and also we followed the PG Guidelines which was prepared by the dean faculty. The revised syllabi will be implemented with effect from the academic year 2016-17 admission onwards.

The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for the two M.Sc. Programmes in Chemistry currently approved by the Mahatma Gandhi University. The BoS has taken keen interest in collecting expert opinion from the renowned experts in the field as well as from the faculties of the affiliated colleges handling the subjects. We have also referred to the syllabi of various other Universities such as that of Cochin University of Science and Technology, Calicut University, Pune University, Delhi University besides, that of University Grants Commission and offered in the affiliated colleges.

The BoS prepared draft proposals of revised curricula and syllabi for the two M.Sc. Programmes in Chemistry keeping the Credit and Semester System. The syllabus has been set with an objective of training the students in all the fundamentals of the subject along with good practical exposure. Most of the advanced topics have been incorporated in the fourth semester. In view of creating research aptitude in students, BoS has decided to give sufficient time for project work, at least three months, and as far as possible send the students in reputed research centres/Universities in and outside the state for doing their project. Since specific time is not allotted for project work in the academic calendar, students can go for project after their final semester examinations.

The BoS feels that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the faculty and BoS. I would like to express my sincere thanks to all my fellow members of the BOS and faculty for all their whole hearted time-bound help, cooperation and encouragement. I also express my sincere gratitude to Prof. S. Suganan (CUSAT), Prof.(Rtd.) K. K Vijayan (Calicut University), Prof. Abraham Joseph (Calicut University), Dr. M. K Muraleedharan Nair (Maharajas College), Dr. Mahesh Hariharan (IISER – TVM) and Dr. Pramod Padmanabhan (IISER – Pune) for their meaningful contributions.

Dr. Joseph John

Chairman

PG & UG Board of Studies

Sacred Heart College (Autonomous). Thevara.

Board of Studies in Chemistry

1. **Dr. Joseph John (HoD) Chairman.**
2. **Prof. (Dr.) P Raveendran**

   Department of Chemistry.

University of Calicut.

3. **Dr. Jude Martin Mendez.**
   Associate Prof .Department of Chemistry.
   St. Alberts College, Ernakulam.
4. **Prof.(Dr.) Abraham Joseph**
   Department of Chemistry
   University of Calicut.
5. **Dr. K.B Jose.**
6. **Dr. Joseph T Moolayil.**
7. **Dr.Thommachan Xavier.**
8. **Dr. V. S. Sebastian.**
9. **Dr. M. George.**
10. **Dr. Jorphin Joseph.**
11. **Dr. Franklin J.**
12. **Dr. Jinu George.**
13. **Dr. Grace Thomas.**
14. **Dr. Ignatious Abraham.**
15. **Mr. Midhun Dominic C D.**
16. **Mr. Senju Devassykutty.**
17. **Ms. June Cyriac.**
18. **Dr. Ramakrishnan.S.**
19. **Dr. Abi T. G.**
20. **Dr. Kochubaby Manjooran.**
    Manager, Energy and Environmental Division.
    Kochi Refineries Ltd. Ambalamukal, Kochi.
21. **Dr. K Krishnakumar. I. M.**
    General Manager, R&D
    AkayFlavours and Aromatics Pvt. Ltd.

Semester	Code	Course	Hours/ Week	Total Hours	Credit	Remarks
SEM.I	16P1CHET01	Inorganic Chemistry-I	4	72	4	
	16P1CHET02	Basic Organic Chemistry	4	72	4	
	16P1CHET03	Physical Chemistry-I	3	54	3	
	16P1CHET04	Quantum chemistry and group theory	4	72	3	
	16P2CHEP01	Inorganic Chemistry Practical-I	3	54	Evaluation at the end of 2nd Semester.	
	16P2CHEP02	Organic Chemistry Practical-I	3	54		
	16P2CHEP03	Physical Chemistry Practical-I	4	72		
		Total	**25**	**450**	**14**	
SEM.II	16P2CHET05	Inorganic Chemistry-II	4	72	4	
	16P2CHET06	Organic Reaction Mechanism.	4	72	4	
	16P2CHET07	Physical Chemistry-II	3	54	3	
	16P2CHET08	Theoretical and Computational Chemistry	4	72	3	
	16P2CHEP01	Inorganic Chemistry Practical-I	3	54	3	
	16P2CHEP02	Organic Chemistry Practical-I	3	54	3	
	16P2CHEP03	Physical Chemistry Practical-I	4	72	3	
		Total	**25**	**450**	**23**	
SEM.III	16P3CHET09	Inorganic chemistry-III	4	72	4	
	16P3CHET10	Organic Syntheses	4	72	4	
	16P3CHET11	Physical Chemistry-III	4	72	4	
	16P3CHET12	Spectroscopic methods in Chemistry	3	54	3	
	16P4CHEP04	Inorganic Chemistry Practical-II	3	54	Evaluation at the end of IVth Semester.	
	16P4CHEP05	Organic Chemistry Practical-II	3	54		
	16P4CHEP06	Physical Chemistry Practical-II	4	72		
		Total	**25**	**450**	**15**	
SEM.IV	16P4CHET13EL	Advanced Inorganic Chemistry (Elective 1)	5	90	4	
	16P4CHET14EL	Advanced Organic Chemistry (Elective 2)	5	90	4	
	16P4CHET15EL	Advanced Physical Chemistry(Elective 3)	5	90	4	
	16P4CHEP04	Inorganic Chemistry Practical-II	3	54	3	
	16P4CHEP05	Organic Chemistry Practical-II	3	54	3	
	16P4CHEP06	Physical Chemistry Practical-II	4	54	3	
	16P4CHECV	Comprehensive Subject Viva Voce			2	
	16P4PRCHE07	Project			5	
		Total	**25**		**28**	
		Grand Total			**80**	

Distribution of course, teaching Hours and credit for PG Branch III Chemistry

SEMESTER I

16P1CHET01 - INORGANIC CHEMISTRY-I

Credits: 4 **Total Contact Hours 72**

Unit 1: Organometallic Compounds- Synthesis, Structure and Bonding 18 Hrs

1.1 Hapto nomenclature of organometallic compounds and 16 and 18 electron rule, Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding. Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Metal carbene and alkylidenes, carbine and alkylidynes complexes, Fisher- type and Schrock- type complexes.

1.2 Metal Carbonyls: CO- as a π acid ligand, synergism, Molecular electronic structure and18-electron rule. Binary Carbonyl complexes- Mononuclear and Binuclear carbonyls. Preparation, properties, structure, bonding in metal carbonyls, bridging modes of CO, Polynuclear metal carbonyls with and without bridging, oxygen bonded metal carbonyls, Ligands similar to CO-Cyanide, nitrosyls, dinitrogen, Hydrogen and dihydrogen complexes.

1.3 Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons, Synthesis of clusters.

Unit 2: Reactions and catalysis of Organometallic Compounds 18 Hrs

2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands. Carbonylate anions as nucleophiles.

2.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

2.3 Redistribution reactions, fluxional isomerism.

2.4 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.

2.5 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, synthesis gas based reactions - the Fischer-Tropsch reaction(synthesis of gasoline).

2.6 Hydroformylation of olefins using cobalt or rhodium catalyst. Application - Synthesisof diethyhexylphthalate.

2.7 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.

2.8 Carbonylation reactions-Monsanto acetic acid process, Alkoxycarbonylation reactions-carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis.

2.9 Olefin methathesis, photodehydrogenation catalyst ("Platinum Pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

References

1. J. E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.
2. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.
5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. B.D. Guptha, A. J Elias, Basic Organometallic Chemistry, Universities Press, 2010.
7. G.L. Miessler, D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007.

Unit 3: Nuclear Chemistry **18 hrs**

3.1 Radioactive decay. Alpha decay-Alpha ray spectrum, Beta decay-Types of beta decay, β^+, β^-, β-ray spectrum, neutrino antineutrino and Positron emission, Dirac theory, pair production, positron-electron annihilation, electron capture, double β decay. Gamma decay- de-excitation of excited molecules, change of Energy, spin, parity during photon emission, nuclear isomerism and isomeric transition, internal conversion, auger electrons and auger effect.

3.2 Nuclear reactions**.**
Q-Value and reaction threshold, reaction cross section-definition, and units , cross section and reaction rate, neutron capture cross section, variation of neutron cross section with energy(1/V law). Photonuclear, Thermonuclear and Fusion reactions, Magnetic confinement, internal confinement.
Nuclear fission - Fission fragment and mass distribution, fission yield, fission energy, fission cross section and threshold, fission neutrons, prompt and delayed neutrons, fission by high energy neutrons.

3.3 Nuclear Reactors.
Fissile and fissionable nuclei, fast and thermal neutrons, Terms and symbols used in reactor technology- average no. of fission neutrons, fast fission factor, fast neutrons loss factor, resonance capture, thermal neutrons loss factor, thermal utilization factor, relative fission cross section, reproduction factor, critical size of reactor. Breeder reactor, fast breeder test reactor.

3.4 Reactor Safety precaution, Management of radioactive waste- Low level Waste, Intermediate level Waste, High level Waste.

3.5 Principles of counting techniques- G.M. counter, proportional, ionization and scintillation counters.

3.6 Applications of radioisotopes.
Physico-chemical study-Solubility of sparingly soluble salts. Analytical applications-Isotope dilution analysis, radiometric titrations, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.
Applications of radio isotopes medicine-Thyroiditis, Tumour identification, Determination of volume of blood in patient.

References:

1. G. Friedlander,J.W.Kennedy,E.S.Macias,and J.M. Miller,Nuclear and Radiochemistry, John Wiiley and Sons, 2nd Ed.1981.
2. H.J. Arnikar, Essentials of Nuclear Chemistry, New Age International,4th Edn., 2011.
3. B.R Puri,L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone,2011.
4. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

Unit 4: Bioinorganic Chemistry. 18 Hrs

4.1 Biochemistry of Iron
Oxygen Carriers- Structure and functions of haemoglobin and myoglobin, Oxygen transport mechanism of Hemoglobin, cooperativity in haemoglobin. Hemerythrin Structure and function. Bohr effect and phosphate effect.
Redox Metalloenzymes-Cytochromes, Classification, Structure and function, Role in oxidative Phosphorylation of ADP to ATP.
Iron Sulphur Proteins-Rubredoxin, Ferredoxin, Nitrogenase,Structure and function, Nitrogen Fixation. Peroxidases and catalases, Cytochrome P_{450}- Structure and functions.
Storage and transport of iron in biological systems-Ferritin, transferrin and Siderophores.

4.2 Biochemistry of Zn and Copper.
Structure and functions of carboxypeptidase and carbonicanhydrase, Superoxide dismutase.
Structure and functions of various Copper proteins and enzymes.
Blue copper proteins (Type-1) - Electron transfer agents - Plastocyanin, Stellacyanin and Azurin.
Blue copper Enzymes (Type II) - Ascorbateoxidase, Laccase and ceruloplsmin.
Non Blue copper enzyme (Type III) - Cytochrome oxidase, Amine oxidases, Structure and functions of Hemocyanin.

4.3 Other Important metal containing Biomolecules.
Vitamin B_{12}- Structure and biological importance. Chlorophyll-Photosynthesis, PS I & PS II.

4.4 Metals in medicine - Therapeutic applications of *cis*-platin, Mechanism of action, MRI agents, Mechanism of muscle contraction, blood clotting mechanism.

4.5 Essential and trace elements in biological systems, Toxic effects of metals (Cd, Hg, Cr and Pb). Mechanism of ion transport across membranes, Sodium Potassium pump.

References.

1. G. Wulfberg, Inorganic Chemistry, Ind. Edition, Viva, 2014.
2. Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Cengage Learning 2nd Edn., 2014.
4. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
5. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th

edition, Wiley-Interscience, 1999.
6. G.L. Miessler, D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007.
7. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
8. I. Bertini,H. B Gray, S. J Lippard, J. S Valentine, Bioinorganic Chemistry.

16P1CHET02 BASIC ORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Basic Concepts in Organic Chemistry (12 Hrs)

1.1 IUPAC nomenclature of polycyclic, heterocyclic, benzenoid, non-benzenoid and spiro compounds.
1.2 Review of basic concepts in organic chemistry: Electron displacement effects-inductive effect, electrometric effect, resonance effect, hyperconjugation, steric effect. Steric inhibition of resonance.
1.3 Bonding weaker than covalent bonding- H-bonding, π- π interactions, Other non-covalent interactions
1.4 Concept of aromaticity: delocalization of electrons –Huckel's and Craig rule- criteria for aromaticity -examples of neutral and charged aromatic systems, annulenes[10],[14],[18],[22], Tropolone, Azulene. NMR as a tool for aromaticity. Anti- and homo-aromatic systems– Alternate and non-alternate hydrocarbons, Fullerenes, Carbon nanotubes and Graphene.

Unit 2: Physical Organic Chemistry (11 Hrs)

2.1 Energy profiles. Hammond postulate, Kinetic versus thermodynamic control of product formation, Captodative effect –- kinetic isotope effects with examples - Stereochemical studies- use of isotopesHammet equation, Taft equation, cross-over experiments, Hammond postulates.
2.2 Salt and Solvent effect. Intermediates *vs*. Transition state, linear free energy relationship.
2.3 Introduction to carbon acids - pK_a of weak acids - Kinetic and thermodynamic acidity.
2.4 Introduction to organic bases- pK_b of weak bases.

Unit 3: Review of basic reaction mechanisms (8 Hrs)

3.1 Mechanism of SN1, SNAr, SRN1 and Benzyne mechanisms.
3.2 Catalysis by acids and bases and nucleophiles with examples from acetal, cyanohydrin and ester formation and hydrolysis reactions –A_{AC}^2, A_{AC}^1, A_{AL}^1, B_{AC}^2 and B_{AL}^1 mechanisms.

Unit 4: Stereochemistry of Organic Compounds (15Hrs)

4.1 Introduction to molecular symmetry and chirality – examples from common objects to molecules – axis, plane, centre, alternating axis of symmetry.

4.2 Centre of chirality – molecules with C, N, S based chiral centres – absolute configuration - enantiomers – racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules – molecules with a chiral centre and Cn – molecules with more than one center of chirality – definition of diastereoisomers – constitutionally symmetrical and unsymmetrical chiral molecules - erythro, threo nomenclature.

4.3 Axial, planar and helical chirality – examples – stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spirans, exo-cyclic alkylidenecycloalkenes.

4.4 Identification of enantiotopic, homotopic, diastereotopic hydrogens, prochirality, Topicity and prostereoisomerism – topicity of ligands and faces, and their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.Stereospecific, stereoselective and assymetric synthesis.

4.5 Geometrical isomerism: Nomenclature - E-Z notation - methods of determination of geometrical isomers. Geometrical isomerism of oximes-Interconversion of geometrical isomers.

Unit 5: Conformational Analysis (20Hrs)

5.1 Stereoisomerism: Definition based on symmetry and energy criteria – configuration and conformational stereoisomers.

5.2 Conformational descriptors - factors affecting conformational stability of molecules. potential energy diagrams

5.3 Conformational analysis of acyclic systems: substituted ethanes, aldehydes, ketones and olefins.

5.4 Conformational analysis of cyclic systems -Cyclohexane and its derivatives. Cyclohexanone.

5.5 Conformational analysis of Fused and bridged bicyclic systems.-decalins, adamantane hexamethylene diamine and congressane,

5.6 Conformation of sugars-glucose, sucrose and lactose

5.7 Conformation and reactivity of elimination -dehalogenation, dehydrohalogenation, dehydration, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations, substitution and oxidation of 2^0 alcohols.

5.8 Chemical consequence of conformational equilibrium - Curtin-Hammett principle.

Unit 6: Organic Photochemistry (6Hrs)

6.1 Jablonski diagram, triplet and singlet states.

6.2 Photoreactions of carbonyl compounds: Norrish reactions of acyclic and cyclic ketones. Patterno-Buchi reaction. Barton, Di-π-methane and photo reduction of ketones.

6.3 Photochemistry of Nitro and Azo groups.

6.4 Photochemistry of vision

References

1. D. Hellwinkel, Systematic nomenclature of organic chemistry, Springer international edition

2. R. Bruckner, *Advanced Organic Chemistry*: Reaction Mechanisms, Academic Press, 2002.

3. F. A. Carey and R. A. Sundberg, *Advanced Organic Chemistry*, Part A: Structure and Mechanisms, Fifth Edition, Springer, New York, 2007.

4. J.Clayden, N.Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.

5. Aditi Sangal, *Krishna's Advanced Organic Chemistry*; Volume 1 – Krishna Prakashn Media(P) Ltd.
6. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Second Edition, Harper & Row, New York, 1981.
7. N. S. Isaacs, *Physical Organic Chemistry*, ELBS, Longman, UK, 1987.
8. Jack Hine,*Physical Organic Chemistry*, McGraw-Hill; 2nd Edition,1962.
9. Anslyn, E. V.; Dougherty, D. A. *Modern Physical Organic Chemistry*, University Science Books, 2006
10. D. Nasipuri,*Stereochemistry of Organic Compounds: Principles and Applications*, Third Edition, New Age Publications, New Delhi, 2010.
11. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
12. N. J. Turro, V. Ramamurthy and J. C. Scaiano, *Principles of Molecular Photochemistry: An Introduction*, University Science books 2009.
13. N.J Turro, *Modern Molecular Photochemistry*, Benjamin Cummings Publishing Company, Menlopark, 1978.
14. K.K.R.Mukherjee, *Fundamentals of Photochemistry*, New Age Publications, New Delhi, 1978.

16P1CHET03 PHYSICAL CHEMISTRY I

Credit: 3 **Contact Lecture Hours: 54**

Unit 1: Classical Thermodynamics -Fundamentals **(9Hrs)**

1.1 Introduction: Entropy- Free energy-Systems of Variable Compositions - Fugacity and Activity-Clausius Inequality, Maxwell's relations – significance, Partial molar properties – Chemical potential, Fugacity and Activity.

1.2 Thermodynamics of mixing: Thermodynamic functions of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume.

1.3 Chemical Equilibrium: Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff equations.

1.4 Third law of thermodynamics: Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions.

1.5 Three component systems: Gibbs phase rule, graphical representation of three component systems. Solid-liquid equilibria, ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

Unit 2: Thermodynamics of Irreversible Processes &Bioenergetics **(10hrs)**

2.1 Thermodynamics of Irreversible Processes: Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The Onsager reciprocal relations - principle of microscopic reversibility. Electrokinetic phenomena. Thermoelectric phenomena.

2.2 Bioenergetics: Coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Unit 3: Statistical Thermodynamics **(27 Hrs)**

Permutation, probability, apriori and thermodynamic probability, Stirlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength. Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, super cooled liquids. Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.

Heat capacity of solids- the vibrational properties of solids, Einstein's theory and its limitations, Debye theory and its limitations.

Unit 4: Gaseous State (8 Hrs)

Derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, effusion, the rate of effusion, transport properties of gases-viscosity, thermal conductivity and diffusion.

References

1. R.P. Rastogi, R.R. Misra, An introduction to Chemical Thermodynamics, Vikas publishing house, 2009.
2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.
3. M.C. Gupta, Statistical Thermodynamics, New age international, 2007.
4. M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.
5. P.W. Atkins, Physical Chemistry, ELBS, 1994.
6. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4thEdn. Houghton Mifflin, 2003.
7. L.K. Nash, Elements of Classical and Statistical Mechanics, 2ndEdn., Addison Wesley, 1972.
8. D.A. McQuarrie, J.D. Simon, Physiacl Chemistry: A Molecular Approach, University Science Books,1997
9. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.
10. R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill,1999.
11. I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall, 2002.
12. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.
13. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971

16P1CHET04 QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 3 **Contact Lecture Hours: 72**

Unit 1: Postulates of Quantum Mechanics (9 Hrs)

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, Laplacian operator, commuting and non commuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator. Eigen value postulate: eigen value equation, eigen functions of commuting operators. Expectation value postulate. Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

Unit 2: Application to Exactly Solvable Model Problems (18 Hrs)

Translational motion: free particle in one-dimension, particle in a one dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box separation of variables, degeneracy.

Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.

Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators Lz and L2. Ladder operator method for angular momentum. Space quantization.

Unit 3: Quantum Mechanics of Hydrogen-like Atoms (9 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Unit 4 : Group Theory and Molecular Symmetry (18 Hrs)

Symmetry elements, symmetry operations, point groups and their symbols, subgroups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.

Matrices: addition and multiplication of matrices, inverse and orthogonalmatrices, character of a matrix, block diagonalisation, matrix representation ofsymmetry operations, representation of groups by matrices, construction ofrepresentation using vectors and atomic orbitals as basis.

Reducible and irreducible representations-construction of irreduciblerepresentation by standard reduction formula. Statement of Great OrthogonalityTheorem (GOT). Properties of irreducible representations. Construction ofirreducible representation using GOT-construction of character tables for C2v,C2h, C3, C3v and C4v. Direct product of representations.

Unit 5 Application of group theory in Spectroscopy and Chemical bonding (18 Hrs)

Applications in vibrational spectra: transition moment integral, vanishing ofintegrals, symmetry aspects of molecular vibrations, vibrations of polyatomicmolecules-selection rules for vibrational absorption. Determination of thesymmetry of normal modes of H2O, C_2H_4,Trans N_2F_2,$CHCl_3$and NH_3 using Cartesiancoordinates and internal coordinates. Complementary character of IR and Raman spectra-determination of the IR and Raman active vibrational modes.

Application in electronic spectra: selection rules for electronic transition,electronic transitions due to the carbonyl chromophore in formaldehyde.

Applications in chemical bonding, construction of hybrid orbitals with H_2O, NH_3, BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC).

MO diagram for water and ammonia.

Reference

For Units 1,2&3
1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition*, Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press, 2005.
5. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.
6. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books, 2003).
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.

For Units 4& 5
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.
4. R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.
5. P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., New York, 1998.
6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood 1998.
7. A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry,* PHI Learning Pvt. Ltd. 2010.
8. Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer Academic Publishers,2004.
9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.
10.A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.
11. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.
12. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.
13. S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn**.,** Wiley, 2007.
14. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.

SEMESTER 2

16P2CHET05 INORGANIC CHEMISTRY II

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Structural Aspects and Bonding (18 Hrs)

1.1 Sigma and pi bonding ligands such as CO, NO, CN^-, R_3P, and Ar_3P Macrocycles-crown ethers, cryptands, macrocyclic effect, applications of crown ethers, template synthesis, Inverse crown ether complexes.

1.2 Classification of complexes based on coordination numbers and possible geometries. Stability of complexes, thermodynamic aspects of complex formation, chelate effect, Determination of stability constant.Irving William order of stability.

1.3 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields, CFSE, Jahn Teller (JT) effect, theoretical failure of crystal field theory,

1.4 Molecular orbital theory-Evidence of covalency in the metal-ligand bond, nephelauxetic effect, M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

2.1 Electronic Spectra of complexes-Term symbols of d^n and f^n system, splitting of terms, *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and *β* (Nephelauxetic ratio) values, Racah parameters,

Charge transfer spectra, luminescence spectra, Intra Valence charge transfer transition Prussian blue.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Anomalous magnetic moments,quenching of magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Antiferromagnetism-inter and intra molecular interaction. Application of magnetic moment measurement in structural elucidation of complexes.(Co and Ni complexes)

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, Factors affecting the reactivity of square planar complexes of Pt(II) and other d^8 metal ions, *trans* effect-theory and applications.

3.2 Kinetics and mechanism of octahedral substitution- water exchange reactions, Dissociative and associative mechanisms, hydrolysis under acidic conditions, rate and stereochemistryof aquation of cis and trans isomers of Co(III) complexes, base hydrolysis – conjugate base mechanism, base hydrolysis of different isomers of $[Co(tren)(NH_3)Cl]^{2+}$,racemization reactions.

3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism. Nature of bridging ligand.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,

4.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism.
Symbiosis-hard and soft ligands

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)

5.1 General characteristics of lanthanides-Electronic configuration, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents. Separation of Lanthanides.

5.2 General characteristics of actinides-difference between *4f* and *5f* orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008.
9. G.L. Miessler,D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007.

16P2CHET06 ORGANIC REACTION MECHANISM

Credit : 4 **Contact Lecture Hours:72**

Unit1: Review of substitution reaction Mechanisms (11Hrs.)

1.1 A comprehensive study on the effect of substrate, reagent, leaving group, solvent, ambident nucleophile and neighbouring group on nucleophilic substitution(SN_1 and SN_2) and elimination (E_1, E_2andE_{1CB}) reactions. Stereochemistry of E_2 reaction, Intramolecular pyrolytic elimination, Cope elimination. Elimination *vs* substitution.

1.2 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN^i, SE_1, SE_2 and SE^i). Substitution at the aromatic centre, unimolecular mechanism, bimolecular mechanism. Kinetics of SE_2-Ar reaction. Ortho-para selectivity ratio.

1.3 Electrophilic substitution via enolization and stork-enamine reaction. Benzyne mechanism. Von Ritcher, Vilsmeyer formylation, Jacobson and Gatterman-Koch reactions.

Unit2: Chemistry of Carbanions (10Hrs.)

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates-lithium and boron enolates in aldol Alkylation and acylation of enolates.

2.2 Electrophilic additions to alkenes, kinetics, effect of structure, orientation and stereochemistry. Ozonolysis and hydroboration.Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry –Mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 Ylids: Chemistry of Phosphorous and Sulphur ylids - Wittig and related reactions, Peterson olefination.

Unit3: Chemistry of Carbocations (9Hrs.)

3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: Oxymercuration, halolactonisation.

3.4 Structure and reactions of α, β- unsaturated carbonyl compounds - electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.

Unit4: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

4.1 Structure of carbenes (singlet and triplet) - generation of carbenes - addition and insertion reactions.

4.2 Rearrangement reactions of carbenes such as Wolff rearrangement - generation and reactions of ylids by carbenoid decomposition.

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann,Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: Generation, structure, stability and reactions. Orientation effect- amination of haloarenes.

Unit5: Radical Reactions (9Hrs)

5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements – Hydroperoxide: formation, rearrangement and reactions. Auto-oxidation.

5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Concerted reactions: (24Hrs)

7.1 Classification: Electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method.

7.2 Pericyclic reactions in organic synthesis such as Claisen,Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition (introductory).

7.3 Pyrolytic elimination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

7.4 Introduction to Click reactions -Mechanism of the Huisgen Azide-Alkyne 1, 3-Dipolar Cycloaddition, Staudinger ligation and Staudinger reduction.

References

1. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press,2002.
2. F. A. Carey, R. A. Sundberg,*Advanced Organic Chemistry*, Part B: Reactions and Synthesis, 5thEdn.,, Springer, New York, 2007.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition, Cambridge University Press, 2005.
4. J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6thEdn., Wiley, 2007.
5. http://www.organic-chemistry.org/namedreactions.
6. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011.
7. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.
8. Fleming, Wiley, *Frontier Orbitals and Organic Chemical Reactions*, London, 1976.
9. S. Sankararaman, *Pericyclic Reactions-A Text Book*, Wiley VCH, 2005.

16P2CHET07 PHYSICAL CHEMISTRY II

Credits 3 **Contact Lecture Hours 54**

Unit 1 Microwave, Infrared and Raman Spectroscopy (14hours)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), and relaxation time.

1.2 Microwave spectroscopy: Classification of molecules; rigid rotor model; rotational spectra of diatomics and polyatomics; effect of isotopic substitution and nonrigidity; selection rules and intensity distribution.

1.3 Vibrational spectroscopy: Vibrational spectra of diatomics; effect of anharmonicity; Morse potential; Vibration-rotational spectra of diatomics, polyatomic molecules-P,Q,R branches, normal modes of vibration, overtones, hot bands drawbacks of dispersive IR, FTIR

1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence. Principle of SERS, selection rules, application. Comparison of IR and Raman.

Unit 2 Electron & Electronic Spectroscopy & Lasers (13hours)

2.1 Electron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, selection rules-Electron spectroscopy for chemical analysis (ESCA)-UPS, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES).

2.2Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-Condon principle, Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.

2.3 Lasers: Laser action, population inversion, properties of laser radiation, two stage, three stage-examples of simple laser systems.

Unit 3: Resonance Spectroscopy (27 Hrs.)

3.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship. FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, ^{19}F, ^{31}P, NMR spectroscopy.

3.2 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation. An elementary study of NQR spectroscopy.

3.3 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to the structural elucidation of metal complexes

References

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
3. P.W. Atkins, Physical Chemistry, ELBS,1994
4. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.
5. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
6. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2ndEdn. CBS, 1999.
7. W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986.
8. H. Kaur, Spectroscopy, 6thEdn. Pragati Prakashan, 2011.
9. H. Gunther, NMR Spectroscopy, Wiley, 1995.
10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.
12. D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007.
13. D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, 2009.
14. J. D. Graybeat. Molecular Spectroscopy, McGraw-Hill International Edition, 1988

16P2CHET08 Theoretical and Computational Chemistry

Credit: 3 **Contact Lecture Hours: 72**

Unit 1: Approximate Methods in Quantum Mechanics (21 Hrs)

Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

Perturbation method, time-independent perturbation method (non-degenerate caseonly), first order correction to energy and wave function, illustration byapplication to particle in a 1D-box with slanted bottom, perturbation treatment ofthe ground state of the helium atom.

Hartree-Fock method. Multi-electron atoms. The antisymmetry principle and the Slater determinant. Hartree-Fock equations (no derivation). The Fock operator. Core Hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Electron correlation energy. The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations.

Unit 2: Chemical Bonding (21 Hrs)

Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H2 molecule, singlet and triplet state functions (spin orbitals) of H2.

Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, $O_2$and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel MolecularOrbital (HMO) theory of ethene, allyl systems, butadiene and benzene.Calculation of charge distributions, bond orders and free valency.

Froniter Molecular Orbitals- Woodward-Hoffmann rule-Introduction to global and local reactivity descriptors-electrophilicity index

Unit 3: Computational Quantum Chemistry (18 hrs)

Introduction and scope of computational chemistry. Potential energy surface - Conformational search - Global minimum, Local minima, saddle points. Conformational analysis of ethane and butane.

Ab initio methods: A review of Hartee-Fock method. Self Consistent Field Procedure. Roothan concept basis functions. Basis sets, Slater type and Gaussian type basis sets, Minimal basis set. Pople style basis sets - Classification - double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Hartree-Fock limit. Post Hartree-Fock methods.Introduction to Møller Plesset Perturbation Theory, Configuration Interaction, Coupled Cluster and semi empirical methods.

Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohntheorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).
Comparison of ab initio, semi empirical and DFT methods.

Unit 4: Model Chemistry and Molecular Simulations (12 Hrs)

Introduction to computational chemistry software packages. Generating molecular structures Cartesian coordinates, internal coordinates and Z-matrix of simple molecules. Introduction to computational chemistry calculations using simple molecular structures of water, ammonia, methane, butane, benzene. Input file format - Method, Basis Set, Calculation type, Spin Multiplicity, Coordinate format. Single Point Energy, Geometry Optimization, Frequency Analysis.

Computational Chemistry using Statistical mechanics, Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions. Commonly used force fields AMBER and CHARMM. Molecular dynamics simulations. Introduction to simulation softwares. Protein data bank (PDB) and Protein structure file (PSF) formats. Practical aspects of computer simulation. Analyzing the results of a simulation.

Reference

For **Unit 1 & 2**

1. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

2. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
3. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
4. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd., 1998.
5. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill, 1968.
6. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
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. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.

12. Density functional theory of atoms and molecules, R G Parr and W Yang;
13. Chemical hardness: Applications from Molecules to Solids, R G Pearson.

For Unit 3 & 4

1. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
2. F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.
3. Michael Springborg, Methods of Electronic-Structure Calculations: From Molecules to Solids John Wiley & Sons, 2000.
4. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000
5. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.
6. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.
7. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
8. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*,
9. Gaussian Inc., 2000.
10. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.
11. D. Rogers *Computational Chemistry Using the PC, 3rd Edition*, John Wiley & Sons (2003).
12. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.
13. J. M. Haile (2001) *Molecular Dynamics Simulation: Elementary Methods*.
14. Stote, R. H., Dejaegere, A. and Karplus, M. (1997). Molecular Mechanics and Dynamics Simulations of Enzymes. Computational Approaches to Biochemical Reactivity. Netherlands, Kluwer Academic Publishers.

   (For pdb,psf file formats and molecular dynamics simulations)
15. http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win.pdf
16. http://www.ks.uiuc.edu/Training/Tutorials/vmd/vmd-tutorial.pdf

17. List of some Free and Commercial Computational Chemistry Softwares
   Drawing & Visualization
   Chem Draw, Avagadro, Discovery Studio Client, Gabedit, Open Babel, Gauss view, Pymol, VMD
   Quantum Chemistry Softwares
   Firefly, Gamess, Spartan, Molpro, Gaussian, Dmol3, Turbomole
   Molecular Mechanics and Dynamics Softwares
   NAMD, Tinker, DL-POLY, CHARMM, AMBER

SEMESTERS 1 AND 2

16P2CHEP01 INORGANIC CHEMISTRY PRACTICAL-1

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.
(a) Tris (thiourea)copper(I) complex
(b) Potassium tris (oxalate) aluminate (III).
(c) Hexammine cobalt (III) chloride.
(d) Tetrammine copper (II) sulphate.
(e) Schiff base complexes of various divalent metal ions.

PART IV

Chromatography
Separation, Identification and determination of Rf values of
a) Pb, Hg, Cu, Cd ions using paper chromatography
b) Fe, Al, Cr ions using paper chromatography
c) Ni, Mn, Co and Zn ions using TLC

References

01. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
02. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
03. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic analysis, 3rd Edn., McMillian, 1968.
04. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

16P2CHEP02 ORGANIC CHEMISTRY PRACTICAL- 1

CREDIT: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction.
2. Soxhlet extraction of a natural product from its source.
3. Fractional crystallization.
4. TLC and Paper Chromatography
5. Column Chromatography.

PART II

1. Separation of Organic binary mixtures by chemical/physical separation methods.
2. Purification of organic compounds by column chromatography.
3. Record the IR spectrum of simple organic compounds and Identification of the functional groups.

PART III

Drawing the structures of organic molecules and reaction schemes by Chemsketch.

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

References

1. A.I.Vogel, *A Textbook of Practical Organic Chemistry, Longman*, 1989.
2. A.I.Vogel, *Elementary Practical Organic Chemistry*, Longman, 1957.
3. F.G.Mann and B.C Saunders, *Practical Organic Chemistry*, 2009.
4. J. R.Johnson, J.F.Wilcox, *Laboratory Experiments in Organic Chemistry*, Macmillan, 1979.

16P2CHEP03 PHYSICAL CHEMISTRY PRACTICAL-I

Credit: 3 Contact Lab Hours: 72+72 =144

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.

2. Effect of (KCl/succinic acid) on miscibility temperature.

3. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.

2. Distribution coefficient of benzoic acid between benzene and water.

3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by

a) Drop number method

b) Drop weight method

2. Determination of the composition of two liquids by surface tension measurements

3. To determine the critical Micelle concentration of sodium lauryl sulphate

4. Determine the surface excess of amyl alcohol.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.

03. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005

04. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency,2012

05. Practical Physical Chemistry Paperback, 1974 by A.M. James , F.E. Prichard.

Part B

List of Computational Chemistry Experiments

(Second Module of Physical Chemistry Practical -I)

(These experiments are related to the topics in organic chemistry and physical chemistry covered in BSc-MSc Chemistry courses. From the list of experiments we can select the performable experiments depend on the availability of time and suitable computational chemistry software)

1. Geometry optimization and single point energy calculations of simple organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis
5. Calculation of Resonance energy of aromatic compounds
6. Prediction of the stability of ortho, meta, para products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
8. Calculation of dimerization energy of carboxylic acids
9. Perform the conformational analysis of butane using potential energy scan
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.

12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.

13. Spectral analysis (UV, IR and NMR) of simple organic molecules.

14. Perform molecular dynamic simulations of smaller molecules in water.

15. Calculation of pK_a of simple organic molecules and compare it with experimental values

16. Docking studies involving protein ligand interactions.

17. Calculation of electrophilicity index in hard-soft acids and bases.

Reference

1. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.

2. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

3. D. Rogers *Computational Chemistry Using the PC, 3rd Edition*, John Wiley & Sons (2003).

4. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, 2001.

5.J. M. Haile (2001) *Molecular Dynamics Simulation: Elementary Methods*.

SEMESTER 3

16P3CHET09 INORGANIC CHEMISTRY-III

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Solid State Chemistry (18 Hrs)

1.1 Close Packing. Imperfections in solids-point defects, Stoichiometric and non-stoichiometric defects, Non stoichiometric defects in the monoxides of 3d series, Vegard's rule. Line defects and plane defects.

1.2 Structure of solids:. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), ABX_3 (Perosvskite, Ilmenite). Spinels. Inverse spinel structures.

1.3 Diffusion in solids. Mechanisms- vacancy diffusion, Interstitial diffusion, Interstitialcy diffusion, Ring mechanism. Diffusion equation- Coefficient of diffusion atomic approach.

1.4 Solid state reactions-Factors affecting the rate of solid state reactions- Reaction condition, Structural factor, Nucleation and growth, Surface area of solids, Surface structure and reactivity, Wagner reaction mechanism, Kirkendall effect, Nucleation and reactivity, Topotactic and epitactic reaction.

1.5 Synthesis of solids- Direct reactions (Shake n bake method) Examples $L_{i4}Si_{O4}$,$YB_{a2}C_{u3O7}$ and Na β/β'', Sol-gel method, (Synthesis of Silica glass,Indium tin oxide, Zeolites),Intercalation and deintercalation, Vapour phase transport, and Chemical vapour deposition.

1.6 Phase transition in solids- Buerger's Classification of phase transitions, Reconstructive and Displacive Transitions. Thermodynamic Classification-first and second order phase transitions (Brief study only).Nucleation, growth and critical size in phase transition. Order-disorder transitions and Martensitic transformations.

1.7 Crystal Growth. Growth of Single crystal. Various Techniques-Crystal growth from melt-Czohralski method, Bridgman and Stockbarger method, Zone melting. Crystallization from solution-Hydro thermal method, gel method. Crystal growth from Vapour- Chemical Vapour Deposition.

1.8 Solid Electrolytes- Solid cationic electrolytes, Solid anionic electrolytes, Mixed ionic electronic conductors.

1.9 Solid solution-Substitutional Solid Solution, Requirments for formation,Interstitial Solid Solution, Metal alloys,Engel-Brewer rule, Intermetallic compounds, Hume-Rothery Compounds, Zintal Phase.

Unit 2: Electrical, Magnetic and Optical Properties of Solids. (18 Hrs)

2.1 Classical free electron theory of metals(Lorentz-Drude theory)-Drift velocity-current density J-mobility of charge carriers-conductivity-advantages and disadvantages of classical free electron theory-Quantum free electron theory(Sommerfield)-Fermilevel and calculation of Fermi energy-Density of states-Calculation of average energy of free electrons-specific heat in quantum free electron theory-Lorenz number in Quantum free electron theory

2.2 Zone theory of solids (Quantum mechanical approach)-Kronig-Penney model-K space-Wigner Seitz cell- K space- Brillouin Zone-Extended Zone scheme- MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors.

2.3 Hall Effect- Significance of Hall coefficient-Pyroelectricity- Piezo electricity -ferro electricity

2.4 Metal oxides- Structure and properties.

Electronic and Magnetic properties of monoxides of elements in 3d series. Higher oxide and complex oxides of Transition elements-Oxides with M_2O_3 Corundum structure, Rhenium trioxide and related oxides. Conductivity in mixed oxides, Isomorphous Substitution, Principles and applications. Spinels and inverse spinels, LFSE and spinel structure.

Cooperative magnetism-Ferromagnetic materials, Curie temperature, Anti ferromagnetism, Neel temperature, Super exchange, Ferrimagnetisms.

Perovskite and related Phases. Perovskite structure

Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties.TiO_2 as Photocatalyst.

2.5 Super conductivity-Type I and Type II superconductors- Meisner effect and its applications Cooper pairs- theory of low temperature super conductors, BCS theory of superconductivity (derivation not required)-Josephson Tunneling- Super conducting cuprates – Preparation, properties and application of-YBaCu oxide system -, Meisner effect and its applications- conventional superconductors , high temperature superconductors.

Unit 3: Inorganic Chains, Rings and Cages **(24Hrs)**

3.1 Chains - catenation, heterocatenation. Silicate minerals. Structure of silicates- common silicates, silicates containing discrete anions, silicates containing infinite chains, silicatescontaining sheets, framework silicates. Silicones. Zeolites-synthesis, structure and applications.Isopoly acids of vanadium, molybdenum and tungsten.Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Polythiazyl – one dimensional conductor.

3.2 Rings-topological approach to boron hydrides, Styx numbers. Synthesis, structure and bonding in borazines, ring silicates and silicones, Sunthesis, structure and bonding ofphosphazenes. Heterocyclic inorganic ring systems- Synthesis, structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems- synthesis, structure and bonding in sulphur, selenium and phosphorous compounds.

3.3 Cages: synthesis, structure and bonding of cage like structures of phosphorous – phosphorous-oxygen compounds. Boron cage compounds-Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes.

Unit 4: Metal clusters: **(5 Hrs)**

4.1 Halide Clusters: Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Unit 5: Chemistry of Materials **(7 Hrs)**

5.1 Glasses-glassy state, glass formers, glass modifiers. Ceramics-ceramic structures- mechanical properties. refractories-characterisations, properties and applications

5.2 One dimensional Solids. Magnetic, Electrical and optical properties of the following Solids. KCP and other Pt compounds,$Hg_{3-x}AsF_6$, $[(CH_3)_4N]MnCl_6$,$KCuF_3$,and,RbF_3.

Reference:

1. Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press,2006.
2. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.
3. G.L. Miessler,D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007. Further Reading.
4. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
5. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
6. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
7. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
8. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
9. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
10. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
11. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.
12. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
13. P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.
14. C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.
15. W.L Jolly, Modern Inorganic Chemistry, 2nd Edn. Tata McGraw Hill,2007.
16. C. N. R. Rao and J. Gopalakrishnan, New directions in Solid state Chemistry, 2nd Edition, Cambridge University Press1997.

16P3CHET10 ORGANIC SYNTHESES

Credit : 4 **Contact Lecture Hours: 72 Hrs.**

Unit1: Organic Synthesis via Oxidation and Reduction (18 Hrs)

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium and DMSObased reagents). (b) alkenes to epoxides (peroxides/per acids based)- Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(c) alkenes to diols (Manganese and Osmium based)- Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage- hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger.

1.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson).(b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, Selectrides,trialkylsilanes and trialkylstannane, Meerwein-Pondorff-Verleyreducxtion, Baker's yeast.

Unit2: Modern Synthetic Methods and Reagents (15Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction, Noyori reaction. Brook rearrangement,Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi and Sonogashira reactions, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions.Wohl-Ziegler reaction. Mitsunobu reaction, Michael additionand Reformatsky reactions

2.2 Reagents such as: NBS, DDQ, DCC. Gilmann reagent.

Unit3: Construction of Carbocyclic and Heterocyclic Ring Systems (12Hrs)

3.1 The synthesis of four, five and six-membered rings- ketene cycloaddition (inter- and intramolecular)- Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, radical cyclization, Robinson annulation.

3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction,. Construction of macrocyclic rings - ring closing metathesis.

3.3 Formation of heterocyclic rings: Preparation and structure of the following heterocyclics- azeridine, oxirane, thirane, oxaziridine, azetidine and thietane, 5-membered ring heterocyclic compounds with one or more than 1 hetero atom like N, S or O- Pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Unit4: Protecting Group Chemistry (9Hrs)

4.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo- and regioselective protection and deprotection. Illustration of protection and deprotection in synthesis.

4.2 Protection and deprotection in peptide synthesis: Common protecting groups used in peptide synthesis- Protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

4.3 Role of trialkyl silyl group in organic synthesis.

Unit5: Retrosynthetic Analysis (9Hrs)

5.1 Basic principles and terminology of retrosynthesis:synthesis of aromatic compounds- one group and two group C-X disconnections - one group C-C and two group C-C disconnections.

5.2 Amine and alkene synthesis: important strategies of retrosynthesis - functional group transposition - important functional group interconversions. Enantioselective synthesis of Corey lactone, longifolene and luciferin. Umpolung equivalence - Peterson olefination - enolate formation - Ireland method.

Unit6: Molecular Recognition and Supramolecular Chemistry (9Hrs.)

6.1 Concept of molecular recognition- host-guest complex formation- Forces involved in molecular recognition.
6.2 Molecular receptors: Cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes.
6.3 Importance of molecular recognition in nucleic acids and protein.
6.4 Applications of supramolecular complexes in medicine- targeted drug delivery.

References

1. M. B. Smith, *Organic Synthesis,*3rdEdition, WavefunctionsInc, 2011.
2. F.A. Cary and R. I. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5th Edition, Springer, 2009.
3. S. Warren, *Organic Synthesis, The disconnection Approach*, John Wiley & Sons, 2004.
4. V.K.Ahluwalia, *Oxidation in Organic Synthesis*, Ane Books, New Delhi, 2012.
5. Ojima, Catalytic *Asymmetric Synthesis*, 2nd edition, Wiley−VCH, New York, 2000.
6. W. Carruthers and I Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 2005.
7. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
8. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.
9. L. Kuerti, B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press, 2005.
10. Solomons, T. W. G., *Organic Chemistry*, 6th ed, 1996.
11. R.O.C Norman, J.M.Coxon, *Principles of Organic Synthesis*, ELBS and Chapmann and Hall, London, 1995.
12. V.K. Ahluwalia, L.S. Kumar, S. Kumar, *Chemistry of Natural Products*, Ane Books, New Delhi, 2009.
13. Joule, J.A. and Mills, K. *Heterocyclic Chemistry*,Fifth Edition, Wiley, 2010.
14. J.M.Lehn, *Supramolecular Chemistry*: Concepts and Perspectives, VCH, 1995.
15. F.Vogtle, *Supramolecular Chemistry*:An Introduction, John Wiley Sons, 1993.

16P3CHET11 PHYSICAL CHEMISTRY III

Credit 3 **72hrs**

UNIT 1 CHEMICAL KINETICS I(14 hours)

1.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces.Conventional transition state theory-Eyring equation, Comparisonof the two theories. Thermodynamic formulation of the two theories. Thermodynamicformulation of the reaction rates. Significance of ΔG^*, ΔH^* andΔS^*.Volume of activation. Effect of pressure and volume on velocity of gas reactions.**Introduction** to Molecular Reaction Dynamics

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory ,chain reactions,free radical and chain reactions, steady state treatment, kinetics of H_2-Cl_2 and H_2-Br_2 reactions,Rice –Herzfeld mechanism,Branching chains H_2-O_2,Semenov-Hinshelwood mechanism of explosive reactions.

1.3 Kinetics of polymerization: mechanism of step growth, ionic and addition polymerization,kinetics of anionic and cationic polymerization.

1.4 Fast reactions: relaxation,Flow and Shock methods,Flash photolysis.NMR and ESR a methods of studying fast reactions.

UNIT 2: CHEMICAL KINETICS -II (14 Hrs.)

2.1 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

2.2 Homogenous catalysis -Acid-base catalysis: van't Hoff and Arrhenius intermediates for prototropic and protolytic mechanisms with examples specific and general catalysis, Skrabal diagram, Bronsted catalysis law, acidity function.

2.3 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

2.4 Heterogeneous catalysis Mechanisms of: unimolecular and bimolecular surface reactions, Langmuir-Hinshelwood and Langmuir-Rideal mechanism-ARRT of surface reactions-mechanisms of catalyzed reactions like ammonia synthesis, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

UNIT 3. ELECTROCHEMISTRY I (12 hours)

3.1Theories of ions in solution, Ion activity, Ion-ion and ion-solvent interaction, Born's model,Debye-Huckel theory, Ionic atmosphere. The Debye-Huckel-Onsager conductance equation-its derivation and experimental verification- validity of DHO equation for aqueous and non-aqueous solutions. Deviations from DHO conductance equation. Extension of DHO equationto ion solvent interactions, Debye-Huckel Bjerrum model, Ion association, triple ions, triple ions andconductance minima. Ionic strength, Ionic activity coefficients of strong electrolytes- Derivation of Debye-Huckel limiting law.

3.2Conductance measurements, results of conductance measurements, Factors affecting conductance, Debye Falkenhagen and Wein effects, Walden rule, abnormal ionic conductance.

UNIT 4. SURFACE CHEMITRY & COLLOIDS (18hrs)

4.1 Gas adsorption at solid surface - influencing factors - bonding of adsorbate to solid – adsorption isotherms - Langmuir (derivation), BET (derivation) - determination of surface area.

4.2 Spectroscopic techniques for probing solid surfaces – Temperature programmed desorption (TPD), Reflection absorption infrared spectroscopy (RAIRS) High resolution electron energy loss spectroscopy (HREELS).

4.3 Surface films - film pressure - criteria for spreading of one liquid on another – surface pressure-structure of surface films - analogy between surface films and gases.

4.4 Adsorption from solutions - electrostatic adsorption - Gibbs adsorption isotherm (derivation) - verifications.

4.5 Colloids & **Micellar systems**–Types of colloids, electrical properties of colloids, electrical double layer, zeta potential- miscelles, and miscellisation - structure of miscelles - ionic miscelles.

4.6Electro kinetic effects - electrophoresis, electro osmosis, streaming potential, sedimentation potential – Donnan membrane equilibrium.

UNIT 5. PHOTOCHEMISTRY (14 Hours)

5.1Laws of Photochemistry: Grothus –Draper Law, Stark-Einstein's Law, Laws of light absorption, Quantum yield. Chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermo luminescence, pulse radiolysis, hydrated electrons, photo stationary state, dimerization of anthracene.

5.2Photo physical processes in electronically excited molecules, Jablonsky diagram, Fluorescence and Phosphorescence. Quenching of fluorescence and its kinetics, Stern-Volmer equation, static and dynamic quenching. Concentration quenching, delayed fluorescence, E-type and P-type. Effect of temperature on emissions, two photon absorption spectroscopy,

5.3Photochemistry of environment, greenhouse effect, principle of utilization of solar energy, solar cells and their working. Photochemistry of vision.

References

1. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. K.J. Laidler, Chemical kinetics, 3rdEdn. Harper & Row, 1987.
3. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
4. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
5. P.W. Atkins, Physical Chemistry, ELBS, 1994.
6. D.A. McQuarrie, J.D. Simon, Physiacl chemistry: A Molecular Approach, University Science Books,1997
8. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2ndEdn. New Age International, 1986.
9. G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007.
10. M.R Wright, An Introduction to Chemical Kinetics, John Interscience-2007
11. A.W &Sons, Adamson, A.P. Gast, Physical chemistry of sufaces,6thEdn,John Wiley, 1997
12. D.O. Cowan ,R.L. Drisko , Elements of Organic Photochemistry, Plenum Press,.1976

16P3CHET12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit : 3 **Contact Lecture Hours:54**

Unit1: Ultraviolet-Visible and Chiroptical Spectroscopy (9Hrs)

1.1 Energy levels and selection rules- Woodward-Fieser and Fieser-Kuhn rules.

1.2 Solvent effect- Stereochemical effect-non-conjugated interactions. Applications.

1.3 Chiroptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

1.4 Problems based on the above topics.

Unit2: Infrared Spectroscopy (9Hrs)

2.1 Fundamental vibrations - Characteristic regions of the spectrum (fingerprint and functional group regions).

2.2 Influence of substituents, ringsize, hydrogen bonding, vibrational coupling and field effect on frequency. Determination of stereochemistry by IR technique.

2.3 IR spectra of olefins and arenes, - C=C bonds and C=O bonds.

2.4 Problems-spectral interpretation with examples.

Unit3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 A comparison of the NMR phenomena of ^{1}H and ^{13}C nuclei. Factors affecting chemical shift - relaxation processes, chemical and magnetic non-equivalence - local diamagnetic shielding and magnetic anisotropy. Proton and ^{13}C NMR scales.

3.2 Spin-spin splitting:AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling - First order and non-first order spectra - Pascal's triangle - coupling constant - mechanism of coupling,heteronuclear couplings-Karplus curve - quadrupole broadening and decoupling -diastereomeric protons - virtual coupling - long range coupling-epi, peri, bay effects. NOE - NOE and cross polarization.

3.3 Simplification non-first order spectra: shift reagents-mechanism, spin decoupling-double resonance and off resonance decoupling.

3.4 2D NMR, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion - DEPT, INEPT and RINEPT- sensitivity enhancement and spectral editing- MRI.

3.6 Problems-Spectral interpretation with examples.

Unit4:Mass Spectrometry (9Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CI, MALDI, Electrospray ionization.

4.2 Mass Analysis- Magnetic and electric fields, Quadrupole TOF and ion trap mass analysers.

4.3 Fragmentation patterns in EI MS,- nitrogen andring rules-

4.4 McLafferty rearrangement - applications.

4.5 HRMS, MS-MS, MIKES,CAD, FTMS

4.6 LC-MS, GC-MS.

4.7 Problems-Spectral interpretation with examples.

Unit5: Structural Elucidation Using Spectroscopic Techniques (9Hrs)

5.1 Identification of structures of unknown organic molecules based on the data from IR, ^{1}HNMR and ^{13}CNMR spectroscopy and mass spectroscopy(HRMS data or Molarmass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR NMR and mass spectra.

References

1. D.L. Pavia, G.M. Lampman, G.S.Kriz, *Introduction to Spectroscopy: A Guide for Students of Organic Chemistry* (3rd Ed.), Thomson. 2004.
2. W. Kemp, *Organic Spectroscopy*, 2nd edition, ELBS-Macmillan, 1987.
3. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, Third Edition, New Age Publications, New Delhi, 2010.
4. D.F.Taber, *Organic Spectroscopic Structure Determination: A Problem Based Learning Approach*, Oxford University Press, 2009.
5. R. M. Silverstein, G.C. Bassler, T. C. Morril, *Spectroscopic Identification of Organic Compounds*,John Wiley, 1991.
6. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Tata McGraw Hill, 1988.
7. F. Bernath, Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press, 2005.
8. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, *Molecular Vibrations: The Theory of Infrared and Raman Spectra*, Dover Publications, 1980.
9. Atta-Ur-Rahman, M.I. Choudhary, *Solving Problems with NMR Specroscopy*, Academic Press, New York, 1996.
10. L. D. Field, S.Sternhell, J. R. Kalman, *Organic Structures from Spectra* (fourth edition), Wiley, 2008.
11. Online spectroscopy problems and solutions like www.orgchem.collarado.edu/Spectroscopy/Problems

    www.chem.ucla.edu/webSpectra

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

16P4CHET13EL ADVANCED INORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Applications of Group Theory (22 Hrs)

1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, Hybrid orbitals as linear combinations of atomic orbitals.

1.2 Ligand field theory-splitting of *d* orbitals in different environments using group theoretical considerations.

1.3 M.O. diagrams, formation of symmetry adapted group of ligands,energy levels, construction of energy level diagrams, correlation diagrams, method of descending symmetry,

1.4 *d-d* transition-selection rules, vanishing integrals. Selection rule for IR Transition, IR and Raman spectra of complexes with oxo anions as ligands.

Unit 2: Inorganic Spectroscopic Methods. (9 Hrs)

2.1 Infrared Spectroscopy: Structural elucidation of coordination compounds containing the following molecules/ions as ligands-NH_3, H_2O, CO, NO, OH^-, SO_4^{2-}, CN^-, SCN^-, NO_2^- and X^- (X=halogen).

2.2 Electron Paramagnetic Resonance Spectroscopy: EPR of $d^1$to d^9 transition metal ions in octahedral ligand fields, evaluation of *g* values and metal hyperfine coupling constants.

2.3 Mössbauer Spectroscopy: Applications of Mössbauer spectroscopy in the study of Fe(II) and Fe(III) complexes.

Unit 3: Photochemistry of Co-ordination complexes (9 Hrs)

3.1 Photochemical reactions of Cr(III), Ru(II) and Ru(III) complexes. Photo substitution, Photo racemization reactions and energy and electron transfer process in ruthenium complexes.

3.2 Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis.

3.3 Dye sensitized photochemical solar cells – Ruthenium and supramolecular sensitizers. Photo induced electron collection

Unit 4: Nanomaterials (18 Hrs)

4.1 General introduction to nanomaterials and emergence of nanotechnology – characterization of nano materials using XRD, SEM, TEM (Basic idea only) Moore's law - Synthesis of Nanomaterials – Precipitation methods, Sol-gel method, chemical vapour deposition, reduction techniques. Synthesis, properties and applications of fullerenes, carbon nanotubes, quantum dots. Green synthesis of nanoparticles of gold, silver-lithography. Thin films-chemical vapor deposition and atomic layer deposition techniques,

4.2. Diversity in nanosystems: self assembled monolayers on gold-growth process and phase transitions. Nanoshells-types of systems, characterization and application.

4.3. Evolving interfaces of nanotechnology- nanobiology, nanosensors, nanomedicines -

nanocomposites.

Unit 5: Advanced topics in Coordination Chemistry. 9Hrs

5.1 Coordination Chemistry of Fullerenes.
Fullerene metal complexes-Fullerides of alkali metals, Fullerenes as π-ligands, Metal fullerides, exohedral fullerenes, endohedral fullerenes. (Only elementary study is expected)

5.2 Metallo supra molecular chemistry and Molecular Architecture. Molecular recognition. Molecular Receptors- Cation binding Hosts- Crown ethers, Heterocrowns, Spherands, Cryptands, Calixarenes. Selectivity of Cation Complexation. Anionic Recognition. From anionic to cationic recognition. Neutral Molecules Recognition- Cyclodextrins, Carcerands, Cyclophane. Metallosupramolecular chemistry- Different Strategies and Types. Helicates, Grid type Metal ion Architecture, Ladder and Racks. Supramolecular Assistance in the Synthesis of Molecular and Supramolecular Structures-Catenanes, Rotaxanes, Knots and Necklaces.

Unit 6: Analytical Methods (9 Hrs)

6.1 Atomic Spectroscopy: Emission Spectra – Absorption Spectra – Fluorescence Spectra. Plasma Emission Spectroscopy – Direct current plasma - Inductively coupled plasma (ICP). Principle and Applications.

6.2 Size Exclusion Chromatography: Column Packings – Applications – Chromatographic Separation of Fullerenes (Bucky Balls). Affinity Chromatography. Chiral Chromatography.

6.3 Supercritical Fluid Chromatography: Important properties of supercritical fluids-Principle and Applications.

6.4 Analytical procedures involved in the environmental monitoring of water quality-BOD, COD, DO, nitrite and nitrate, iron, fluoride.

Unit 7: Acids and Bases. (9 hrs)

Acid –Base Strength. Acid-Base interaction- Ionic and Covalent Interaction(Drago and Wayland Concept). Steric Effect, Solvation Effect, Acid base strength and Proton affinity, Acidity and basicity of Binary Hydrogen compounds, Inductive effect, Non Aqueous solvent and Acid- Base strength, leveling effect, Superacid.
Hard and Soft Acids and Bases.- Classification, Acid Base strength and Hardness and Softness, Symbiosis, HSAB Theory, HOMO – LUMO concept. Applications of HSAB –Solubility of halides and chalcogenides, in qualitative Analysis, In biological function and Toxicology of elements and in Medicinal Chemistry (Chelation).

Unit 8: Structure of Some Inorganic Molecules. (5 hrs)

Hybridization and Structure of molecules- Structure of the following molecules- Trimethylborane, Phosphorus pentafluoride, Ammonium tetrafluoroborate, Aluminium bromide.

Structure of molecules containing lone pairs- Spatial requirements between lone pairs and bond pairs, Sulphur tetrafluoride, Bromine trifluoride, Dichloroiodate(I) anion, Pentafluorate(IV) anion, Tetrachloroiodate(III)anion, Nitrogen Dioxide, Nitrite ion, nitryl ion, Phosphorus trihalides, Carbonylfluoride and Xenon hexafluoride. Bent's rule and energy of Hybrid orbitals.

References:

1. F. A Cotton, Chemical Application of Group theory
2. K.V. Reddy, Symmetry and Spectroscopy of Molecules, New age International,1999.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiely, 2004.
4. T. Pradeep, Nano: the Essentials, Tata Mc Graw Hill, 2007.
5. C.N.R. Rao, A. Govindaraj, Nanotubes and Nanowires, Royal Society of Chemistry, 2011.
6. Wai- Kee Li,Gong-Du Zhou, Thomas Chung Wai Mak. Advanced structural Inorganic Chemistry, Oxford University Press. 2008.
7. Joan Ribas Gispert, Coordination Chemistry, WILEY-VCH , Master 2008.
8. Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press, 2006.
9. G. Wulfberg, Inorganic Chemistry, Ind. Edition, Viva, 2014.
10. K. Nakamoto, IR and Raman Spectra of Inorganic and Coordination Complexes, Part A-Theory and Applications in Inorganic Chemistry, 6th Edn., John Wiley & sons, 1997.
11. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
12. R.L. Dutta, A. Syamal, Elements of Magnetochemistry, Affiliated East-West Press, New Delhi, 1993.
13. D.M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, 1994.
14. V. Balzani, V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, 1970.
15. S.E. Manahan, Environmental Chemistry, 9$_{th}$ Edn., CRC Press, 2010.
16. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.
17. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8$_{th}$ Edn., Saunders College Pub., 2007.

16P4CHET14EL ADVANCED ORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit1:Biosynthesis and Biomimetic Synthesis **(15Hrs)**

1.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, and nucleic acids.
1.2 Biosynthesis of cholesterol, morphine, glucose and phenyl alanine.
1.3 Biogenesis of isoprenoids and alkaloids. Biomimetic synthesis of progesterone and spatreine.
1.4 Structure of DNA and RNA.Replication of DNA - Flow of genetic information - Protein biosynthesis - transcription and translation - Genetic code - regulation of gene expression

Unit2: Green Alternatives to Organic Synthesis **(12Hrs)**

2.1 Principles of Green Chemistry: Basic concepts, atom economy - twelve principles of Green Chemistry - principles of green organic synthesis.

2.2 Green alternatives to Organic Synthesis: Coenzyme catalysed reactions -thyamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: Pinacol-pinacolone and Benzidine rearrangement. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions. Green photochemical reactions.

2.3 Green Solvents: Ionic liquids, supercritical CO_2, fluorous chemistry.

2.4 General principles of microwave and ultrasound assisted organic synthesis.

Unit 3: Advances in Polymer Chemistry **(13Hrs)**

3.1 Degree of polymerization, classification and stereochemistry of polymers. Ziegler-Natta catalyst. Glass transition temperature of polymers, factors affecting glass transition temperature. Natural and synthetic rubber (SBR, Butyl, neoprene and nitrile rubber), vulcanization.
3.2 Conducting polymers - temperature resistant and flame retardant polymers - polymers for medical applications.
3.3 Dendrimers and dendritic polymers: Terminology- classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers.
3.4 Hyper branched polymers: definition, synthesis, applications.

Unit 4: Stereoselective Transformations **(10Hrs)**

4.1 Assymetric induction- chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenationdeveloped by Noyori and Knowels

4.3 Assymetric aldol condensation pioneered by Evans

4.4 Assymetric Diels- Alder reactions

4.5 Assymetric epoxidation using Jacobsen's catalyst

Unit 5: Chemistry of Natural Products and Biomolecules (14Hrs)

5.1 Synthesis of camphor, atropine, papaverine, cyanin, quercetin, β-carotene, testosterone, PGE_2 and $PGF_{2\alpha}$, Vitamine C and Riboflavin.

5.2 Methods for primary structure determination of peptides, proteins.

5.3 Enzymes- classification, structure and mode of action.

Unit 6: Medicinal Chemistry and Drug Designing (16Hrs)

6.1 Drug- Structure-activity relationships- a general idea.
6.2 Drug action - drug selectivity- receptor proteins- drug-receptor tinteraction - drug metabolism.Drug-receptor theory: occupancy theory, rate theory, induced fit theory, activation-aggregation theory. Mechanism of drug acting on DNA- intercalating agent (proflavin), alkylating agent (uracil mustard, cisplatin), chain cutting agents (bleomycin).
6.3 Central nervous system acting drugs (general idea), antidepressants, tranquilizers, sedatives and hypnotics.
6.4 A general idea of cardio-vascular drugs.
6.5 Introduction to Drug design- Concept of combinatorial and parallel synthesis. Computer assisted drug design. Illustration of drug development through a specific exampleof antibacterials- Pencillines.

Unit7: Research Methodology of Chemistry (10Hrs)

7.1 The search of knowledge - purpose of research - scientific methods - role of theory -
7.2 Characteristics of research. Types of research: Fundamental research, applied research, historical and experimental research.
7.3 Statistical calculations: Presentation of data, mean, median, mode, errors in chemical analyses, linear regression and correlation. Method of least squares.

7.4 Chemical literature: Primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, SciFinder. Chemical Abstract.

7.5 Scientific writing: Research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

7.6 Important scientific journals- important Chemistry journals. Impact factor

References

1. D. Voet and J.G. Voet*Biochemistry* Wiley, 2nd ed, 1995
2. J. Mann, *Chemical Aspects of Biosynthesis*, Oxford Chemistry Primer No. 20, 1994.
3. *Biomimetic Organic Synthesis*, First Edition. Edited by Erwan Poupon and Bastien Nay. Wiley-VCH Verlag GmbH & Co., 2011
4. W. Carruthers, *Modern Methods of Organic Synthesis*, Cambridge University Press, 1996.
5. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
6. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, ELBS with Chapman & Hall, 1993.

7. V.K.Ahluwalia, Green Chemistry: *Environmentally Benign Reactions*, ,Ane Books, New Delhi, 2009.

8. Jeremy M. Berg, John L. Tymoczko and LubertStryer, *Principles of Biochemistry* 6th edition, 2006 (W.H. Freeman & Co.).

9. Lehninger, Nelson, D. L. and M. M. Cox. *Principles of Biochemistry 5th edition*(W. H. Freeman &Co.), 2008.

10. V.K.Ahluwalia, M.Gupta, *Medicinal Chemistry*, Ane Books, New Delhi, 2012.

11. Patric, G. L., *An Introduction to Medicinal Chemistry*. 5thEdn.; Oxford University,2013.

12. Silverman, R. B., *The Organic Chemistry of Drug Design and Drug Action*. 2nd ed.; Academic Press: 2004Press: 2005

13. Deyue Yan, Chao Gao, Holger Frey,*Hyperbranched Polymers: Synthesis, Properties and applications:* 2011.

14. S.V.Bhat, B.A.Nagasampaki, M.Sivakumar, *Chemistry of Natural Products*, Narosa Publications, New Delhi, 2005.

15. R.L.Dominoswki, *Research Methods*, Prentice Hall, 1981.

16. J.W.Best, *Research in Education*, Prentice Hall, New Delhi, 1981.

17. H.F.Ebel, C.Bliefert and W.E.Russey, *The Art of Scientific Writing*, VCH, Weinheim, 1988.

18. Durtson, Poole, *Thesis and assignment writing*- Anderson, 1971.

19. John E. Freund.*Modern elementary statistics*,2003, ISBN-13: 978-0131874398

20. S. P. Gupta.*Statistical Methods*: S. Chand, 2014.

16P4CHET15EL ADVANCED PHYSICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Crystallography **(20 Hrs.)**

1.1 Introduction: Miller indices, stereographic projection, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.

1.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.

1.3 Liquid crystals: mesomorphic state, types, examples and application of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals.

Unit 2: Electrochemistry -II **(24Hrs.)**

2.1Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electro capillary, Lippmann equation, membrane potential.

2.2 Storage Cells: Lead, Ni-Cd, Lithium

2.3 Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells – efficiency-electro catalysis.

2.4 Corrosion: stability of metals-theories-Porbaus diagram-Evan diagram-corrosion control

2.5 Dynamic Electrochemistry-kinetics of electron transfer-polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage, Butler-Volmer equation for simple electron transfer reactions, Tafel equation and its significance, transfer coefficient, exchange current density, rate constants.

Unit 3: Diffraction Methods (8 Hrs.)

Electron diffraction of gases. Wierl's equation. Neutron diffraction method-SANS, Comparison of X-ray, electron and neutron diffraction methods. X-ray diffraction techniques, XRD, SAXS, WAXS

Unit 4: Spectroscopic Techniques (14Hrs.)

4.1 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.

4.2 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.

4.3 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation

4.4 Introduction to Fluorescence Spectroscopy

Unit 5: Electro Analytical Techniques (24Hrs.)

5.1 Voltametry: Voltametry-cyclic-voltametry, anodic stripping voltametry.

5.2 Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.

The dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition methods, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.

5.3 Amperometry: general principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, Amperometric titrations - titration procedure, merits and demerits of amperometric titrations.

5.4 Coulometry: coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations. Advantages of coulometry.

5.5 Ion selective electrodes: glass electrodes, sodium, potassium, lithium ion selective electrodes

References

01. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.

02. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

03. R.J. Silbey, R.A. Alberty, M.G. Bawendi, Physical Chemistry, 4th Edn. Wiley, 2005.

04. G.M. Barrow, Physical Chemistry, 5th Edn. Tata McGraw Hill, 2007.

05. A.R. West, Basic Solid State Chemistry, John Wiley & Sons, 1999.

06. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn. Houghton Mifflin, 2003.

07. P.W. Atkins, Physical Chemistry, ELBS, 1994.

08. G.W. Castellan, Physical Chemistry, Addison-Wesley, 1983.

09. B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH 2002.

10. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Edn. Springer, 2006.

11. D.L. Andrews, A.A. Demidov, Resonance Energy Transfer, Wiley, 1999.

12. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, 2011.

13. D. R. Crow, Principles and Applications of Electrochemistry, 4th Edn. S.Thornes, 1994.

14. B.K. Sharma, Electrochemistry, Krishna Prakashan, 1985.

15. H. Kaur, Spectroscopy, 6th Edn. Pragati Prakashan, 2011.

16. A.I. Vogel, A Text Book of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.

17. H.H. Willard, J.A .Dean, L.L. Merritt, Instrumental Methods of Analysis, Van Nostrand, 1965.

18. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn. Saunders College Pub., 2007.

16P4CHET16EL POLYMER CHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Introduction to Polymer Science (9 Hrs)
1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Unit 2: Fundamentals of Polymerization (18 Hrs)
2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

2.2 Ionic polymerization, common features of two types of ionic polymerization, mechanism and kinetics of cationic polymerization, expressions for overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expressions for overall rate of polymerization and the average degree of polymerization, living polymers.

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

2.4 Copolymerization, types of copolymers, the copolymer composition equation, reactivity ratio and copolymer structure-influence of structural effects on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

2.5 Step reaction (condensation) polymerization, Carothers equation, mechanism of step reaction polymerization, kinetics of step reaction polymerization, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point.

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Unit 3: Properties of Polymers (18 Hrs)
3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between T_g and T_m, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Unit 4: Stereochemistry and Conformation of Polymers (9 Hrs)
04.1 Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Unit 5: Morphology and Order in Crystalline Polymers (9 Hrs)
5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability-mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Unit 6: Advances in Polymers (9 Hrs)
6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications.
6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Unit 7: Dendrimers and Dendritic Polymers (18 Hrs)
7.1 Basic concepts and terminology: Dendrons, star shaped and starbust polymers, dendrimer formation and generations, various types of dendrimers.

7.2 Synthesis of dendrimers-convergent and divergent approaches, methods and mechanism. Properties of dendrimers-polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies(MALDI and TOF).

7.4 Dendritic macromolecules: hypergrafted and hyperbranched polymers – definition and classification, synthesis-methods and mechanism, characterization, properties, applications.

References
01. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.
02. F.W. Billmeyer Jr., Textbook of Polymer Science, 3rd Edn., Wiley-India, 2007.
03. L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn, John Wiley & Sons, 2006.
04. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.
05. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.
06. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving approach,

CRC/Taylor & Francis, 2006.
07. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1983.
08. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.
09. G. Odian, Principles of Polymerization, 4th Edn., John Wiley & Sons, 2007.
10. K.J. Saunders, Organic Polymer Chemistry, Chapmann & Hall, 1973.
11. K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, John Wiley & Sons, 2003.
12. H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

16P4CHET17EL ANALYTICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Instrumental Methods (36 Hrs)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentration electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes ($_1H$, $_{13}C$, $_{32}P$). Principle of MRI.

Unit 2: Sampling (18 hrs)

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Unit 3: Applied Analysis (9 hrs)

3.1 Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Unit 4: **Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)**

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection(indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Unit 5: Process instrumentation (9 Hrs)

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Unit 6: Aquatic Resources (9 Hrs)

6.1 Aquatic resources: renewable and non renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.

References

01. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College Pub., 2007.
03. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.
04. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.
05. G.D. Christian, J.E. O’Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
06. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
07. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
08. E.D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.
09. H.G. Heitmann, Saline Water Processing, VCH, 1990.

SEMESTERS III AND IV
16P4CHEP04 INORGANIC CHEMISTRY PRACTICAL-2

Credit: 3 **Contact Lab Hours: 54 + 54 =108**

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Introduction to material science and Nanotechnology

- Green synthesis of nanoAg/nanoAu-Assigning SPR band using UV-Vis Spectroscopy
- Synthesis of nano silica/nano titania- FTIR characterization
- Synthesis of nano Zinc Oxide- FTIR characterization
- Synthesis of nanocellulose- FTIR characterization
- Synthesis of the conducting polymer-poly aniline- FTIR characterization
- Synthesis of PbS/CdS/CdSe/ZnS quantum dot-UV- Vis spectral characterization

References

01. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
02. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.
03. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.
04. N.H. Furman, Standard Methods of Chemical Analysis: Volume 1, Van Nostrand, 1966.
05. F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub., 2006
06. T. Pradeep, Nano: the Essentials, Tata Mc Graw Hill, 2007.
07. C.N.R. Rao, A. Govindaraj, Nanotubes and Nanowires, Royal Society of Chemistry, 2011.

16P4CHEP05 ORGANIC CHEMISTRY PRACTICAL-2

CREDIT: 3 **Contact Lab Hours: 54+54=108**

PART I

Preparation and purification of organic compounds involving Two step Synthetic Sequences by Chemical Methods (Reactions involving nitration, Bromination, deamination, hydrolysis, rearrangement etc.)

PART II

Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods including Enzyme/coenzyme catalyzed reactions

PART III

Microwave assisted Organic Synthesis-oxidation, hydrolysis, condensation, substitution etc.

PART IV

Record the IR spectrum of the compounds synthesised in part I-III.

Generate and interpret the 1H and ^{13}C NMR spectra of selected organic molecules using software.

PART V

Study of enzyme- drug interaction by molecular docking(Minimum three models)

REFERENCES

1 A.I.Vogel, A Textbook of Practical Organic Chemistry, Longman, 1989.

2 A.I.Vogel, Elementary Practical Organic Chemistry, Longman, 1957.

3 F.G. Mann, B.C Saunders, Practical Organic Chemistry, 2009.

4 J.R. Johnson, J.F.Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

5 V.K. Ahluwalia, Green Chemistry:Environmentally Benign Reactions, Ane Books, New Delhi, 2009.

6 Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

7. Patric, G. L., *An Introduction to Medicinal Chemistry*. 5thEdn.; Oxford University,2013.

16P4CHEP06 PHYSICAL CHEMISTRY PRACTICAL-II

Credit: 3 Contact Lab Hours: 72+72=144

I Chemical Kinetics

1. Determination of the rate constant of the hydrolysis of ester by sodium hydroxide/HCl

2. Determination of Arrhenius parameters.

3. Kinetics of reaction between $K_2S_2O_8$ and KI

4. Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI

5. Iodination of acetone in acid medium.

II Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.

2. Determination of the concentration of a sugar solution.

3. Determination of the concentration of HCl.

4. Determination of the relative strength of acids.

III Refractometry

1. Determination of molar refractions of pure liquids.

2. Determination of concentration of solutions (KCl-water, glycerol-water).

3. Determination of molar refraction of solids.

4. Study of complex formation between potassium iodide and mercuric iodide system.

IV Viscosity

1. Determination of viscosity of pure liquids.

2. Determination of the composition of binary liquid mixtures (alcohol-water,

Toluene-nitrobenzene) and verification of Kendall's equation

3. Determination of the molecular weight of a polymer (polystyrene in toluene).

4. Determine the concentration of the given solution of Glycerol/sucrose.

V Conductivity measurements

1. Verification of Onsager equation.

2. Determination of the degree of ionization of weak electrolytes.

3. Determination of pKa values of organic acids.

4. Determination of solubility of sparingly soluble salts.

5. Titration of a strong acid/Weak acid against a strong base.

6. Titration of a dibasic acid against a strong base.

7. Conductometric determination of the rate constant for the alkaline hydrolysis of methyl acetate.

VI Potentiometry

1. Determination of single electrode potentials (Cu and Zn).

2. Application of Henderson equation.

3. Titration of a mixture of acids against a strong base.

4. Redox Titrations and determination of formal redox potential.

VII Photometry

1. Verification of the Beer and Lamberts law.

2. Kinetics of iodination of acetone.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House,

2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry,

8th Edn. McGraw Hill, 2009.

03. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005

04. Saroj Kumar and Naba Kumar,Physical Chemistry Practical,New Central Book Agency,2012

05. Practical Physical Chemistry Paperback, 1974 by A.M. James , F.E. Prichard.

16P4CHECV - Comprehensive Viva Voce

There will be a comprehensive viva at the end of the programme. The viva board consists of three external examiners preferably same as the practical examiners for the respective subject and one internal examiner (Class teacher).

16P4CHEPJ - Project

Each student should submit a project report for evaluation. A minimum of 3 months period shall be given to each student for the project and this may be after the end semester examination of semester 4. Students can do their project in the department or any other reputed research institution in and outside the state. After completing the project the report should be submitted to the department for internal and external evaluation. The external evaluation will be done by the project viva board, which consists of three examiners preferably same as the practical examiners for the respective subjects.