MAR ATHANASIUS COLLEGE (AUTONOMOUS)

KOTHAMANGALAM, KERALA 686 666

NAAC Accredited 'A^{+}' Grade Institution

Email: mac@macollege.in

www.macollege.in

SCHEME AND SYLLABUS

FOR

POST GRADUATE PROGRAMME

UNDER CREDIT SEMESTER SYSTEM

MAC-PG-CSS 2020

IN

M.Sc.CHEMISTRY

EFFECTIVE FROM THE ACADEMIC YEAR 2020-2021

BOARD OF STUDIES IN CHEMISTRY (PG)

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BOARD OF STUDIES IN CHEMISTRY (PG)

ACADEMIC COUNCIL

COMPOSITION – With Effect From 01-06-2020

Chairperson : **Dr. Shanti. A. Avirah**
Principal
Mar Athanasius College (Autonomous), Kothamangalam.

Experts/Academicians from outside the college representing such areas as Industry, Commerce, Law, Education, Medicine, Engineering, Sciences etc.

1. **Dr. Winny Varghese**
   Secretary
   Mar Athanasius College Association
   Kothamangalam.

2. **Prof. Dr. V.N. Rajasekharan Pillai**
   Former Vice-Chairman
   University Grants Commission,
   New Delhi.

3. **Dr. R.K. Chauhan**
   Former Vice-Chancellor, Lingaya's University,
   Faridabad, Haryana -121002

4. **Dr. Sheela Ramachandran**
   Pro-Chancellor,
   Atmiya University
   Rajkot.

5. **Prof. Kuruvilla Joseph**
   Senior Professor and Dean,
   Indian Institute of Space Science and Technology (IIST),
   Department of Space, Govt. of India, Valiyamala, Thiruvananthapuram.

6. **Dr. M.C. Dileep Kumar**
   Former Vice Chancellor
   Sree Sankaracharya Sanskrit University
   Kalady, Kerala, India.

7. **Dr. Mathew. K.**
   Principal
   Mar Athanasius College of Engineering,
   Kothamangalam, Kerala - 686 666

8. **Adv. George Jacob**
   Senior Advocate
   High Court of Kerala
   Ernakulam.

Nominees of the university not less than Professors

9. **Dr. Biju Pushpan**
SAS SNDP Yogam College
Konni.

10. **Dr. Suma Mary Scharia**
UC College
Aluva.

11. **Dr. V.B. Nishi**
Associate Professor
Sree Sankara College, Kalady.

Member Secretary

12. **Dr. M.S.Vijayakumary**
Dean – Academics
Mar Athanasius College (Autonomous)
Kothamangalam.

Four teachers of the college representing different categories of teaching staff by rotation on the basis of seniority of service in the college.

13. **Dr. Bino Sebastian. V** (Controller of Examinations)

14. **Dr. Manju Kurian,** Asst. Professor, Department of Chemistry

15. **Dr. Smitha Thankachan**, Asst. Professor, Department of Physics

16. **Dr. Asha Mathai**, Asst. Professor, Department of Malayalam

Heads of the Departments

17. Dr. Jayamma Francis, Head, Department of Chemistry

18. Dr. Mini Varghese, Head, Department of Hindi

19. Ms. Shiny John, Head, Department of Computer Science

20. Dr. Igy George, Head, Department of Economics

21. Dr. Rajesh.K. Thumbakara, Head, Department of Mathematics

22. Dr. Aji Abraham, Head, Department of Botany

23. Dr. Selven S., Head, Department of Zoology

24. Dr. Deepa. S, Head, Department of Physics
25. Dr. Aswathy Balachandran, Head, Department of English
26. Dr. Diana Ann Issac, Head, Department of Commerce
27. Ms. Seena John, Head, Department of Malayalam
28. Ms. Diana Mathews, Head, Department of Sociology
29. Ms. Sudha. V, Head, Department of Statistics
30. Dr. Jani Chungath, Head, Department of History
31. Sri. Haary Benny Chettiamkudiyil, Head, Department of Physical Education
32. Ms. Shari Sadasivan, Head, Department of Marketing and International Business
33. Dr. Julie Jacob, Head, Department of Biochemistry
34. Ms. Nivya Mariyam Paul, Head, Department of Microbiology
35. Ms. Jaya Vinny Eappen, Head, Department of Biotechnology
36. Ms. Shalini Binu, Head, Department of Actuarial Science
37. Ms. Simi. C.V, Head, Post Graduate Department of History
38. Ms. Sari Thomas, Head, Post Graduate Department of Statistics
39. Ms. Sheeba Stephen, Head, Department of B.Com Model III - Tax Procedure and Practice
40. Ms. Dilmol Varghese, Head, Post Graduate Department of Zoology
41. Ms. Bibin Paul, Head, Post Graduate Department of Sociology

MAR ATHANASIUS COLLEGE, (AUTONOMOUS) KOTHAMANGALAM MEMBERS OF THE BOARD OF STUDIES - PG PROGRAMME Subject: CHEMISTRY	
NAME	DETAILS
CHAIRPERSON	
Dr.JAYAMMA FRANCIS	HOD and Associate Professor in Chemistry, M.A College, Kothamangalam
EXPERTS(2)	
1.DR.S.SUGUNAN	Emeritus Professor in Applied Chemistry CUSAT, Kochi
2.DR.PAULSON MATHEW	Associate Professor in Chemistry St. Thomas College Thrissur.
ONE EXPERT - TO BE NOMINATED BY V C (MGU)	
DR.K.L.SEBASTIAN	Professor Dean, Department of Physical Chemistry, IIT, Palakkad.
MEMBER FROM INDUSTRY	
DR.KOCHUBABY MANJOORAN	Dy. Manager(Energy & Environment) BPCL, Kochi Refinery
MERITORIOUS ALUMNUS	
DR.IGNATIOUS ABRAHAM	Assistant Professor in Chemistry SH College Thevara
FACULTY MEMBERS OF THE DEPARTMENT WITH Ph.D	
1.Dr. DENSELY JOSE	Associate Professor in Chemistry M.A College Kothamangalam
2.Dr. MANJU KURIAN	Assistant Professor in Chemistry M.A. College, Kothamangalam
3. Dr. ANNU ANNA VARGHESE	Assistant Professor in Chemistry M.A. College, Kothamangalam
4. Dr. BINU VARGHESE	Assistant Professor in Chemistry M.A. College, Kothamangalam
5. Dr. MARYMOL MOOTHEDAN	Assistant Professor in Chemistry M.A. College, Kothamangalam

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PREFACE

Chemistry is the science of matter and the changes it undergoes being concerned with the composition, behaviour structure and properties of matter as well as the changes it undergoes during chemical reactions.

Mar Athanasius College Kothamangalam, in its pursuit of academic excellence, was accorded Autonomous status on March 2016. In order to cope with the internationally followed curricula and mode of evaluation, the department was directed to revise the curriculum and syllabi of M.Sc. programme in Chemistry. The guidelines are provided by the College.

Our **Vision** is to provide quality education in Chemistry which aims at global academic competence and sustainable development for the creation of vibrant and inclusive society.

Our **Mission** is to equip the students to build up a career in Chemistry and to contribute towards national development through foster collaboration with leading research institutes in knowledge production.

Teachers of different branches of Chemistry, namely inorganic, organic, physical and analytical chemistry had separate and joint brainstorming sessions and arrived at a draft syllabus in Chemistry for four semesters. The draft syllabus prepared by the members of the faculty was discussed in detail in the meetings of the Board of the Studies held on 17-12-2016, 28-2-2017, 1-12-2018 and 17-10-2019 respectively. Appreciable updating has done in keeping with current developments and trends in Chemistry

I would like to express my sincere gratitude to all the members of the Board of Studies, especially, Dr.K.L.Sebastian, Professor Dean, IIT Palakkad, Dr.S.Sugunan, Emeritus Professor, Dept. of Applied Chemistry, CUSAT and Dr. Paulson Mathew, Associate Professor, Dept. of Chemistry, St. Thomas College, Thrissur for their whole hearted time bound help, cooperation and encouragement. I also thank Dr. Binu Varghese, Assistant professor in Chemistry, M.A College Kothamangalam for coordinating and editing the Post Graduate syllabus in Chemistry.

Dr. Jayamma Francis, Chairperson, PG Board of Studies in Chemistry

LIST OF POST GRADUATE PROGRAMMES IN MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM

SL. NO.	PROGRAMME	DEGREE	FACULTY
1	ENGLISH	MA	LANGUAGE AND LITERATURE
2	ECONOMICS	MA	SOCIAL SCIENCES
3	SOCIOLOGY	MA	SOCIAL SCIENCES
4	HISTORY	MA	SOCIAL SCIENCES
5	MATHEMATICS	M.Sc	SCIENCE
6	CHEMISTRY	M.Sc	SCIENCE
7	PHYSICS	M.Sc	SCIENCE
8	BOTANY	M.Sc	SCIENCE
9	STATISTICS	M.Sc	SCIENCE
10	ZOOLOGY	M.Sc	SCIENCE
11	BIOCHEMISTRY	M.Sc	SCIENCE
12	BIOTECHNOLOGY	M.Sc	SCIENCE
13	MICROBIOLOGY	M.Sc	SCIENCE
14	ACTUARIAL SCIENCE	M.Sc	SCIENCE
15	COMMERCE(SPECIALISATION-FINANCE AND TAXATION)	M.Com	COMMERCE
16	COMMERCE(SPECIALISATION-MARKETING AND INTERNATIONAL BUSINESS	M.Com	COMMERCE

REGULATIONS OF THE POSTGRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM MAC-PG-CSS 2020 (2020 Admission onwards)

1. SHORT TITLE

1.1 These Regulations shall be called "Mar Athanasius College (Autonomous) Regulations (2020) governing Postgraduate Programmes under the Credit Semester System (MAC-PG-CSS2020)".

1.2 These Regulations shall come into force from the Academic Year 2020-2021.

2. SCOPE

2.1 The regulations provided herein shall apply to all Regular Postgraduate (PG) Programmes, M.A. /M.Sc. /M.Com. conducted by Mar Athanasius College (Autonomous) with effect from the academic year 2020-2021 admission onwards.

3. DEFINITIONS

3.1 **'Academic Committee'** means the Committee constituted by the Principal under this regulation to monitor the running of the Post-Graduate programmes under the Credit Semester System (MAC-PG-CSS2020).

3.2 **'Academic Week'** is a unit of five working days in which distribution of work is organized from day one to day five, with five contact hours of one hour duration on each day. A sequence of 18 such academic weeks constitutes a semester.

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

3.4 **'CE' means Continuous Evaluation (Internal Evaluation)**

3.5 **'College Co-ordinator'** means a teacher from the college nominated by the Principal to look into the matters relating to MAC-PG-CSS2020 for programmes conducted in the College.

3.6 **'Comprehensive Viva-Voce'** means the oral examinations conducted by the appointed examiners and shall cover all courses of study undergone by a student for the programme.

3.7 **'Common Course'** is a core course which is included in more than one programme with the same course code.

3.8 '**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.

3.9 '**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/seminar/ project/practical training / assignments/evaluation etc., to meet effective teaching and learning needs.

3.10 **'Course Code'** means a unique alpha numeric code assigned to each course of a programme.

3.11 '**Course Credit**' One credit of the course is defined as a minimum of one hour lecture /minimum of 2 hours lab/field work per week for 18 weeks in a Semester. The course will be considered as completed only by conducting the final examination.

3.12 **'Course Teacher'** means the teacher of the institution in charge of the course offered in the programme.

3.13 **'Credit (Cr)'** of a course is a numerical value which depicts the measure of the weekly unit of work assigned for that course in a semester.

3.14 '**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**.

3.15 '**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. CGPA determines the overall performance of a student at the end of a programme.
(CGPA = Total CP obtained/ Total credits of the programme)

3.16 '**Department**' means any teaching Department offering a programme of study in the institution.

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

3.18 **'Dissertation'** means a long document on a particular subject in connection with the project /research/ field work etc.

3.19 '**Duration of Programme**' means the period of time required for the conduct of the programme. The duration of post-graduate programme shall be 4 semesters spread over two academic years.

3.20 '**Elective Course**' means a course, which can be substituted, by equivalent course from the same subject.

3.21 'Elective Group' means a group consisting of elective courses for the programme.

3.22 'ESE' means End Semester Evaluation (External Evaluation).

3.23 'Evaluation' is the process by which the knowledge acquired by the student is quantified as per the criteria detailed in these regulations.

3.24 External Examiner is the teacher appointed from other colleges for the valuation of courses of study undergone by the student in a college. The external examiner shall be appointed by the college.

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

3.26 '**Grace Grade Points**' means grade points awarded to course(s), recognition of the students' meritorious achievements in NSS/ Sports/ Arts and cultural activities etc.

3.27 '**Grade Point**' (GP) 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.

3.28 '**Grade Point Average(GPA)**' is an index of the performance of a student in a course. It is obtained by dividing the sum of the weighted grade point obtained in the course by the sum of the weights of Course.**(GPA= ∑WGP / ∑W)**

3.29 '**Improvement Course**' is a course registered by a student for improving his performance in that particular course.

3.30 'Internal Examiner' is a teacher nominated by the department concerned to conduct internal evaluation.

3.31 '**Letter Grade**' or '**Grade**' for a course is a letter symbol (A+, A, B+, B, C+, C, D) which indicates the broad level of performance of a student for a course.

3.32 MAC-PG-CSS2020 means Mar Athanasius College Regulations Governing Post Graduate programmes under Credit Semester System, 2020.

3.33 '**Parent Department**' means the Department which offers a particular postgraduate programme.

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

3.35 '**Programme**' means the entire course of study and Examinations.

3.36 **'Project'** is a core course in a programme. It 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 research centre in order to submit a dissertation on the project work as specified. It allows students to work more autonomously to construct their own learning and culminates in realistic, student-generated products or findings.

3.37 '**Repeat Course**' is a course to complete the programme in an earlier registration.

3.38 '**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.

3.39 '**Seminar**' means a lecture given by the student on a selected topic and expected to train the student in self-study, collection of relevant matter from various resources, editing, document writing and presentation.

3.40 '**Semester Grade Point Average(SGPA)**' is the value obtained by dividing the sum of credit points (CP) obtained by the student in the various courses taken in a semester by the total number of credits for the course in that semester. The SGPA shall be rounded off to two decimal places. SGPA determines the overall performance of a student at the end of a semester (SGPA = Total CP obtained in the semester / Total Credits for the semester).

3.41 '**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.

3.42 '**Weight**' is a numeric measure assigned to the assessment units of various components of a course of study.

3.43 **University** means Mahatma Gandhi University Kottayam to which the college is affiliated.

3.44 '**Weighted Grade Point (WGP)**' is grade points multiplied by weight. **(WGP = GP x W)**

3.45 **'Weighted Grade Point Average (WGPA)' is an index of the performance of a student in a course. It is obtained by dividing the sum of the weighted grade points by the sum of the weights. WGPA shall be obtained for CE (Continuous Evaluation) and ESE (End Semester Evaluation) separately and then the combined WGPA shall be obtained for each course.**

4. ACADEMIC COMMITTEE

4.1. There shall be an Academic Committee constituted by the Principal to Manage and monitor the working of MAC-PG-CSS 2020.

4.2. The Committee consists of:

1. Principal
2. Dean, Administration
3. Dean, Academics
4. IQAC Coordinator
5. Controller of Examinations
6. One Faculty each representing Arts, Science, Commerce, Languages, and Self Financing Programmes

5. PROGRAMME STRUCTURE

5.1 Students shall be admitted to post graduate programme under the various Faculties. The programme shall include three types of courses, Core Courses, Elective Courses and Common core courses. There shall be a project with dissertation and comprehensive viva-voce as core courses for all programmes. The programme shall also include assignments / seminars/ practical's etc.

5.2 No regular student shall register for more than 25 credits and less than16 credits per semester unless otherwise specified. The total minimum credits, required for completing a PG programme is 80.

5.3. Elective Courses and Groups

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

5.3.2 The elective courses shall be either in fourth semester or distributed among third and fourth semesters. There may be various groups of Elective courses (three elective courses in each group) for a programme such as Group A, Group B etc. for the choice of students, subject to the availability of facility and infrastructure in the institution.

5.3.3 The selection of courses from different elective groups is not permitted.

5.3.4 The elective groups selected for the various Programmes shall be intimated to the Controller of Examinations within two weeks of commencement of the semester in which the elective courses are offered. The elective group selected for

the students who are admitted in a particular academic year for various programmes shall not be changed.

5.4 P**roject Work**

5.4.1. Project work shall be completed in accordance with the guidelines given in the curriculum.

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

5.4.3. A candidate may, however, in certain cases be permitted to work on the project in an Industrial/Research Organization on the recommendation of the supervising teacher.

5.4.4 There shall be an internal assessment and external assessment for the project work.

5.4.5. The Project work shall be evaluated based on the presentation of the project work done by the student, the dissertation submitted and the viva-voce on the project.

5.4.6 The external evaluation of project work shall be conducted by two external examiners from different colleges and an internal examiner from the college concerned.

5.4.7 The final Grade of the project (External) shall be calculated by taking the average of the Weighted Grade Points given by the two external examiners and the internal examiner.

5.5 **Assignments:** Every student shall submit at least one assignment as an internal component for each course.

5.6 **Seminar Lecture:** Every PG student shall deliver one seminar lecture as an Internal component for every course with a weightage of two. The seminar lecture is expected to train the student in self-study, collection of relevant matter from the various resources, editing, document writing and presentation.

5.7 **Test Papers (Internal):**Every PG student shall undergo at least two class tests as an internal component for every course with a weight one each. The best two shall be taken for awarding the grade for class tests.

5.8. **No courses shall have more than 5 credits unless otherwise specified.**

5.9. **Comprehensive Viva-Voce** -Comprehensive Viva-Voce shall be conducted at the end of fourth semester of the programme and its evaluation shall be conducted by the examiners of the project evaluation.

5.9.1. Comprehensive Viva-Voce shall cover questions from all courses in the Programme.

5.9.2. There shall be an internal assessment and an external assessment for the Comprehensive Viva-Voce.

6. ATTENDANCE

6.1. The minimum requirement of aggregate attendance during a semester for appearing at the end-semester examination shall be 75%. Condonation of shortage of attendance to a maximum of 15 days in a semester subject to a maximum of two times during the whole period of the programme may be granted by the University.

6.2 If a student represents his/her institution, University, State or Nation in Sports, NCC, or Cultural or any other officially sponsored activities such as college union/ university union etc., he/she shall be eligible to claim the attendance for the actual number of days participated subject to a maximum 15 days in a Semester based on the specific recommendations of the Head of the Department or teacher concerned.

6.3 Those who could not register for the examination of a particular semester due to shortage of attendance may repeat the semester along with junior batches, without considering sanctioned strength, subject to the existing University Rules and Clause 7.2.

6.4. A Regular student who has undergone a programme of study under earlier regulation/ Scheme and could not complete the Programme due to shortage of attendance may repeat the semester along with the regular batch subject to the condition that he has to undergo all the examinations of the previous semesters as per the MAC-PG-CSS2020 regulations and conditions specified in 6.3.

6.5 A student who had sufficient attendance and could not register for fourth semester examination can appear for the end semester examination in the subsequent years with the attendance and progress report from the principal.

7. REGISTRATION/ DURATION

7.1 A student shall be permitted to register for the programme at the time of admission.

7.2 A student who registered for the Programme shall complete the Programme within a period of four years from the date of commencement of the programme.

7.3 Students are eligible to pursue studies for additional post graduate degree. They shall be eligible for award of degree only after successful completion of two years (four semesters of study) of college going.

8. ADMISSION

8.1 The admission to all PG programmes shall be done through the Centralised Allotment Process of Mar Athanasius College (Autonomous), Kothamangalam(MAC-PG CAP) as per the rules and regulations prescribed by the affiliating university and the Government of Kerala from time to time.

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

9. ADMISSION REQUIREMENTS

9.1 Candidates for admission to the first semester of the PG programme through CSS 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 Mahatma Gandhi University as eligible thereto.

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

10. PROMOTION:

10.1 A student who registers for the end semester examination shall be promoted to the next semester.

10.2 A student having 75% attendance and who fails to register for examination of a particular semester will be allowed to register notionally and is promoted to the next semester, provided application for notional registration shall be submitted within 15 days from the commencement of the next semester.

10.3 The medium of Instruction shall be English except programmes under faculty of Language and Literature.

11. EXAMINATIONS

11.1 **End-Semester Examinations**: The examinations shall be at the end of each Semester of three hour duration for each centralised and practical course.

11.2 Practical examinations shall be conducted at the end of each semester or at the end of even semesters as prescribed in the syllabus of the particular programme. The number of examiners for the practical examinations shall be prescribed by the Board of Studies of the programmes.

11.3 A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions. Different types of questions shall have different weightage.

12. EVALUATION AND GRADING

12.1 **Evaluation:** The evaluation scheme for each course shall contain two parts; (a) End Semester Evaluation (ESE) (External Evaluation) and (b) Continuous Evaluation (CE) (Internal Evaluation). 25% weightage shall be given to internal evaluation and the remaining 75% to external evaluation and the ratio and weightage between internal and external is 1:3. Both End Semester Evaluation (ESE) and Continuous Evaluation(CE) shall be carried out using direct grading system.

12.2 **Direct Grading: The direct grading for CE (Internal) and ESE (External Evaluation) shall be based on 6 letter grades (A+, A, B, C, D and E) with numerical values of 5, 4, 3, 2, 1 and 0 respectively.**

12.3 **Grade Point Average (GPA): Internal and External components are separately graded and the combined grade point with weightage 1 for internal and 3 for external shall be applied to calculate the Grade Point Average (GPA) of each course. Letter grade shall be assigned to each course based on the categorization provided in 12.16.**

12.4 **Internal evaluation:** The internal evaluation shall be based on predetermined transparent system periodic written tests, assignments, seminars, lab skills, records, viva-voce etc.

12.5 Components of internal (CE) and External Evaluation (ESE): Grades shall be given to the evaluation of theory / practical / project / comprehensive viva-voce and all internal evaluations are based on the Direct Grading System.

Proper guidelines shall be prepared by the BOS for evaluating the assignment, seminar, practical, project and comprehensive viva-voce within the framework of the regulation.

12.6 There shall be no separate minimum grade point for internal evaluation.

12.7 **The model of the components and its weightages for Continuous Evaluation (CE) and End Semester Evaluation (ESE) are shown in below:**

a) For Theory (CE) (Internal)

	Components	Weightage
i.	Assignment	1

ii.	Seminar	2
iii.	Best Two Test papers	2 (1 each)
Total		**5**

(Average grade of the best two papers can be considered. For test paper all the Questions shall be set in such a way that the answers can be awarded A+, A, B, C, D, E grades)

b) For Theory (ESE) (External)

Evaluation is based on the pattern of Question specified **in 12.15.5**

c) For Practical (CE) (Internal)

Components	Weightage
Written / Lab Test	2
Lab Involvement and Record	1
Viva	2
Total	**5**

(The components and weightage of the practical (Internal) can be modified by the concerned BOS without changing the total weightage 5)

d) For Practical (ESE) (External)

Components	Weightage
Written / Lab Test	7
Lab Involvement and Record	3
Viva	5
Total	**15**

(The components and weightage of the practical (External) can be modified by the concerned BOS without changing the total weightage 15)

e) For Project(CE) (Internal)

Components	Weightage
Relevance of the topic and analysis	2
Project content and presentation	2
Project viva	1
Total	**5**

(The components and the weightage of the components of the Project (Internal) can be modified by the concerned BOS without changing the total weightage 5)

f) For Project (ESE) (External)

Components	Weightage
Relevance of the topic and analysis	3
Project content and presentation	7
Project viva	5
Total	**15**

(The components and the weightage of the components of the Project (External) can be modified by the concerned BOS without changing the total weightage 15)

g) Comprehensive viva-voce (CE) (Internal)

Components	Weightage
Comprehensive viva-voce(all courses from first semester to fourth semester)	5
Total	**5**

(Weightage of the components of the Comprehensive viva-voce(Internal) shall not be modified.)

h)Comprehensive viva-voce (ESE) (External)

Components	Weightage
Comprehensive viva-voce(all courses from first semester to fourth semester)	15
Total	**15**

(Weightage of the components of the Comprehensive viva-voce (External) shall not be modified.)

12.8 **All grade point averages shall be rounded to two digits.**

12.9 To ensure transparency of the evaluation process, the internal assessment grade 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.

12.10 **There shall not be any chance for improvement for Internal Grade.**

12.11 The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course and a copy should be kept in the college for verification for at least two years after the student completes the programme.

12.12 **External Evaluation.** The external examination in theory courses is to be conducted by the College at the end of the semester. The answers may be written in English or Malayalam except those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The external evaluation shall be done immediately after the examination.

12.13 Photocopies of the answer scripts of the external examination shall be made available to the students on request as per the rules prevailing in the University.

12.14 The question paper should be strictly on the basis of model question paper set and directions prescribed by the BOS.

12.15. **Pattern of Questions**

12.15.1 **Questions shall be set to assess knowledge acquired, standard, and application of knowledge, application of knowledge in new situations, critical evaluation of knowledge and the ability to synthesize knowledge. Due weightage shall be given to each module based on content/teaching hours allotted to each module.**

12.15.2 The question setter shall ensure that questions covering all skills are set.

12.15.3 A question paper shall be a judicious mix of short answer type, short

essay type /problem solving type and long essay type questions.

12.15.4 The question shall be prepared in such a way that the answers can be awarded A+, A, B, C, D, E grades.

12.15.5 Weight: Different types of questions shall be given different weights to quantify their range as follows:

Sl.No.	Type of Questions	Weight	Number of questions to be answered
1	Short Answer type questions	1	8 out of 10
2	Short essay / problem solving type questions	2	6 out of 8
3	Long Essay Type questions	5	2 out of 4

12.16. **Pattern of question for practical**. The pattern of questions for external evaluation of practical shall be prescribed by the Board of Studies.

12.17. **Direct Grading System**

Direct Grading System based on a 6- point scale is used to evaluate the Internal and External examinations taken by the students for various courses of study.

Grade	Grade point(G)	Grade Range
A+	5	4.50 to 5.00
A	4	4.00 to 4.49
B	3	3.00 to 3.99
C	2	2.00 to 2.99
D	1	0.01 to 1.99
E	0	0.00

12.18. **Performance Grading**

Students are graded based on their performance (GPA/SGPA/CGPA) at the examination on a 7-point scale as detailed below.

Range	Grade	Indicator
4.50 to 5.00	**A+**	**Outstanding**
4.00 to 4.49	**A**	**Excellent**
3.50 to 3.99	**B+**	**Very good**
3.00 to 3.49	**B**	**Good(Average)**
2.50 to 2.99	**C+**	**Fair**
2.00 to 2.49	**C**	**Marginal**
up to 1.99	**D**	**Deficient(Fail)**

12.19 **No separate minimum is required for Internal Evaluation for a pass, but a minimum grade is required for a pass in an External Evaluation.**

However, a minimum C grade is required for pass in a Course

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

12.21 **Improvement of Course-** The candidate who wish to improve the grade/grade point of the external examination of the of a course/ courses he/ she has passed can do the same by appearing in the external examination of the semester concerned along with the immediate junior batch. This facility is restricted to first and second semester of the programme.

12.22 **One Time Betterment Programme-** A candidate will be permitted to improve the **CGPA** of the programme within a continuous period of four semesters immediately following the completion of the programme allowing only once for a particular semester. The **CGPA** for the betterment appearance will be computed based on the **SGPA** secured in the original or betterment appearance of each semester whichever is higher.

If a candidate opts for the betterment of **CGPA** of a programme, he/she has to appear for the external examination of the entire semester(s) excluding practical /project/comprehensive viva-voce. One time betterment programme is restricted to students who have passed in all courses of the programme at the regular (First appearance)

12.23 **Semester Grade Point Average(SGPA) and Cumulative Grade Point Average (CGPA) Calculations.** The SGPA is the ratio of sum of the credit point of all courses taken by a student in a semester to the total credit for that semester. 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.

Semester Grade Point Average -SGPA (S_j) = $\sum(C_i \times G_i) / \sum C_i$

(SGPA= Total credit Points awarded in a semester / Total credits of the semester)

Where 'S_j' is the j^{th} semester, 'G_i' is the grade point scored by the student in the i^{th} course 'C_i' is the credit of the i^{th} course.

12.24 **Cumulative Grade Point Average (CGPA)** of a programme is calculated using the formula:-

Cumulative Grade Point Average (CGPA) = $\sum(C_i \times S_i) / \sum C_i$

(CGPA= Total credit Points awarded in all semester / Total credits of the programme)

Where 'C_i' is the credit for the i^{th} semester, 'S_i' is the SGPA for the i^{th} semester. The **SGPA** and **CGPA** shall be rounded off to 2 decimal points.

For the successful completion of semester, a student shall pass all courses and score a minimum **SGPA** of 2.0. However a student is permitted to move to the next semester irrespective of her/his **SGPA**

13. GRADE CARD

13.1 The Institution under its seal shall issue to the students, a consolidated grade card on completion of the programme, which shall contain the following information.

a) Name of the University.

b) Name of college

c) Title of the PG Programme.

d) Name of Semesters

e) Name and Register Number of students

f) Code, Title, Credits and Max GPA(Internal, External & Total) of each course (theory &practical), project, viva etc in each semester.

g) Internal, external and Total grade, Grade Point (G), Letter grade and Credit point (P) in each course opted in the semester.

h) The total credits and total credit points in each semester.

i) Semester Grade Point Average (SGPA) and corresponding Grade in each semester

j) Cumulative Grade Point Average (CGPA), Grade for the entire programme.

k) Separate Grade card will be issued.

l) Details of description of evaluation process- Grade and Grade Point as well as indicators, calculation methodology of SGPA and CGPA as well as conversion scale shall be shown on the reverse side of the grade card.

14. AWARD OF DEGREE - The successful completion of all the courses with 'C' grade within the stipulated period shall be the minimum requirement for the award of the degree.

15. MONITORING COMMITTEE

There shall be a Monitoring Committee constituted by the Principal to monitor the internal evaluations conducted.

16. RANK CERTIFICATE

Rank certificate shall be issued to candidates who secure positions 1st and 2nd . Candidates shall be ranked in the order of merit based on the CGPA secured by them.

Grace grade points awarded to the students shall not be counted for fixing the rank. Rank certificate shall be signed by the Principal and the Controller of Examinations.

17. GRIEVANCE REDRESSAL COMMITTEE

17.1 Department level: The College shall form a Grievance Redressal Committee in each Department comprising of the course teacher and one senior teacher as members and the Head of the Department as Chairperson. The Committee shall address all grievances relating to the internal assessment grades of the students.

17.2. College level: There shall be a college level Grievance Redressal Committee comprising of faculty advisor, college co-ordinator, one senior teacher and one staff council member and the Principal as Chairperson.

18. **FACTORY VISIT / FIELD WORK/VISIT:** Factory visit / field work/visit to a reputed research institute/ student interaction with renowned academicians may be conducted for all Programmes before the commencement of Semester III.

19**.** **INTERNSHIP/ON THE JOB TRAINING:** Each student may undertake internship/on the job training for a period of not less than 15 days. The time, duration and structure of internship/on the job training can be modified by the concerned Board of Studies.

20. **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.

21. **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 Credit Semester System in their application to any course offered in a College, the latter shall prevail.

22. **Credits allotted for Programmes and Courses**

22.1 Total credit for each programme shall be **80**.

22.2 Semester-wise total credit can vary from 16 to 25

22.3 The minimum credit of a course is 2 and maximum credit is 5

23. **Common Course:** If a course is included as a common course in more than one programme, its credit shall be same for all programmes.

24. **Course Codes:** The course codes assigned for all courses (Core Courses, Elective Courses, Common Courses etc.) shall be unique.

25. **Models of distribution of courses, course codes, type of the course, credits, teaching hours for the M Sc Chemistry programme are given in the following table.**

Programmes with practical -Total Credits 80 - M SC Chemistry

Semester	Course code	Course	Hours/ week	Contact hours	Credit
I	PG20CH101	INORGANIC CHEMISTRY-I	4	72	4
	PG20CH102	ORGANIC CHEMISTRY-I	4	72	4
	PG20CH103	THEORETICAL CHEMISTRY-I	4	72	4
	PG20CH104	PHYSICAL CHEMISTRY-I	3	54	4
	PG20CHP1	INORGANIC CHEMISTRY PRACTICAL-1	3	54	Evaluation at the end of second semester
	PG20CHP2	ORGANIC CHEMISTRY PRACTICAL-1	3	54	
	PG20CHP3	PHYSICAL CHEMISTRY PRACTICAL-1	4	72	
		Total	25	450	16
II	PG20CH205	INORGANIC CHEMISTRY- II	4	72	4
	PG20CH206	ORGANIC CHEMISTRY-II	4	72	4
	PG20CH207	THEORETICAL CHEMISTRY-II	4	72	3
	PG20CH208	PHYSICAL CHEMISTRY-II	3	54	3
	PG20CHP1	INORGANIC CHEMISTRY PRACTICAL-1	3	54	3
	PG20CHP2	ORGANIC CHEMISTRY PRACTICAL-1	3	54	3

	PG20CHP3	PHYSICAL CHEMISTRY PRACTICAL-1	4	72	3
		Total	25	450	23
III	PG20CH309	INORGANIC CHEMISTRY-III	4	72	4
	PG20CH310	ORGANIC CHEMISTRY-III	4	72	4
	PG20CH311	PHYSICAL CHEMISTRY-III	4	72	4
	PG20CH312	ORGANIC CHEMISTRY-IV	3	54	4
	PG20CHP4	INORGANIC CHEMISTRY PRACTICAL-2	3	54	Evaluation at the end of fourth semester
	PG20CHP5	ORGANIC CHEMISTRY PRACTICAL-2	3	54	
	PG20CHP6	PHYSICAL CHEMISTRY PRACTICAL-2	4	72	
		Total	25	450	16
IV	PG20CH413	Elective-01-ADVANCED INORGANIC CHEMISTRY	5	90	4
	PG20CH414	Elective-02-ADVANCED ORGANIC CHEMISTRY	5	90	4
	PG20CH415	Elective-03-ADVANCED PHYSICAL CHEMISTRY	5	90	4
	PG20CH416	Elective-04-POLYMER CHEMISTRY	5	90	4
	PG20CH417	Elective-05-ANALYTICAL CHEMISTRY	5	90	4
	PG20CHP4	INORGANIC CHEMISTRY PRACTICAL-2	3	54	3
	PG20CHP5	ORGANIC CHEMISTRY PRACTICAL-2	3	54	3
	PG20CHP6	PHYSICAL CHEMISTRY PRACTICAL-2	4	72	3
	PG20CH4P	DISSERTATION/PROJECT			2
	PG20CH4V	VIVA			2
		Total	25	450	25
Grand Total					80

Appendix

1. **Evaluation first stage – Both internal and external to be done by the teacher)**

Grade	Grade Points	Range
A+	5	4.50 to 5.00

A	**4**	**4.00 to 4.49**
B	**3**	**3.00 to 3.99**
C	**2**	**2.00 to 2.99**
D	**1**	**0.01 to 1.99**
E	**0**	**0.00**

The final Grade range for courses, SGPA and CGPA

Range	Grade	Indicator
4.50 to 5.00	**A+**	**Outstanding**
4.00 to 4.49	**A**	**Excellent**
3.50 to 3.99	**B+**	**Very good**
3.00 to 3.49	**B**	**Good**
2.50 to 2.99	**C+**	**Fair**
2.00 to 2.49	**C**	**Marginal**
Upto1.99	**D**	**Deficient(Fail)**

Theory-External-ESE

Maximum weight for external evaluation is 30. Therefore Maximum Weighted Grade Point (WGP) is 150

Type of Question	Qn. No.'s	Grade Awarded	Grade Point	Weights	Weighted Grade Point
Short Answer	1	A+	5	1	5
	2	-	-	-	-
	3	A	4	1	4
	4	C	2	1	2
	5	A	4	1	4
	6	A	4	1	4
	7	B	3	1	3
	8	A	4	1	4
	9	B	3	1	3
	10	-	-	-	
Short Essay	11	B	3	2	6
	12	A+	5	2	10
	13	A	4	2	8
	14	A+	5	2	10
	15	-	-	-	-
	16	-	-	-	-
	17	A	4	2	8
	18	B	3	2	6
Long Essay	19	A+	5	5	25
	20	-	-	-	-
	21	-	-	-	-

	22	B	3	5	15
			TOTAL	**30**	**117**
Calculation : **Overall Grade of the theory paper = Sum of Weighted Grade Points /Total Weight = 117/30 = 3.90 = Grade B**					

Theory-Internal-CE

Maximum weight for internal evaluation is 5. Therefore Maximum Weighted Grade Point (WGP) is 25.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W *GP	Overall Grade of the Course
Assignment	1	A	4	4	**WGP/Total Weight= 24/5 =4.8**
Seminar	2	A+	5	10	
Test Paper 1	1	A+	5	5	
Test Paper 2	1	A+	5	5	
Total	**5**			**24**	**A+**

Practical-External-ESE

Maximum weight for external evaluation is 15. Therefore Maximum Weighted Grade Point (WGP) is 75

Components	Weight(W)	Grade Awarded	Grade Point(GP)	WGP=W* GP	Overall Grade of the Course
Written/Lab Test	7	A	4	28	**WGP/Total Weight= 58 / 15 = 3.86**
Lab involvement & record	3	A+	5	15	
Viva	5	B	3	15	
Total	**15**			**58**	**B**

Practical-Internal-CE

Maximum weight for internal evaluation is 5. Therefore Maximum Weighted Grade Point (WGP) is 25

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W *GP	Overall Grade of the Course
Written/ Lab Test	2	A	4	8	**WGP/Total Weight=17/5 =3.40**
Lab involvement & record	1	A+	5	5	

Viva	2	C	2	4	
Total	**5**			**17**	**B**

Project-External-ESE
Maximum weight for external evaluation is 15. Therefore Maximum Weighted Grade Point (WGP) is 75

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W*GP	Overall Grade of the Course
Relevance of the topic & Analysis	3	C	2	6	**WGP/Total Weight = 56/15= 3.73**
Project Content &Presentation	7	A+	5	35	
Project Viva- Voce	5	B	3	15	
Total	**15**			**56**	**B**

Practical-Internal-CE
Maximum weight for internal evaluation is 5. Therefore Maximum Weighted Grade Point (WGP) is 25

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W *GP	Overall Grade of the Course
Relevance of the topic & Analysis	2	B	3	6	**WGP/Total Weight= 21/5 = 4.2**
Project Content & Presentation	2	A+	5	10	
Project Viva-Voce	1	A+	5	5	
Total	**5**			**21**	**A**

Comprehensive viva-voce-External-ESE
Maximum weight for external evaluation is 15. Therefore Maximum Weighted Grade Point (WGP) is 75

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W*GP	Overall Grade of the Course
Comprehensive viva-voce	15	A	4	60	**WGP/Total Weight = 60 / 15 = 4**

Total	**15**			**60**	**A**

Comprehensive viva-voce-Internal-CE
Maximum weight for internal evaluation is 5. Therefore Maximum Weighted Grade Point (WGP) is 25

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W *GP	Overall Grade of the Course
Comprehensive viva-voce	5	A+	5	25	**WGP/Total Weight = 25/ 5 = 5**
Total	**5**			**25**	**A+**

2. Evaluation Second stage-(to be done by the College)

Consolidation of the Grade(GPA) of a Course PC-1

The End Semester Evaluation (ESE) (External evaluation) grade awarded for the course PC-1 is A and its Continuous Evaluation (CE) (Internal Evaluation) grade is A. The consolidated grade for the course PC-1 is as follows

Evaluation	Weight	Grade awarded	Grade Points awarded	Weighted Grade Point
External	3	A	4.20	12.6
Internal	1	A	4.40	4.40
Total	**4**			**17**
Grade of a course.	GPA of the course =Total weighted Grade Points/Total weight= **17/4 =4.25 = Grade A**			

3. Evaluation Third stage-(to be done by the College)
Semester Grade Point Average (SGPA)

Course code	Titleof the course	Credits (C)	Grade Awarded	Grade Points(G)	Credit Points (CP=C X G)
01	**PC-1**	**5**	**A**	**4.25**	**21.25**
02	**-----**	**5**	**A**	**4.00**	**20.00**
03	**-----**	**5**	**B+**	**3.80**	**19.00**
04	**-----**	**2**	**A**	**4.40**	**8.80**
05	**-----**	**3**	**A**	**4.00**	**12.00**

TOTAL		**20**			**81.05**
SGPA	**Total credit points / Total credits = 81.05/20 = 4.05= Grade- A**				

4. **Evaluation Third stage-(to be done by the College)**

Cumulative Grade Point Average (CGPA)

If a candidate is awarded three **A+** grades in semester 1(SGPA of semester 1), semester 2(SGPA of semester 2), semester 4(SGPA of semester 4) and **B** grades in semester 3(SGPA of semester 3). Then CGPA is calculated as follows:

Semester	Credit of the Semesters	Grade Awarded	Grade point (SGPA)	Credit points
I	20	A+	4.50	90
II	20	A+	4.60	92
III	20	B	3.00	60
IV	20	A+	4.50	90
TOTAL	**80**			**332**
CGPA= Total credit points awarded / Total credit of all semesters = 332 / 80= 4.15 (Which is in between 4.00 and 4.49 in 7-point scale) Therefore the overall Grade awarded in the programme is A				

ELIGIBILITY FOR ADMISSION

Academic eligibility should be satisfied as on the last date of submission of academic data. No candidate shall be admitted to the PG programme unless he/she possess the qualifications and minimum requirements thereof, as prescribed by Mahatma Gandhi University from time to time.

If an applicant for admission is found to have indulged in ragging in the past or if it is noticed later that he/she had indulged in ragging, admissions shall be denied or he/she will be expelled from Mar Athanasius College (Autonomous), Kothamangalam.

Candidates should have passed the corresponding Degree Examination under the 10 + 2 + 3 pattern with one core/main subject and two complementary/subsidiary subjects from any of the Universities in Kerala or of any other University recognized by Mahatma Gandhi University as equivalent thereto for admission, subject to the stipulation regarding marks.

OR

Candidates who have passed Degree examination with Double or Triple main subject and candidates who have passed the Degree Examination in Vocational or Specialized Programmes are also eligible for admission. However, they have to submit copy of the Equivalency/Eligibility Certificate from Mahatma Gandhi University, stating that, their Qualifying Examination is recognized for seeking admission to the relevant P.G. Degree Programme(s) as applicable, at the time of admission. This provision is not applicable in the case of those applicants who have passed their qualifying examination from MG University.

The minimum requirements for admission to PG Degree Programmes are:

M.Sc. Chemistry (Branch III)

Graduates who have passed qualifying examination in CBCS (2017)/CBCSS (2013) pattern	**Graduates who have passed qualifying examination in CBCSS (2009) pattern**	**Graduates who have passed qualifying examination in other patterns**
Graduation in Chemistry/Petrochemicalswith not less than CGPA/CCPA of 5.00 out of 10.00 in Core Group (Core + Complementary + Open Courses).	Graduation in Chemistry/Petrochemicals with not less than CGPA of 2.00 out of 4 in Core Group (Core + Complementary + Open Courses).	Graduation in Chemistry/ Petrochemicals with not less than 50% marks in Part III subjects (Main/Core +subsidiaries/Complementaries).
No weightage marks.		

The Open course under core group is taken only for reckoning the eligibility for applying for the PG programmes concerned. But a candidate cannot apply for the respective PG programmes solely on the basis of the open course selected under core group.

Relaxation in Marks in the qualifying examination:

(i) **Kerala Scheduled Caste/Scheduled Tribe Category**: The minimum grade in the qualifying examination for admission to the PG Degree programmes is 'C' in the seven point scale for CBCSS and a pass for pre CBCSS applicants.

(ii) **SEBC Category**: A relaxation of 3% marks in the qualifying examination from the prescribed minimum is allowed i.e. CGPA of 4.7 for CBCS (2017), CCPA of 4.7 for CBCSS (2013), and CGPA of 1.88 for CBCSS (2009) applicants and 47% marks for pre-CBCSS applicants for admission to M Sc. Programme in Chemistry.

(iii) **OEC Category:** A relaxation of 5% marks in the qualifying examination from the prescribed minimum is allowed i.e. CGPA of 4.5 for CBCS (2017), CCPA of 4.5 for CBCSS (2013), CGPA of 1.80 for CBCSS (2009) applicants and 45% marks for pre - CBCSS applicants for admission to M Sc. Programme in Chemistry.

(iv) **Persons with Disability category**: A relaxation of 5% marks in the qualifying examination from the prescribed minimum is allowed i.e. CGPA of 4.5 for CBCS (2017), CCPA of 4.5 for CBCSS (2013), CGPA of 1.80 for CBCSS (2009) applicants and 45% marks for pre – CBCSS applicants for admission to M Sc. Programme in Chemistry.

PROGRAMME OBJECTIVES AND OUTCOMES

PROGRAMME OBJECTIVES

To extend the depth and breadth of knowledge in all branches of chemistry to provide an excellent foundation for any kind of career of scientific leadership in academia and industry.

CAREER OPPORTUNITIES

1. Chemists or scientists in private and government research institutions.

2. Lecturers or researchers in higher learning institutions, following further their degree qualifications at Masters of PhD levels.

3. Officers in agencies or industries in which sound knowledge of chemistry and high levels of generic skills are required.

POSTGRADUATE PROGRAMME OUTCOME

PO No.	Upon completion of postgraduate programme, the students will be able to:
PO-1	Create, apply and disseminate knowledge leading to innovation
PO-2	Think critically, explore possibilities and exploit opportunities positively
PO-3	Work in teams, facilitating effective interaction in work places.
PO-4	Lead a sustainable life
PO-5	Embrace lifelong learning

MSc. CHEMISTRY PROGRAMME

PROGRAMME SPECIFIC OUTCOMES (PSO)

PSO No.	Upon completion of M.Sc. CHEMISTRY programme, the students will be able to:	PO No.
PSO-1	Acquire the depth and breadth of knowledge in the core areas of Inorganic, Organic ,Physical and Theoretical Chemistry	1,2,5
PSO-2	Demonstrate advanced knowledge in the relevant areas of chemistry research such as Computational Chemistry, Spectroscopy, Organic Synthesis, Polymer Chemistry and Nano Chemistry.	1,2,3,5
PSO-3	Develop critical thinking and analysis skills to solve complex chemical problems such as data analysis, structure and modeling, synthetic logic, spectroscopy and team-based problem solving.	1,2,3,5
PSO-4	Perform accurate quantitative measurements using contemporary chemical instrumentation, interpret experimental results, do calculations based on theoretical understanding and draw valid conclusions.	1,2,3,4,5

PSO-5	Achieve laboratory competence in relating chemical structure to spectroscopic phenomena	1,2,3,5
PSO-6	Acquire a broader understanding of research strategies, scientific thinking and data analysis	1,2,3,4,5
PSO-7	Conduct independent research under limited supervision and communicate the concepts of chemistry, through multimedia and research articles.	1,2,3,5

CAREER OPPORTUNITIES

1. Scientists or Chemists in private, government and research institutions.
2. Academicians or researchers in higher educational institutions, following further degree qualifications at Masters or Ph.D levels.
3. Officers in agencies or industries in which sound knowledge of chemistry and higher levels of generic skills are required.

DETAILED SCHEME AND PROGRAMME STRUCTURE OF M Sc CHEMISTRY PROGRAMME-TOTAL CREDITS-80

Semester	Course code	Course	Hours/ week	Contact hours	Credit
I	PG20CH101	INORGANIC CHEMISTRY-I	4	72	4
	PG20CH102	ORGANIC CHEMISTRY-I	4	72	4
	PG20CH103	THEORETICAL CHEMISTRY-I	4	72	4
	PG20CH104	PHYSICAL CHEMISTRY-I	3	54	4
	PG20CHP1	INORGANIC CHEMISTRY PRACTICAL-1	3	54	Evaluation at the end of second semester
	PG20CHP2	ORGANIC CHEMISTRY PRACTICAL-1	3	54	
	PG20CHP3	PHYSICAL CHEMISTRY PRACTICAL-1	4	72	
		Total	25	450	16
II	PG20CH205	INORGANIC CHEMISTRY- II	4	72	4
	PG20CH206	ORGANIC CHEMISTRY-II	4	72	4
	PG20CH207	THEORETICAL CHEMISTRY-II	4	72	3
	PG20CH208	PHYSICAL CHEMISTRY-II	3	54	3

	PG20CHP1	INORGANIC CHEMISTRY PRACTICAL-1	3	54	3
	PG20CHP2	ORGANIC CHEMISTRY PRACTICAL-1	3	54	3
	PG20CHP3	PHYSICAL CHEMISTRY PRACTICAL-1	4	72	3
		Total	25	450	23
III	PG20CH309	INORGANIC CHEMISTRY-III	4	72	4
	PG20CH310	ORGANIC CHEMISTRY-III	4	72	4
	PG20CH311	PHYSICAL CHEMISTRY-III	4	72	4
	PG20CH312	ORGANIC CHEMISTRY-IV	3	54	4
	PG20CHP4	INORGANIC CHEMISTRY PRACTICAL-2	3	54	Evaluation at the end of fourth semester
	PG20CHP5	ORGANIC CHEMISTRY PRACTICAL-2	3	54	
	PG20CHP6	PHYSICAL CHEMISTRY PRACTICAL-2	4	72	
		Total	25	450	16
IV	PG20CH413	Elective-01-ADVANCED INORGANIC CHEMISTRY	5	90	4
	PG20CH414	Elective-02-ADVANCED ORGANIC CHEMISTRY	5	90	4
	PG20CH415	Elective-03-ADVANCED PHYSICAL CHEMISTRY	5	90	4
	PG20CH416	Elective-04-POLYMER CHEMISTRY	5	90	4
	PG20CH417	Elective-05-ANALYTICAL CHEMISTRY	5	90	4
	PG20CHP4	INORGANIC CHEMISTRY PRACTICAL-2	3	54	3
	PG20CHP5	ORGANIC CHEMISTRY PRACTICAL-2	3	54	3
	PG20CHP6	PHYSICAL CHEMISTRY PRACTICAL-2	4	72	3
	PG20CH4P	DISSERTATION/PROJECT			2
	PG20CH4V	VIVA			2
		Total	25	450	25
Grand Total					80

Semester **I**	Code: **PG20CH101**	**INORGANIC CHEMISTRY-I**	Total Hrs:72 Hrs/Week:4	Credits :4

- To understand the theories of bonding and reaction mechanisms in coordination complexes.
- To interpret the electronic spectra & magnetic properties of complexes.
- To provide a perspective of the coordination chemistry of lanthanoids and actinoids.

Unit 1: Structural Aspects and Bonding in Coordination Complexes (18 hrs)

1.1 Sigma and pi bonding ligands such as CO, NO, CN^-, and R_3P.

1.2 Stability of complexes-thermodynamic aspects of complex formation-stepwise and overall stability constant, chelate effect. Irving William order of stability. Macrocycles- crown ethers, cryptands, porphyrins, macrocyclic effect, applications of crown ethers, template synthesis, Inverse crown ether complexes.

1.3 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, CFSE, Jahn Teller effect- effect on electronic spectra, theoretical failure of crystal field theory.

1.4 Molecular orbital theory-Evidence of covalency in the metal-ligand bond, nephelauxetic effect, MO 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 systems, splitting of terms, effect of spin orbit coupling, selection rules for electronic transition- d-p mixing and vibronic coupling-d-d transition.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams of d^1-d^9, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, Racah parameters. Charge transfer spectra.

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. Structural elucidation of complexes (Co and Ni complexes) using electronic spectra and magnetic moments

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

3.1 Kinetic stability of complexes, Labile and inert complexes, 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, effect of entering ligand, effect of

leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways, *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 stereochemistry of aquation of cis and trans isomers of Co(III) complexes, base hydrolysis – conjugate base mechanism, base hydrolysis of different isomers of $[Co(en)_2(NH_3)Cl]^{2+}$. Water exchange reactions.

3.3 Electron transfer reactions: outer sphere mechanism-Potential energy diagrams- Factors affecting outer sphere mechanism- Marcus theory, inner sphere mechanism- Taube mechanism. Nature of bridging ligand. Factors affecting inner sphere mechanism - remote and adjacent attack -Two electron transfer reactions.

3.4 Racemization reactions of octahedral complexes.

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. Prussian blue and related structures.

Unit 5: Coordination Chemistry of Lanthanoids and Actinoids (9 Hrs)

5.1 General characteristics of lanthanoids- Electronic configuration, Oxidation state, Lanthanide contraction- Cause and Consequences. Coordination compounds of lanthanoids. Electronic spectra, and magnetic properties of lanthanide complexes. Lanthanoid chelates. Uses of coordination complexes of lanthanoids as NMR shift reagents.

5.2 General characteristics of actinoids-difference between *4f* and *5f* orbitals, comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties. Actinide hypothesis. Trans actinoid elements

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	**10**	**8**	**4**	**22**
No.of Questions to be answered	**8**	**6**	**2**	**16**
CO No.	**Upon completion of this course, the students will be able to:**	**Knowledge Level**	**PSO No.**	
1	Demonstrate the theories of bonding to explain the structure, stability and properties of coordination compounds.	K2	1	
2	Analyze & interpret the electronic spectra & magnetic behavior of complexes.	K4	3	
3	Apply electronic spectra & magnetic moments for structure elucidation of coordination	K3	3	

	complexes.		
4	Analyze the kinetics and reaction pathways of complex formation	K4	1,3
5	Recognize the stereochemistry of coordination compounds.	K4	2,3
6	Acquire a comprehensive knowledge of coordination chemistry of inner transition compounds	K2	1
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **I**	Code: **PG20CH102**	**ORGANIC CHEMISTRY-I**	Total Hrs:72 Hrs/Week:4	Credits :4

- To apply the concepts of aromaticity, electron displacement effects and steric effect to explain physico-chemical properties of organic compounds.
- To elucidate the conformational analysis and stereochemistry of organic compounds.
- To explain the photochemistry and the mechanism of named organic reactions of carbonyl compounds.

Unit 1: Basic Concepts in Organic Chemistry (15 Hrs)

1.1 IUPAC nomenclature of organic compounds: polycyclic and spiro compounds.

1.2 Review of basic concepts in organic chemistry-Bonding-hybridization-MO picture of butadiene and allyl systems- Electronic displacement and steric effects and its applications with examples-H bonding: Inter and intramolecular hydrogen bonding.

1.3 Concepts of aromaticity-qualitative application of Huckel's MO theory to systems containing delocalized electron. Antiaromatic, non-aromatic and homoaromatic compounds -Non-benzenoid aromatic compounds-Examples of neutral and charged aromatic and non aromatic systems: cyclopropenyl cation, cyclopentadienyl anion, tropylium cation, azulene, fulvene, fulvalenes, annulenes. Effect of aromaticity on the stability and reactivity of aromatic systems.

Unit 2: Reactions of Carbonyl Compounds (12 Hrs)

2.1 Nucleophilic additions to carbonyls groups: addition of cyanide, ammonia, alcohol, Grignard reagent. Chemistry of enolates and enamines- lithium and boron enolates in aldol and Michael reactions-alkylation and acylation of enolates-Applications of Claisen, Claisen-Schmidt, Benzoin, Aldol, Perkin, Knoevenagel, Cannizzaro's, Wittig, Favorskil -Stork enamine reactions-Oxidation-reduction reactions: Baeyer-Villiger- Meerwein-Ponndorf-Verley reduction-Clemmensen reduction, Wolf- Kishner reduction (Problem solving type).

2.2 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition-Michael addition, Mannich reaction, Robinson annulations, Ene reaction.

Unit 3: Organic photochemistry (9 Hrs)

3.1 Jablonski diagram-triplet and singlet states-sensitization and quenching-photoreactions of carbonyl compounds, enes, dienes, dienones and arenes: Norrish type I and Norrish type II reactions- Patterno-Buchi reaction-Barton reaction-Di-π-methane rearrangement-photo Fries rearrangement- Hofmann-Loffler-Freytag reaction-photo oxidation of conjugated dienes- cis-trans isomerisation-photochemistry of nitro and azo groups-photochemistry of vision.

Unit 4: Stereochemistry of Organic Compounds (18 Hrs)

4.1 Concept of chirality-symmetry elements and chiral structures-conditions for optical activity-enantiomers-diastereoisomers-racemisation-resolution- relative and absolute configuration-R &S nomenclature-Cahn-Ingold-Prelog rules-optical purity-determination of enantiomeric excess-molecules with C based chiral centers- molecules with more than one center of chirality-constitutionally symmetrical and unsymmetrical chiral molecules-erythro, threo nomenclature.

4.2 Stereochemistry of sulphur and nitrogen compounds.

4.3 Axial, planar and helical chirality with examples-stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidene cycloalkanes.

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 assymmetric synthesis.

4.5 Geometrical isomerism-nomenclature-E-Z notation of compounds with one and more double bond in acyclic systems-methods of determination of geometrical isomers-interconversion of geometrical isomers-stereochemistry of aldoximes, ketoximes-naming-isomerism-methods of determining configuration.

Unit 5: Conformational Analysis **(18 Hrs)**

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. Anchoring group and conformationally biased molecule.

5.4 Conformational analysis of cyclic systems-cyclohexane and mono and disubstituted cyclohexanes- Cyclohexanone and substituted 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 (E_1 & E_2)-dehalogenation, dehydrohalogenation, dehydration, Saytzeff and Hofmann elimination, semipinacolic deamination and pyrolytic elimination- substitution (SN^1 & SN^2)-oxidation of 2^0 alcohols. Esterification of menthols-carboxyl group-hydroxyl group. Hydrolysis of esters and tosylates.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. of Questions to be answered	8	6	2	16

CO No.	Upon completion of this course, the students will be able to:	Knowledge Level	PSO No.
1	Interpret the aromaticity of organic molecules.	K4	1, 3
2	Predict the physiochemical properties of organic molecules based on electron displacement and steric effect.	K3	3
3	Analyze the reaction mechanism of carbonyl compounds.	K4	1
4	Acquire a comprehensive knowledge of organic photochemical reactions.	K2	1
5	Develop skills to predict the stereochemistry of organic molecules	K4	3
6	Relate the conformation and reactivity of cyclic, acyclic, fused and	K4	1,3

	bridged bicyclic systems.		
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **I**	Code: **PG20CH103**	**THEORETICAL CHEMISTRY-I**	Total Hrs:72 Hrs/Week:4	Credits :4

- Refresh the mathematical concepts of vectors and tensors to chemical systems by solving eigen value and eigen vector problems in matrices and differential equations.
- Solve elementary model problems in quantum mechanics exactly.
- Discuss the molecular symmetry operations of the group and its characterization by irreducible representations.
- Apply the great orthogonality theorem to derive simple point groups.

Unit 1: Introduction to Quantum Mechanics (18 Hrs)

1.1 Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator.

1.2 Eigen value postulate, eigen value equation, eigen functions of commuting operators; Expectation value postulate; Postulate of time dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((Lx, Ly, Lz), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

1.3 Derivation of time independent SWE–Wave functions and SWE of all simple systems. 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.

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

2.1 Vibrational motion: Simple harmonic oscillator – force constant – zero point energy –Hermite equations and Hermite polynomials (qualitative idea only) Rotational Motion: co-ordinate systems, cartesian, The wave equation in spherical polar coordinates. Particle moving in a ring, particle on a sphere - Rigid rotator – reduced mass – moment of inertia rotational energy levels –Legendre equations and Legendre polynomials (qualitative idea only)

2.2 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.

2.3 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 3: Group Theory and Molecular Symmetry (18 Hrs)

3.1 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.

3.2 Symmetry in crystals-Hermann-Mauguin symbols. Screw axis, Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.

3.3 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations.

3.4 Reducible and irreducible representations- construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v},C_{2h}, C_{3v}, C_3 and C_{4v}. Direct product of representations.

Unit 4: Application of group theory in Spectroscopy (18 Hrs)

4.1 Applications in vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra.

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

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For Units 1 & 2

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For Units 3 &4

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QUESTION PAPER PATTERN

Module	**Part A (Wt. : 1) Short Answer**	**Part B (Wt. : 2) Short Essay**	**Part C (Wt. : 5) Long Essay**	**Total**
Total No. of Questions	**10**	**8**	**4**	**22**
No.of Questions to be answered	**8**	**6**	**2**	**16**
CO No.	**Upon completion of this course, the students will be able to:**	**Knowledge Level**	**PSO No.**	
1	Use mathematical techniques in linear algebra for eigen values and eigen vectors and first and second order differential equations.	K1, K2	1	
2	Solve the model problems in quantum mechanics.	K3, K4	1,3	
3	Explore quantum mechanical operators corresponding to angular momenta.	K5	1,2,3	

4	Apply Ladder operator method for angular momentum.	K4	3
5	Explain the space quantization of orbital and spin angular momenta.	K2	2
6	Differentiate the features of symmetry of molecules and crystals.	K2	2,3
7	Apply group theory in vibrational, Raman and Electronic Spectroscopy.	K3	3
8	Explore new areas of research both in group theory and Quantum mechanics.	K6	8
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **I**	Code: **PG20CH104**	**PHYSICAL CHEMISTRY-I**	Total Hrs:54 Hrs/Week:3	Credits :4

- To understand the inter relation between thermodynamic properties in closed and open systems.
- To study the dependence of fugacity on state variables.
- To evaluate the changes in thermodynamic properties on mixing of ideal as well as real systems.
- To interpret third law of thermodynamics.
- To analyse the phase equilibria of three component system.
- To understand the thermodynamics of irreversible processes.
- To formulate the thermodynamics of bioenergetics.
- To study the transport phenomenon in gases.
- To quantify thermodynamic properties by bridging quantum mechanics and probability theory.

Unit 1: Thermodynamics **(18 Hrs)**

1.1 Thermodynamic equations of state, Maxwell relations and significance.

1.2 Partial molar quantities, determination of partial molar properties- intercept method, density method to determine partial molar volume.

1.3 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

1.4 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's first and second laws, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.

1.5 Third law of thermodynamics: Nernst heat theorem, determination of absolute entropies using third law.

1.6 Three component systems-graphical representation. 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.

1.7 Thermodynamics of irreversible processes with simple examples. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermal osmosis and thermoelectric phenomena.

1.8 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 2: Gaseous State **(9 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 frequency in a single gas and in a mixture of two gases, mean free path, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states, transport properties of gases – viscosity, thermal conductivity and diffusion

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

3.1 Permutation, probability, thermodynamic probability, macro states and microstates Stirling's approximation, 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 function according to forms of energy. Sackur-Tetrode equation. Calculation of equilibrium constant by using partition function.

3.2 Thermodynamic probability and entropy, statistical formulation of third law of thermodynamics, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

3.3 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, supercooled liquids. Fermi Dirac distribution: examples of particles. Comparison of three statistics.

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

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QUESTION PAPER PATTERN

Module	**Part A (Wt. : 1) Short Answer**	**Part B (Wt. : 2) Short Essay**	**Part C (Wt. : 5) Long Essay**	**Total**
Total No. of Questions	**10**	**8**	**4**	**22**
No. of Questions to be answered	**8**	**6**	**2**	**16**
CO No.	**Upon completion of this course, the students will be able to:**	**Knowledge Level**	**PSO No.**	
1	Evaluate the thermodynamic properties (ideal and real) in closed and open systems.	K5	1	
2	Interpret phase equilibria of three component systems	K4	1	
3	Apply the kinetic theory to the transport phenomena in gases.	K3	1	
4	Compute the absolute value of thermodynamic properties from classical and	K5	2,3	

	statistical Principles		
5	Relate the thermodynamic properties and partition function	K3	1,3
6	Explain Bose - Einstein statistics and the behaviour of liquid helium	K4	1,8
7	Apply thermodynamic principles to irreversible process and bioenergetics.	K3	2,4,8
8	Formulate the theory of heat capacity of solids	K5	1,3
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **II**	Code: **PG20CH205**	**INORGANIC CHEMISTRY-II**	Total Hrs:72 Hrs/Week:4	Credits :4

- The learners should be able to apply, analyse and evaluate structure and bonding aspects of different kinds of compounds of the main group elements and the basic concepts of defects in crystals & solid state reactions.
- To know the synthetic techniques in inorganic chemistry.
- To give an insight into the theories of bonding in solids.
- To know the synthesis, structure and bonding in inorganic chains, rings, cages and clusters.

Unit 1: Solid State Chemistry (18 Hrs)

1.1 Close Packing. Imperfections in solids-point defects, Stoichiometric and non-stoichiometric defects, Vegard's rule. Line defects and plane defects.

1.2 Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), AXO_3 (Perovskite) AX_2O_4 (spinel), Spinels and inverse spinels, stability of spinels.

1.3 Diffusion in solids. Mechanisms- vacancy diffusion, Interstitial diffusion, Diffusion equation-Coefficient of diffusion.

1.4 Solid state reactions-Factors affecting the rate of solid state reactions, Sintering.

1.5 Phase transition in solids- Thermodynamic Classification-first and second order phase transitions (Brief study only). Nucleation, growth and critical size in phase transition. Order-disorder transitions, spinodal decomposition.

1.6 Crystal Growth. Growth of Single crystal. Crystal growth from melt. Crystallization from solution-Hydro thermal method, gel method. Crystal growth from Vapour- Chemical Vapour Deposition.

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

2.1 Free electron theory of solids- advantages and disadvantages of free electron theory- , Zone theory-Kronig Penney model.

2.2 Band theory of solids-MO theory. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Drift velocity-current density J-mobility of charge carriers-conductivity Hall Effect- Significance of Hall coefficient-Pyroelectricity- Piezo electricity- Ferro electricity-hysteresis.

2.3 Metal oxides- Structure and propertiesHigher oxide and complex oxides of Transition elements-Oxides with M_2O_3-Corundum structure, Rhenium trioxide. Conductivity in mixed oxides, Magnetic properties of solids- Cooperative magnetism-Ferromagnetic materials-Curie temperature, Antiferromagnetism, Neel temperature, Super exchange, Ferrimagnetism. . Magnetic properties of transition metal oxides, garnets, spinels, Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties-phosphors, solid state lasers.

2.4 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)- High temperature superconductors- Super conducting cuprates – Synthesis, structure and applications of-YBaCu oxide system. Josephson Tunneling-Conventional and organic superconductors, fullerenes.

Unit 3: Chemistry of Materials –Structure, Properties and Applications. (18 Hrs)

3.1 Chains - catenation, heterocatenation. Silicate minerals. Structure of silicates-common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets,

Frame work silicates. Zeolites. Silicones. Infinite metal chains.

3.2 Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications.

3.3 One dimensional Solids. Magnetic, Electrical and optical properties of KCP and other Pt compounds, $KCuF_3$ and RbF_3. One dimensional conductor-Polythiazyl.

3.4 Rings-topological approach to boron hydrides, styx numbers. Synthesis, structure and bonding in borazines, ring silicates, silicones, and phosphazenes. Heterocyclic inorganic ring systems-Synthesis, structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems: Structure and bonding in sulphur, selenium and phosphorous compounds.

Unit 4. Inorganic Materials and Cluster Compounds. (18 Hrs)

4.1 Cages: synthesis, structure and bonding of cage like structures of phosphorous – phosphorous-oxygen compounds. Boron cage compounds-Wade's rule, MNO rule, boranes, carboranes, metallacarboranes.

4.2 Clusters: Halide clusters- Trinuclear, tetranuclear and hexanuclear clusters. Polyatomic Zintl anions and cations.

4.3 Carbon allotropes- Synthesis, properties and applications. sp3 forms- Diamond, Lonsdaleite, carbon dots, sp^2 forms- graphite, graphite intercalation compounds, graphene, graphene quantum dots, carbon nanotubes, fullerenes, glassy carbon, sp form-Linear acetylenic carbon, Mixed sp3sp2 forms- Q carbon.

4.4 Boron nitrides- hexagonal and cubic, Carbon nitride, structure, properties and applications, other superhard materials- Osmium diboride, Rhenium boride.

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Chemistry, Wiley, 1974.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No.of Questions to be answered	8	6	2	16
CO No.	Upon completion of this course, the students will be able to:	Knowledge Level	PSO No.	
1	Familiarize the structure of inorganic solids and defects in crystals	K2	1	
2	Understand the basic concepts of solid state reactions	K2	2	
3	Acquire a comprehensive knowledge about the synthetic techniques of crystal growth	K2	2	
4	Demonstrate the theories of bonding in inorganic solids and concepts of superconductivity	K2	2	

5	Develop skills to correlate structure-composition – properties (magnetic, electrical and optical) in inorganic crystalline solids	K3	3
6	Explain the synthesis, structural and bonding aspects of different kinds of compounds of main group elements	K1, K2	1
7	Get advanced knowledge about the synthesis, structure bonding aspects and properties of inorganic cages and cluster materials.	K2	1, 2
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **II**	Code: **PG20CH206**	**ORGANIC CHEMISTRY-II**	Total Hrs:72 Hrs/Week:4	Credits :4

- To get insight of organic reaction mechanisms and methods of determining the reaction mechanisms
- To acquire a deep knowledge of reactive intermediates and pericyclic reactions
- To introduce the physical organic concepts that allows the outcome of organic reactions to be rationalised and understood**.**

Unit 1: Organic Reaction Mechanisms **(18 Hrs)**

1.1 Organic reaction mechanisms of aliphatic nucleophilic substitution reactions: SN^1, SN^2, SE^1, SE^2- Elimination reactions: $E^1$and E^2.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent, neighbouring group participation, salt effect and special salt effect on nucleophilic substitution (SN^2 and SN^1)

and elimination (E^1 and E^2) reactions. Elimination at bridge head carbon-Bredt's rule-Chugav reaction-elimination vs substitution.

1.3 Mechanisms of addition reactions-regioselectivity-Markovnikov's addition: carbocation mechanism-anti-Markovnikov's addition: radical mechanism.

1.4 Mechanisms of electrophilic and nucleophilic aromatic substitution reactions: Arenium ion, SN^2Ar, SN^1Ar, S_{RN}^1 and Benzyne mechanisms

1.5 Mechanisms of esterification and ester hydrolysis-acyl oxygen and alkyl oxygen cleavage: AAC^2, AAC^1, AAL^1, BAC^2 and BAL^1 mechanisms.

Problems based on the above topics

Unit 2: Physical Organic Chemistry (9 Hrs)

Methods of determining reaction mechanisms-primary and secondary kinetic isotope effects-kinetic versus thermodynamic control of product formation-linear free energy relationship-Hammet and Taft equation-Curtin-Hammett principle-Hammond postulate-bulk and specific solvent effects-solvent polarity parameters: Y, Z and E parameters

Unit 3: Reactions of Carbanions (6 Hrs)

3.1 C-X bond (X = C, O, N) formations through the intermediary of carbanions-named reactions under carbanion chemistry: Mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination, Woodward and Prevost hydroxylation reactions.

3.2 Ylides: chemistry of phosphorous and sulphur ylides - Wittig and related reactions, Peterson olefination.

Problems based on the above topics.

Unit 4: Reactions of Carbocations (6 Hrs)

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

Problems based on the above topics

Unit 5: Reactions of Free radicals (6 Hrs)

5.1 Addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules-fragmentation and rearrangements. Hydroperoxide: formation, rearrangement and reactions-Autooxidation.

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

Problems based on the above topics.

Unit 6: Carbenes and Nitrenes (9 Hrs)

6.1 Structure of carbenes: singlet and triplet-generation of carbenes-addition and insertion reactions.
6.2 Rearrangement reactions of carbenes such as Wolff rearrangement-generation and reactions of ylides by carbenoid decomposition.
6.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.
6.4 Hoffmann, Curtius, Lossen, Schmidt reactions.

Problems based on the above topics.

Unit 7: Concerted reactions (18 Hrs)

7.1 Conservation of molecular orbital symmetry-methods to explain pericyclic reactions- Thermal and photochemical reactions- Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - Huckel-Mobius method-PMO method-Correlation diagram method analysis. Classification: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions.
7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), 1,3- dipolar cycloaddition (introductory).
7.3 Unimolecular pyrolytic elimination reactions: chelotropic elimination, decomposition of cyclic azo compounds.

Problems based on the above topics.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	**10**	**8**	**4**	**22**
No.of Questions to be answered	**8**	**6**	**2**	**16**
CO No.	**Upon completion of this course, the students will be able to:**	**Knowledge Level**	**PSO No.**	
1	Discuss the mechanism of different organic reactions and factors which affect the reaction rate	K2	1,2	
2	Recognize the different reaction intermediates in organic reactions.	K2	1	
3	Familiarize with different types of pericyclic reactions in organic chemistry and orbital correlation approaches.	K2	1	
4	Highlight the applications of pericyclic reactions in organic synthesis	K3	3	

5	Understand the concept of physical organic chemistry.	K2	1
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester	Code: **PG20CH207**	**THEORETICAL CHEMISTRY-II**	Total Hrs:72 Hrs/Week:4	Credits :3

II				

- Recognize the most significant and elementary solutions of Schrodinger equation in molecular quantum mechanics through a study of time independent perturbation theory, valence bond and molecular orbital theories.
- Apply the concept of linear combination of atomic orbitals to hybridization and directed bonding in polyatomic molecules.
- Solve real-world problems using advanced numerical programs through GAMESS software.

Unit 1: Approximation Methods in Quantum Mechanics (18 Hrs)

1.1 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.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, 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.

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

Unit 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_{3v} and D_{3h} point groups. Woodward-Hoffmann rule.

Unit 4: Computational Chemistry (18 hrs)

4.1 Introduction and scope of computational chemistry. Potential energy surface - Global minimum, Local minima, saddle points.

4.2 Molecular mechanics methods: Force fields-bond stretching, angle bending, torsional terms, non-bonded interactions. Mathematical expressions. Parameterisation from experiments or quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.3 Ab initio methods: 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, Hartree-Fock limit. Post Hartree-Fock methods. Introduction to Møller Plesset Perturbation Theory, Configuration Interaction.

4.4 General introduction to semiempirical methods: Basic principles and terminology.

4.5 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.6 Comparison of ab initio, semiempirical and DFT methods.

Unit 5: Computational Chemistry Calculations (9 Hrs)

5.1 Introduction to computational chemistry software packages. Molecular geometry input-cartesian coordinates and internal coordinates. Z-matrix of single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules.

5.2 Computational chemistry calculations using simple molecular structures of water and ammonia. Input file format - Method, Basis Set, Calculation type, Spin Multiplicity, Coordinate format. Single Point Energy, Geometry Optimization.

5.3 General format of GAMESS input file. GAMESS key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization and frequency calculation.

References

For **Units 1, 2 & 3**

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2. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
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11. Density functional theory of atoms and molecules, R G Parr and W Yang; Chemical hardness: Applications from Molecules to Solids, R G Pearson.

For Units 4 & 5

1. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of
2. Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
3. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	**10**	**8**	**4**	**22**
No. Questions to be answered	**8**	**6**	**2**	**16**
CO No.	**Upon completion of this course, the students will be able to:**	**Knowledge Level**	**PSO No.**	
1	Use mathematical techniques in linear algebra for eigen values and eigen vectors and first and second order differential equations.	K1,K2	1	
2	Solve the model problems in quantum mechanics.	K3,K4	1,3	
3	Explore quantum mechanical operators corresponding to angular momenta.	K5	1,2,3	
4	Apply Ladder operator method for angular momentum.	K4	3	
5	Explain the space quantization of orbital and spin angular momenta.	K2	2	
6	Differentiate the features of	K2	2,3	

	symmetry of molecules and crystals.		
7	Apply group theory in vibrational, Raman and Electronic Spectroscopy.	K3	3
8	Explore new areas of research both in group theory and Quantum mechanics.	K6	8
Knowledge Levels: K1-Remembering; K2-Understanding; K3-Applying; K4-Analyzing; K5-Evaluating; K6-Creating.			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **II**	Code: **PG20CH208**	**PHYSICAL CHEMISTRY-II**	Total Hrs:54 Hrs/Week:3	Credits :3

1. To study the interaction of electromagnetic radiation with matter.
2. To study the principles, instrumentation and applications of microwave, IR, electronic, NMR, ESR, NQR and Mossbauer spectroscopy.

Unit 1: Foundations of Spectroscopic Techniques **(27 Hrs)**

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.

1.2 Microwave spectroscopy: classification of molecules (linear, symmetric tops, spherical tops and asymmetric tops), rigid rotor model, selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max} , effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Vibrational spectra of diatomics, Morse potential energy diagram, effect of anharmonicity, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, breakdown of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, introduction to FTIR spectroscopy. Instrumentation of 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, applications of Raman spectroscopy.

1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

Unit 2: Resonance Spectroscopy (27 Hrs)

2.1 **NMR spectroscopy** : Interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift and its representation- **δ** scale of PMR and CMR. Spin- spin coupling: Theory and illustration with AX system.

2.2 **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, introduction to solid state NMR, magic angle spinning.

2.3 **EPR spectroscopy**: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values , fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

2.4 **Theory and important applications of NQR spectroscopy**.

2.5 **Mossbauer spectroscopy**: Principle, Doppler Effect, recording of spectrum, isomer shift, factors determining isomer shift, effect of electrical and magnetic field, application to iron complexes.

References

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn.,Tata McGraw Hill, 2013.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2nd Edition 2007.
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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Study the interaction of electromagnetic radiation with matter.	K2	2,3
2	Apply quantum mechanical principles to calculate various energy levels and transitions between these levels in atoms and molecules.	K3	.3
3	Explain Fourier Transform spectroscopic technique to record IR, PMR and CMR spectrum.	K2	1,2,3,
4	Translate the second order spectra to first order one.	K3	1,3
5	Relate structure of organic compounds with spectroscopic data.	K6	1,2,3,8
6	Compute the molecular parameters like from spectral data.	K6	1,2,3
7	Investigate the mechanism of the reaction from ESR spectrum using g values.	K6	1,2,3,4
8	Investigate the stereochemistry of compounds from NOE effect.	K6	1,2,3,8
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semesters	Code:	INORGANIC CHEMISTRY	Total Hrs:108	Credits
I &II	**PG20CHP1**	**PRACTICAL-1**	Hrs/Week:3	:3

1: Understand the principles of intergroup separation of cations.
2: Learn semi micro qualitative analysis for a mixture containing common and less common cations
3: Expertise in the preparation, drying and recrystallisation of inorganic complexes

4: Accrue the ability to correlate the IR and electronic spectra of various inorganic complexes with their structures
5: Develop skills in the spectrophotometric method of estimation of metal ions
6: Set up glass wares and apparatus to conduct experiments with minimum or without error.

PART I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as Ag^{+} , Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, $Sn^{2+,}$ Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+} , Mn^{2+}, Co2+, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+} , Na^{+} , K^{+} and $NH4^{+}$ and 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 of complexes using IR 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.

References

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4. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

COURSE OUTCOME

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Understand the principles of intergroup separation of cations.	K2	1,2
2	Learn semi micro qualitative analysis for a mixture containing common and less common cations	K4	4

3	Expertise in the preparation, drying and recrystallisation of inorganic complexes	K3	4,5
4	Accrue the ability to correlate the IR and electronic spectra of various inorganic complexes with their structures	K5	3
5	Develop skills in the spectrophotometric method of estimation of metal ions	K4	4
6	Set up glass wares and apparatus to conduct experiments with minimum or without error	K4	4,5
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Semesters	Code:	**ORGANIC CHEMISTRY**	Total Hrs:108	Credits
I &II	**PG20CHP2**	**PRACTICAL-1**	Hrs/Week:3	:3

Course outcome:

1: Understand the general methods of separation and purification of organic compounds.

2: Develop skills for the separation of organic binary mixtures by chemical/solvent separation methods.

3: Familiarize with the identification of organic compounds by TLC / paper chromatography.

4: Acquire skills for the separation/ purification of organic mixtures by column chromatography.

5: Familiarize to draw structure of organic compounds and mechanisms of reactions using chemsketch software.

PART I

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

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Identification of organic compounds by TLC/Paper chromatography (mixture of aminoacids)
3. Separation/ purification of organic mixtures by column chromatography

PART III

Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

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, 1974.
2. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
3. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.
4. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 5th edition, 1989.

COURSE OUTCOME

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.

1	Understand the general methods of separation and purification of organic compounds.	K2	5
2	Develop skills for the separation of organic binary mixtures by chemical/solvent separation methods.	K4	5
3	Familiarize with the identification of organic compounds by TLC / paper chromatography.	K2	5
4	Acquire skills for the separation/ purification of organic mixtures by column chromatography.	K2	5
5	Familiarize to draw structure of organic compounds and mechanisms of reactions using chemsketch software.	K2	3
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Semesters **I &II**	Code: **PG20CHP3**	**PHYSICAL CHEMISTRY PRACTICAL-1**	Total Hrs:144 Hrs/Week:3	Credits :3

1. Analyze the extent of adsorption and verify adsorption isotherms.
2. Construct and interpret the phase diagrams of binary and tertiary systems.
3. Apply the distribution law to various solutes in different solvent pairs.

4. Determine the composition using surface tension measurements.

5. Compare and apply theoretical approaches in stimulating various scientific problems and calculating properties of molecules

(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. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. 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) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements.

Part B

Computational chemistry experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
3. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
4. GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html

COURSE OUTCOME

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Analyze the extent of adsorption and verify adsorption isotherms.	K4	4
2	Construct and interpret the phase diagrams of binary and tertiary systems.	K4	4
3	Apply the distribution law to various solutes in different solvent pairs.	K3	4
4	Determine the composition using surface tension measurements.	K3	4
5	Compare and apply theoretical approaches in stimulating various scientific problems and calculating properties of molecules	K3	2,4

Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create

Semester **III**	Code: **PG20CH309**	**INORGANIC CHEMISTRY-III**	Total Hrs:72 Hrs/Week:4	Credits :4

1. Identify the structure and bonding aspects of simple organometallic compounds.
2. Analyse the mechanism of selected catalytic organic reactions from the structure – bonding aspects and reactivity of simple organometallic compounds.

3. Identify the occurrence, active site, structure and functions of some transition metal ion containing metalloproteins and enzymes.
4. To learn the fundamentals, instrumentation and Concepts of nuclear energy.
5. To familiarize the students with nuclear and radioisotopic techniques.

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

1.1 Hapto nomenclature of organometallic compounds, 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, ferrocene and dibenzene chromium -structure and bonding. Metal carbene complexes, Fischer-type and Schrock-type complexes and carbyne complexes.

1.2 Metal Carbonyls: CO- as a π acid ligand, synergism, Molecular electronic structure –EAN rule. Binary Carbonyl complexes- Mononuclear and Binuclear carbonyls. Preparation, properties, structure, bonding in metal carbonyls, bridging modes of CO, IR spectral studies of bridging and non-bridging CO ligands. Polynuclear metal carbonyls with and without bridging, Carbonyl clusters- LNCCS and HNCCS, Isoelectronic and isolobal analogy, cluster valence electrons, Wade Mingos rules. Ligands similar to CO- Cyanides, nitrosyls, dinitrogen. Metal cyanides, metal nitrosyls and dinitrogen complexes.

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

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

2.3 Redistribution reactions - fluxional isomerism of allyl, cyclopentadienyl and allene systems.

Unit 3: Catalysis by Organometallic Compounds (9 Hrs)

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

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

3.3 Hydroformylation of olefins using cobalt and rhodium catalyst - Oxo process

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

3.5 Carbonylation reactions-Monsanto acetic acid process.

3.6 Olefin metathesis, photo dehydrogenation catalyst (“Platinum Pop”).

3.7 .Oxidation of olefins: Palladium catalysed oxidation of ethylene-the Wacker process

Unit 4: Nuclear Chemistry (18 Hrs)

4.1 Nuclear structure: Composition, nuclear size, shape, density, nuclear spin and parity, nuclear binding forces. Nuclear models-shell model, liquid drop model, collective model, optical model.

4.2 Radioactive decay. Alpha decay. Beta decay-Types of beta decay, β^+, β^-, neutrino, antineutrino, Dirac theory and Positron emission, electron capture. Gamma decay- de-excitation of excited molecules, nuclear isomerism and isomeric transition.

4.3 Nuclear reactions-Q-Value and reaction threshold, reaction cross section, neutron capture cross section. Photonuclear, Thermonuclear and Fusion reactions.
Nuclear fission - Fission fragment and mass distribution, fission yield, fission cross section and threshold, fission neutrons, prompt and delayed neutrons, fission by high energy neutrons.

4.4 Nuclear reactors- Fast Breeder Reactor, Reactor Safety precaution, Management of radioactive waste- Low level Waste, Intermediate level Waste, High level Waste.

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

4.6 Applications of radioisotopes-Analytical applications-Isotope dilution analysis, Determination of volume of blood in patient, radiometric titrations, Neutron Activation Analysis, Prompt Gamma Neutron Activation Analysis. Applications of radio isotopes in industry, agriculture.

4.7 Radiation chemistry of water, Relevance of radiation chemistry in biology. Radiation polymerization.

Unit 5: Bioinorganic Chemistry **(18 Hrs)**

5.1 Biochemistry of Iron
Oxygen Carriers- Structure and functions of haemoglobin and myoglobin, Oxygen transport mechanism of Haemoglobin, cooperativity in haemoglobin. Bohr effect and phosphate effect. Hemerythrin-Structure and function. Redox Metalloenzymes-Cytochromes- Classification. Role in oxidative phosphorylation of ADP to ATP. Cytochrome P_{450}-Structure and functions. Iron Sulphur Proteins- Structure and function of Rubredoxin, Ferridoxin. Nitrogenase. Storage and transport of iron in biological systems-Ferritin, transferrin and Siderophores.

5.2 Biochemistry of Zn and Copper.
Structure and functions of carboxypeptidase and carbonic anhydrase, Superoxide dismutase. Copper proteins – Classification (Type 1, II and III) – Plastocyanin, cytochrome oxidase, Hemocyanin.

5.3 Biochemistry of alkali and alkaline earth metals.
Mechanism of ion transport across membranes, Sodium Potassium pump, Ionophores-Valinomycin. Chlorophyll-Photosynthesis, PS I & PS II.

5.4 Vitamin B_{12}-Structure and biological importance.

5.5 Metals in medicine - Therapeutic applications of *cis*-platin- Mechanism of action

5.6 Essential and trace elements in biological systems, Toxic effects of metals (Cd, Hg, Cr and Pb).

References

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3 F. A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999

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6 Shriver & Atkins , Inorganic Chemistry (Solution Manual), Fourth edition . Oxford University Press 2007

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9 B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	**10**	**8**	**4**	**22**
No. Questions to be answered	**8**	**6**	**2**	**16**

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Understand the structure, bonding aspects and chemical reactions of organometallic compounds	K2	2

2	Analyse the role of organometallic compounds as catalysts in selected organic reactions	K4	3
3	Acquire a comprehensive knowledge and understanding about the concepts of nuclear chemistry , nuclear reactions and nuclear reactors	K2	2
4	Recognise the applications of radioisotopes in theoretical, analytical and industrial fields.	K4	3
5	Elucidate the structure and functions of some biologically important inorganic transition metal complexes.	K5	3
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **III**	Code: **PG20CH310**	**ORGANIC CHEMISTRY-III**	Total Hrs:72 Hrs/Week:4	Credits :4

1. To introduce the concept of protecting groups in organic synthesis.
2. To equip students with the skills to plan how to prepare organic molecules.

3. To introduce a range of key reactions for application in organic synthesis**.**
4. To introduce the different chemical reagents and reactions used in organic synthesis.

Unit 1: Retrosynthetic Analysis **(9 Hrs)**

1.1 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.

1.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Retrosynthesis of luciferin. Umpolung equivalent - Peterson olefination, Ireland-Claisen rearrangement.

Unit 2: Organometallics **(9 Hrs)**

2.1 Preparation and applications in organic synthesis of (i) Organo lithium compounds and addition to $-C=O$, $-COOH$ and $-CONR_2$ (ii) Lithium dialkylcuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents and Glaser coupling (iv) Dialkyl cadmium compounds and (v) Benzene tricarbonyl chromium and reaction with carbanions.

Unit 3: **Organic Synthesis via Oxidation and Reduction** **(18 Hrs**)

3.1 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 Silver based 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 oxidation.

3.2 (a) Catalytic hydrogenation (Heterogeneous and Homogeneous) (b) Metal based reductions- Birch reduction, Pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - LiAlH4, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkylstannane. Meerwein-Pondorff-Verley Reduction, Baker's yeast.

Unit 4: Modern Synthetic Methods and Reagents **(18 Hrs)**

4.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Noyori reaction, Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald- Hartwig, Ullmann reactions. Kumuda coupling, Wohl-Ziegler reaction. Reagents such as NBS, DDQ, DCC, Gilmann reagent.

4.2 Introduction to multicomponent reactions- Three component reactions (Mannich reaction, Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (Triazole synthesis).

Unit 5: Construction of Carbocyclic and Heterocyclic Ring System (9 Hrs)

5.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization. Construction of macrocyclic rings-ring closing metathesis.

5.2 Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Unit 6: Protecting Group Chemistry (9 Hrs)

6.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection.

6.2 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).

6.3 Role of trimethyl silyl group in organic synthesis.

References

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Understand the role of protecting groups in organic synthesis.	K2	1
2	Describe the preparations of organometallics and apply in organic synthesis.	K1	1,2
3	Explain the key reactions in organic chemistry including substitution reactions of heterocycles, reactions involving enols and enolates.	K1,K2	3
4	Discuss the role of reagents in organic synthesis	K3	4
5	Execute retrosynthetic analysis of organic molecules.	K4	5
6	Design different approaches towards the synthesis of three, four, five and six membered rings	K5,K6	4
7	Formulate modern synthetic methods in coupling reactions.	K6	6
8	Investigate the scope of metal and non metal based oxidation reactions in organic synthesis.	K5	6
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester **III**	Code: **PG20CH311**	**PHYSICAL CHEMISTRY-III**	Total Hrs:72 Hrs/Week:4	Credits :4

1. To understand the basic principles of chemical kinetics
2. To impart knowledge of applications of reaction kinetics
3. To appreciate the area of surface chemistry and its role in catalysis
4. To gain knowledge about photochemistry and photophysical principles
5. To help the student understand about solar cells, fluorescence, greenhouse effect etc.

Unit 1: Chemical kinetics **(36 Hrs)**

1.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces. Conventional transition state theory-Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

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,Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

Mechanisms of heterogeneous catalysis : unimolecular and bimolecular surface reactions.

1.3 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, kinetic isotope effect.

1.4 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.5 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

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

1.7 Introduction to oscillating chemical reactions : autocatalysis, autocatalytic mechanism of oscillating reactions, the Lotka- Volterra mechanism, the brusselator, the oreganator, bistability.

Unit 2: Surface Chemistry **(18 Hrs)**

2.1. Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification.

2.2. Adsorption: Physisorption and chemisorption. The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Freundlich's adsorption isotherm, Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption, Surface heterogeneity.

Collision theory and absolute rate theory as applied to chemisorptions. Chemisorption on semiconducting metal oxides and metals, catalysis by metal oxides and metals, Ligand field theory of surface bonding, charge transfer theory of catalysis.

2.3. Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Unit 3: Photochemistry (18 Hrs)

3.1. Quantum yield - Reasons for low and high quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, Rate of formation of ozone layer in the atmosphere.

3.2. Principle of utilization of solar energy, solar cells, types of solar cells-amorphous silicon solar cell, cadmium telluride solar cell,copper indium gallium selinide solar cell.

3.3. Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, photochemistry of environment, greenhouse effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total

Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Apply the laws of chemical kinetics in understanding the mechanism of various chemical reactions	K2,K3	1, 3
2	Understand free radical and chain reactions leading to explosive reactions	K2,K4	1
3	Acquire knowledge of heterogeneous catalysis, kinetics of chain reactions, polymerization reactions etc.	K2,K3	1,3
4	Explain the techniques to study fast reactions and factors affecting enzyme catalysis	K2,K5	1
5	Familiarize with Oscillating chemical reactions	K2	1,2
6	Utilize the principles of kinetics in understanding catalytic activity at the surfaces	K3,K4	1,3
7	Apply adsorption techniques in surface catalyzed reactions	K2,K3	3
8	Apply the principles of photochemistry in studying various effects of transient intermediates	K3	1,3

Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester	Code: **PG20CH312**	**ORGANIC CHEMISTRY-IV**	Total Hrs:72 Hrs/Week:4	Credits :4

III				

1. To study the chiro optical properties.
2. To determine the structure of organic compounds from the deep knowledge of the principles of UV-Visible IR, NMR spectroscopy.
3. To study the principles of Mass spectrometry.

Unit 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.
1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.
1.3 Chirooptical properties- ORD, CD, octant rule, axial halo ketone rule, Cotton effect.
1.4 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.
2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.
2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, anisotropic effects-concentration and temperature effects-H bonding- ^{1}H and ^{13}C NMR scales-Solvents used in NMR- Solvent Shifts.
3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order spectra, Pascal's triangle, coupling constant, factors influencing coupling constant, Karplus curve, germinal, vicinal, long range and heteronuclear coupling, quadrupole broadening and decoupling-proton exchange reactions-NOE and cross polarization.
3.3 Non-first order spectra-simplification non-first order spectra to first order spectra-shift reagents, spin decoupling on double resonance, off resonance decoupling. Deuterium exchange-chemical shifts and homonuclear/heteronuclear couplings. Spectra of fluxional molecules.
3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY-Analysis of simple organic molecules.
3.5 Polarization transfer. Selective Population Inversion. DEPT, INEPT and RINEPT. Sensitivity enhancement and spectral editing, MRI.
3.6 Problems on spectral interpretation with examples.

Unit 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR,^{13}C NMR and mass spectroscopy (HRMS data or Molar mass or molecular formula may be given).

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

References

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11. Online spectral databases including RIO-DB.

QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Elucidate the structure of compounds by analysis and interpretation of UV-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectral data.	K3,K4	2, 3
2	Interpret UV-Vis, IR and NMR spectra	K3,K4	2,3,4
3	Gain advanced knowledge in stereochemistry of compounds.	K2,K4	2,3
4	Acquire knowledge in the interpretation of 2-D NMR, COSY, HOMOCOSY, HETROCOSY.	K4,K5	1, 2
5	Predict the molecular mass of a compound by analysing the mass spectrum.	K4	2,3
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination.

Semester IV	Code: PG20CH413	Elective-01-ADVANCED INORGANIC CHEMISTRY	Total Hrs:90 Hrs/Week:5	Credits :4

1. To understand the application of group theory in coordination compounds.
2. To learn the applications of inorganic spectroscopic methods for the study and structure elucidation of complexes.
3. To understand the importance of the emerging field of nanotechnology.
4. To know the photochemical behaviour of coordination compounds.
5. To introduce and give an insight into the fascinating area of material science.

Unit 1: Applications of Group Theory (27 Hrs)

1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding -octahedral and tetrahedral complexes. Hybrid orbitals as linear combinations of atomic orbitals.

1.2 Ligand field theory-splitting of *d* orbitals in different environments using group theoretical considerations, construction of energy level diagrams , Energy levels, Correlation diagrams, method of descending symmetry.

1.3 M.O.Theory-formation of symmetry adapted group of ligands- diagram approach, MO. Diagrams, MO theory of tetrahedral, octahedral complexes with sigma bond alone, with sigma and pi bonds –MO diagram of ferrocene.

1.4 *d-d* transition-Selection rules, vanishing integrals. Selection rule for IR and Raman Transition. Determination of modes of vibrations in IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes. Mutual Exclusion principles.

Unit 2: Inorganic Spectroscopic Methods. (9 Hrs)

2.1 Infrared and Raman 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: Advanced topics in Coordination Chemistry. (9 Hrs)

3.1 Photochemistry of Co-ordination complexes- Photochemical reactions of Cr(III), Ru(II) and Ru(III) complexes. Photo substitution, Photo racemization reactions 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: Nanoscience **(24 Hrs)**

4.1 Introduction to nanoscience and nanotechnology: Fundamental physicochemical principles - size dependence of the properties of nanostructured matter - quantum confinement, single electron charging, importance of nanoscale morphology.

4.2 Synthesis of Nano materials: Top down and Bottom up approaches- Ball milling, Lithography, Sol gel process, chemical vapour deposition, atomic layer deposition, Electrophoretic deposition.

4.3 Basic tools of nanotechnology: Basic principles and applications of Scanning electron microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and X-ray diffraction. Band gap measurement using UV-Vis spectrophotometers, light scattering methods.

4.4 Diversity in nanosystems: self-assembled monolayers on gold-growth process and phase transitions. Preparation, characterisation and applications of Nanostructured Materials- quantum dots, nanoshells. Metal nanoparticles: Size control of metal nanoparticles and their characterization, study of their properties-optical, electronic, magnetic.

4.5 Evolving interfaces of nanotechnology- nanobiology, Nanobiotechnology, nano-biosensors, nanotechnology for manipulation of biomolecules- optical tweezers, dielectrophoresis, biochips, labs on chips, and integrated systems, nanocatalysts, nanomedicines- importance of nanomaterials in the pharmaceutical industry and future possibilities for medical nanotechnology, nanoparticles for medical imaging, nanoparticles for targeting cancer cells, nanoencapsulation for drug delivery to tumors. Nanosensors, Nanocatalysts, Nanocomposites- natural nanocomposites, polymer nanocomposites, metal and ceramic nanocomposites and clay nanocomposites.

Unit 5: Chemistry of New Materials **(12 Hrs)**

5.1 Metal Oxides – Silicon dioxide, Zinc oxide, Titanium dioxide, Aluminium oxide- Applications.

5.2 Intercalation Compounds: graphite interlayer compounds (GILC), pillared clays (PILC).

5.3 Microporous materials – zeolites and zeolitic materials, $AlPO_4$- $GaPO_4$.

5.4 Fibres and Composites - microscopic composites, particle reinforced, Fibre-glass reinforced composites, hybrid composites.

Unit 6: Industrially important Materials **(9 Hrs)**

6.1 Ceramic Structures- mechanical properties, clay products, refractories- characterisation, properties and applications, non-silicon semiconductors as light emitting diodes, thermoelectric (TE) materials, applications of metals and alloys in hydrogen storage, inorganic organic hybrid composites- sol-gel ceramics, fillers in elastomers, polymer- modified ceramics.

6.2 Synthetic strategies for inorganic material design- direct Combination, low temperature techniques, combinatorial synthesis.

References

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Reactivity, 4th Edn., Harper Collins College Publishers, 1993.

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	**10**	**8**	**4**	**22**
No. Questions to be answered	**8**	**6**	**2**	**16**

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Apply the principles of group theory in explaining the bonding & electronic spectra of coordination compounds.	K3	3,4
2	Develop a skill to use inorganic spectroscopic tools for the structure elucidation of coordination compounds.	K4	4
3	Acquire a sound knowledge about the photochemistry of inorganic complexes.	K2	2
4	Investigate the importance of inorganic complexes in photo chemical applications.	K4	2
5	Develop a thorough knowledge about the synthesis, characterisation and interdisciplinary applications of nano structured materials.	K2	2
6	Gain an advanced knowledge about the chemistry and applications of some industrially important materials	K2	2
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

Semester IV	Code: PG20CH414	Elective-02-ADVANCED ORGANIC CHEMISTRY	Total Hrs:90 Hrs/Week:5	Credits :4

1. To impart thorough idea in the chemistry of carbohydrates, heterocyclic compounds, amino acids, proteins and nucleic acids. To study the fundamentals of terpenoids, alkaloids, vitamins, lipids and steroids.
2. To have an elementary idea of supramolecular chemistry and molecular recognition.
3. To understand the importance of medicinal chemistry and drug design.
4. To give an idea of scientific writing.

1.1 Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition.

1.2 Molecular receptors: cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes, carbon nanocapsules.

1.3 Importance of molecular recognition in biological systems like DNA and protein. Controlled release phenomena.

1.4 Applications of supramolecular complexes in perfumery and medicine. Targeted drug delivery.

Unit 2: Green Alternatives to Organic Synthesis (9 Hrs)

2.1 Green alternatives to Organic Synthesis: coenzyme catalysed reactions, thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: pinacol-pinacolone and benzidine rearrangements. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions. Green photochemical reactions.

2.2 Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.

2.3 General principles of microwave and ultrasound assisted organic synthesis.

Unit 3: Stereoselective Transformations (9 Hrs)

3.1 Assymmetric induction-chiral auxiliaries and chiral pool.

3.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

3.3 Assymetric aldol condensation pioneered by Evans.

3.4 Assymmetric Diels-Alder reactions.

3.5 Assymmetric epoxidation using Jacobsen's catalyst.

Unit 4: Chemistry of Natural Products and Biomolecules (18 Hrs)

4.1 Basic aspects of structure and classification of carbohydrates, terpenoids, alkaloids, steroids, nts, lipids, vitamins, amino acids, proteins and nucleic acids. Nomenclature of prostaglandins.

4.2 Synthesis of atropine, papaverine, quinine, quercetin, β-carotene, testosterone, PGE_2 and $PGF_{2\alpha}$.

4.3 Methods for primary structure determination of peptides, proteins and nucleic acids. End group analysis, Replication of DNA, flow of genetic information, protein biosynthesis, transcription and translation, Genetic code, regulation of gene expression, DNA sequencing. The Human Genome Project. Polymerase Chain Reaction (PCR).

Unit 5: Medicinal Chemistry and Drug Designing (18 Hrs)

5.1 Introduction to Drug design: modeling techniques, receptor proteins, drug receptor interaction, drug action, drug selectivity, drug metabolism, structure activity relationship (SAR and QSAR).
5.2 Classification of drugs with examples- Antibiotics, Antitubercular agents anticoagulants, anti-anginal drugs, antihypertensive agents, antimalarial drugs, Antileprotic drugs, Antiviral drugs, CNS Drugs, Antisyphilitic agents, Cholesterol lowering agents, Immuno suppressants, Vasodialators, Sulphonamide, Narcotics Drugs for cancer, AIDS and diabetes
5.3 Synthesis of important drugs-Penicillin, chloramphenicol, Sulphanilamide, N-substituted sulphanilamide derivatives, mechanism of action, sulphones- dapsone
5.4 Antibiotics: Important penicillins, tetracyclins and cephalosporins.
5.5 Antitubercular agents: Isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin
5.6 Antileprotic drugs: Dapsone, phenazine derivatives- clofazimine
5.7 Antiviral drugs: A brief study of infection, its development and social significance. Principles of antiviral drugs. Nucleoside and non-nucleoside analogues.
5.8 Antiherpes virus drugs- Idoxuridine, vidarabine and acyclovir.

Unit 6: Advances in Polymer Chemistry (9 Hrs)

6.1 Conducting polymers, self healing polymers, temperature resistant and flame retardant polymers, polymers for medical applications.
6.2 Dendrimers and dendritic polymers: terminology, classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers. Hyperbranched polymers: definition, synthesis, applications.

Unit 7: Research Methodology of Chemistry (9 Hrs)

7.1 The search of knowledge, purpose of research, scientific methods, role of hypothesis and theory, characteristics of research.
7.2 Types of research: fundamental, applied, historical and experimental research.
7.3 Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, SciFinder. Chemical Abstract.
7.4 Scientific writing: Structure of research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.
7.5 Important scientific and Chemistry Journals. Impact factor, h index.

References

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Understand the applications of important medicines and the need of drug designing.	K2	1
2	Discuss the importance of research methodology in chemistry.	K1,K2	1,2

3	Recognize the alternatives to organic syntheses like green, ultrasound and microwave.	K4	7
4	Explain the methods of stereoselective transformations in organic synthesis	K2	3,4
5	Describe the synthesis and structure determination of natural products and biomolecules	K2,K3	5
6	Apply the importance of molecular recognition in supramolecular chemistry.	K3	6
7	Investigate the scope of conducting polymers, hyperbranched polymers and dendrimers in medical applications.	K5	4,5
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination.

Semester IV	Code: PG20CH415	Elective-03-ADVANCED PHYSICAL CHEMISTRY	Total Hrs:90 Hrs/Week:5	Credits :4

1. To study the crystal structure of different compounds using various methods
2. To gain an understanding of the diffraction and spectroscopic methods of analysis
3. To understand the theories and concepts of electrochemistry
4. To obtain knowledge about modern areas of electrochemistry
5. To acquire knowledge of electroanalytical techniques

Unit 1: Crystallography (9 Hrs)

1.1. 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.

Unit 2: Diffraction Methods, Atomic Spectroscopic Techniques and thermal methods of analysis (18 Hrs)

2.1. Diffraction methods

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

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

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

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

2.3. Fluorescence spectroscopy

Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers. Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorephores: long life time metal-ligand complexes.

2.4 Thermal methods-TG, DTA, DTG, DSC-Theory and applications

Unit 3: Surface Characterisation Techniques (9 Hrs)

3.1 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces. Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.

Unit 4: Electrochemistry and Electromotive Force (36 Hrs)

4.1. Conductance measurements at high frequency and high voltage, results of conductance measurements, ionic mobilities, influence of pressure and temperature on conductance of ions, Walden equations, abnormal ionic conductance.

4.2. Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, ionic atmosphere, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL. Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes, association constant, solubility product principle, solubility in presence of common ion, instability constant, activity coefficient and solubility measurement, determination of activity coefficient from equilibrium constant measurement.

4.3. Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.

4.4 Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density.

4.5. Fuel cells- theory and working of fuel cells, H_2-O_2 fuel cells, methanol fuel cell, solid oxide fuel cells.

4.6 Corrosion and methods of prevention, Pourbaix diagram and Evans diagram

Unit 5: Electroanalytical Techniques (18 Hrs)

5.1. Voltametry and polarography: Voltametry-cyclic voltametry, ion selective electrodes, Anodic stripping voltametry. Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.

5.2. 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 anion, advantages of polarography.

5.3. Amperometry: general principles of amperometry, application in qualitative analysis of anions and cations in solution, instrumentation, 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 Electrogravimetry : Electrogravimetric analysis, types of electrogravimetric methods- constant current electrolysis, constant potential electrolysis.

References

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QUESTION PAPER PATTERN

Module	Part A (Wt. : 1) Short Answer	Part B (Wt. : 2) Short Essay	Part C (Wt. : 5) Long Essay	Total
Total No. of Questions	10	8	4	22
No. Questions to be answered	8	6	2	16

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Analyse the type and behaviour of crystal structure in solids.	K2,K4	1, 2
2	Apply theories in electrochemistry to analyse electrode kinetics.	K3,K4	1,3
3	Acquire knowledge of Debye- Huckel theory, Debye- Huckel-Onsager equation, Debye Huckel Limiting Law etc.	K2,K3	1,3
4	Explain the working of fuel cells	K5	1
5	Apply the spectroscopic and thermal methods of analysis in instrumentation.	K2,K3	1, 3
6	Acquaint with the advanced techniques in surface characterization and electro analytical techniques.	K2,K4	2, 3
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Assessment Tools

Chalk and talk, Multimedia projection, Group discussion, Seminar, Interactive sessions, Tutorials, Assignment

Learning Pedagogy

Assignments, Seminar, Test papers, End semester examination

ELECTIVE COURSE-4
PG20CH416 -POLYMER CHEMISTRY

Credits: 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 Tg and Tm, 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)

4.1 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

1. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.
2. F.W. Billmeyer Jr., Textbook of Polymer Science, 3rd Edn., Wiley-India, 2007.
3. L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn, John Wiley & Sons, 2006.
4. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.
5. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press,2002.
6. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving approach, CRC/Taylor & Francis, 2006.
7. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1983.
8. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.
9. 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.

ELECTIVE COURSE-5
PG20CH417 -ANALYTICAL CHEMISTRY

Credits: 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, 13C, 32P). 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, H2SO4, HNO3, HClO4, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na2O2, KNO3, NaOH, K2S2O7,B2O3 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. Waterquality-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-SO2, NO2, NH3, O3 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, electrochemical mass, 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

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.
4. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.
5. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
6. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

Semesters	Code:	INORGANIC CHEMISTRY	Total Hrs:108	Credits
III &IV	**PG20CHP4**	**PRACTICAL-II**	Hrs/Week:3	:3

1: Understand the principles of volumetric and gravimetric analysis.

2: Develop skills in volumetric and gravimetric analysis for the separation and estimation of cations from a solution containing binary mixture of cations.

3: Acquire skills to analyse some common ores and alloys.

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

Analysis of one of the alloys of brass, and bronze. Analysis of one of the ores from dolomite, monazite, illmenite.

References

1. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
2. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.
3. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.
4. N.H. Furman, Standard Methods of Chemical Analysis: Volume 1, Van Nostrand,1966.
5. F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub.,2006.

COURSE OUTCOME

CO No	**Upon completion of this course, the students will be able to**	**Cognitive level**	**PSO No.**
1	Understand the principles of volumetric and gravimetric analysis	K2	4
2	Develop skills in volumetric and gravimetric analysis for the separation and estimation of cations from a solution containing binary mixture of cations	K3	4

3	Acquire skills to analyse some common ores and alloys	K4	4,5
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

Semesters **III &IV**	Code: **PG20CHP5**	**ORGANIC CHEMISTRY PRACTICAL-II**	Total Hrs:108 Hrs/Week:3	Credits :3

1. Understand the principles and techniques involving Preparation of compounds by two stages.
2. Expertise in the Preparation Involving Green Alternatives of Chemical Methods.
3. Understand the principles of Microwave assisted Organic Synthesis
4. Predict and interpret FTIR, ^{1}H and ^{13}C NMR spectra of the synthesized products
5. Relate the IR and NMR spectra of various organic compounds with their structures
6. Set up glass wares and apparatus to conduct experiments with minimum or without error.

PART I

Preparation of compounds by two stages.

1) Acetanilide - p-nitroacetanilide - p-nitroaniline
2) Methyl benzoate - m-nitromethylbenzoate - m-nitrobenzoic acid
3) Acetanilide - p-bromoacetanilide - p-bromoaniline
4) Benzophenone – benzophenone oxime - benzanilide
5) Aniline - 2,4,6-tribromoaniline - 1,3,5-tribromoaniline
6) Benzaldehyde-benzoin-benzilic acid
7) Aniline-sulphanilic acid-methylorange
8) O-Toluidine-o-methyl acetanilide-N-acetyl anthranilic acid
9) Aniline-acetanilide-p-nitroacetanilide

PART II

Preparation Involving Green Alternatives of Chemical Methods

1) Acetanilide from aniline
2) Ortho-methyl acetanilide from ortho-toluidine
3) 1,1-Bis-2-Naphthol from 2-Naphthol

PART III

Microwave assisted Organic Synthesis

1) Benzoic acid from benzyl alcohol
2) Ethyl-3-nitrobenzoate from 3-nitro benzoic acid

3) Benzoic acid from ethyl benzoate

PART IV

Prediction of FTIR, ^{1}H and ^{13}C NMR spectra of the products at each stage synthesized by the above methods

PART V – Viva – voce

References

1. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 5th edition, 1989.
2. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 2016.
3. F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.
4. J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 6th edition, 1989.
5. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

COURSE OUTCOME

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Understand the principles and techniques involving Preparation of compounds by two stages.	K2	1
2	Expertise in the Preparation Involving Green Alternatives of Chemical Methods	K5	7
3	Understand the principles of Microwave assisted Organic Synthesis	K2	1
4	Predict and interpret FTIR, ^{1}H and ^{13}C NMR spectra of the synthesized products	K3	5
5	Relate the IR and NMR spectra of various organic compounds with their structures	K4	7
6	Set up glass wares and apparatus to conduct experiments with minimum or without error.	K6	5

Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create

Semesters	Code:	PHYSICAL CHEMISTRY	Total Hrs:144	Credits
III &IV	**PG20CHP6**	**PRACTICAL-II**	Hrs/Week:4	:3

1. To study the kinetics of first and second order reactions.
2. To familiarize the polarimeter for optical rotation measurement
3. To use a potentiometer for the emf measurements
4. To evaluate refractive index of liquids using Refractometer
5. To evaluate the viscosity of liquids using an Ubbelohde Viscometer
6. To quantify electrolytes by conductivity measurements.

I Chemical Kinetics

1. Determination of the rate constant of the hydrolysis of ester by sodium hydroxide.
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. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water).
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

IV Viscosity

1. Determination of viscosity of pure liquids.
2. Verification of Kendall's equation.
3. Determination of the composition of binary liquid mixtures (alcohol-water, benzene-nitrobenzene).
4. Determination of the molecular weight of a polymer (polystyrene in toluene).

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

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. Determination of end point of a titration using Gran Plot.
5. Determination of the concentration of a mixture of Cl^- and I^- ions.

References

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005.

COURSE OUTCOME

CO No	Upon completion of this course, the students will be able to	Cognitive level	PSO No.
1	Study Kendall's equation by viscosity measurements	K3	1,4
2	Evaluate the concentrations of acids and sugar solutions, and to determine rate constant of inversion of cane sugar in the presence of HCl by polarimetry	K5	1,4
3	Evaluate the concentrations and molar refractions of liquids and complexes using refractive index measurements	K5	1,4
4	Compare the viscosities of various liquids and to determine the composition of liquid mixtures	K4	1,4
5	Evaluate the rate constant of first and second order reactions.	K5	1,4
6	Quantify acids, mixture of acids, using conductivity measurements experiments and to verify Onsager Equation.	K5	1,4

7	Quantify acids, mixture of acids by potentiometric titrations.	K5	1,4
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

PG20CH4P – PROJECT/DISSERTATION

Credits: 2

COURSE OUTCOME

CO No.	**Upon completion of this course, the students will be able to**	**Cognitive level**	**PSO No.**
1	Acquire a knowledge in literature review	K2	5
2	Identify a research problem	K3	6
3	Obtain skills in the characterization using analytical tools and data interpretation	K5	5
4	Gain knowledge about the presentation of reference material	K5	6
5	Get expertise in doing novel experiments.	K6	4
6	Develop industry-academia linkage	K3	8
7	Attain knowledge in data analysis and scientific writing.	K6	6
Cognitive level: **K1**-Remember, **K2**-Understanding, **K3**-Apply, **K4**- Analyze, **K5**-Evaluate, **K6**-Create			

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- I Semester
PG20CH101 – INORGANIC CHEMISTRY-I
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Obtain the relation between stepwise formation constant & overall formation constant
2. How many d – d bands would be expected in the electronic spectrum of an octahedral Cr (III) complex?
3. Derive the ground term symbol for (i) Cr^{3+} (ii) $[Co(H_2O)_6]^{2+}$
4. Which of the following might be expected to exhibit distorted octahedral geometry ?Why? $[Cr(H_2O)_6]^{3+}$, $[Ti(H_2O)_6]^{3+}$, & $[Mn(H_2O)_6]^{3+}$
5. Give any two evidences for covalency in metal – ligand bonds.
6. Give the possible optical isomers of $[Co(en)_2Cl_2]Cl$
7. How is CD spectra useful in determining the absolute configuration of metal complexes?
8. Actinides have greater tendency to form complexes than lanthanides. Why?
9. Explain the steric factor affecting linkage isomerism
10. What is trans effect? Write any two applications of trans effect.

Section B (Answer any **6** questions. Each question carries weight of 2)

11. Distinguish between Orgel diagram and Tanabe Sugano diagrams.
12. Write a note on charge transfer spectra
13. The stepwise stability constant for the complex formed between Cu and en are in the order $k_1 > k_2 >> k_3$. Explain.
14. Discuss the structure elucidation of cobalt metal complex using electronic spectra and magnetic moment measurements
15. Write a note on rearrangement reactions
16. Discuss on the Marcus theory of octahedral complexes
17. Differentiate the magnetic and electronic properties of actinides, lanthanides and transition elements
18. Using suitable examples, explain chelate effect and macrocyclic effect.

Section C (Answer any **2** questions. Each question carries weight of 5)

19. a) Discuss the structure of the following complexes on the basis of crystal field theory
    (i) $[Co(NH_3)_6]^{3+}$ (ii) $[Co\ F_6]^{3-}$ (iii) $[Fe(H_2O)_6]^{2+}$
    b) State and explain the selection rules for electronic spectra
20. Construct a MO energy level diagram for an octahedral complex involving Pi bonding ligands.
21. Discuss in detail the mechanisms for redox reactions of octahedral complexes with suitable examples.
22 Write notes on (a) geometrical isomerism in octahedral complexes
(b) Base hydrolysis of octahedral complexes.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- I Semester
PG20CH102 -ORGANIC CHEMISTRY-I
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Write a note on optical purity and enantiomeric excess.
2. Give an example of Di - π - methane rearrangement.
3. What are the conditions necessary for delocalisation.
4. Give the application of Stork enamine reaction.
5. Write a note on sensitization and quenching
6. What types of allenes are chiral? What is the reason for their chirality?
7. Outline a method for the interconversion of cis and trans isomers?
8. Write the Fischer, Newman, Sawhorse and Flying wedge projection of erythro 3-bromo 2 butanol.
9. What do you mean by prochirality?
10. Write the plain projection formula of the following :-
    (a) 2 R, 3S-2,3 dibromo pentane (b) E – 1 Deuterio-1-hexene.

Section B (Answer any **6** questions. Each question carries weight of 2)

11. Explain the mechanism of Paterno-Buchi reaction. What are factors that limit the synthetic utility of this reaction
12. Discuss the aromaticity, antiaromaticity, and homo aromaticity with examples
13. Give the mechanism of (i) MPV reduction (ii) Baeyer-Villiger oxidation
14. Draw the π molecular orbital diagram of the following molecules:-(a) 1,3-butadiene (b) Benzene (c) Allyl cation
15. What are ansa compounds? Explain the effect of substituent on optical activity of these compounds.
16. Explain with example homotopic and heterotopic atoms and faces.
17. Write a short account on Wittig and Cannizzaro's reactions.
18. Give an account of the stereochemistry of oximes, commenting on nomenclature and determination of configuration.

Section C (Answer any **2** questions. Each question carries weight of 5)

19**.** Discuss (a) Mechanism of (i) Michael addition (ii) Mannich reaction (iii) Robinson annulations (iv) Ene reaction b) Photoreactions of carbonyl compounds.

20. Explain a) Steric Inhibition of resonance b) Aromaticity of non benzenoid aromatic compounds
21. Write notes on a) Methods of resolution of racemic mixture (b) Conformational analysis of substituted cyclohexanes and decalins
22. (a) Describe briefly the optical isomerism of Nitrogen and Sulphur compounds.
    (b) Describe any four methods to determine the configuration of geometrical isomerism.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM

M.Sc. Chemistry (PGCSS) Degree Examination- I Semester
PG20CH103 – THEORETICAL CHEMISTRY-I
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. What is a well behaved function? Explain.
2. For a 2p electron in Hydrogen like atoms what is the magnitude of orbital angular momentum. What are the possible values of L_Z?
3. In a cubic box the energy of free electron is given by $E= (1.125h^2/ml^2)$. Give wave function.
4. Plot the radial portions of the 4s, 4p, 4d and 4f hydrogen like wave functions.
5. Give the postulate of spin by Uhlenbeck.
6. What is similarity transformation?
7. Discuss the selection rule for IR spectroscopy.
8. What is a glide plane?
9. What is mutual exclusion principle?
10. Give the Schoenflies notation for the following point groups
    a) 4/m b) 4/m 2/m 2/m

Section B (Answer any **6** questions. Each question carries a weight 2)

11. Commutate [L^2, Lx] and [Lx ,Ly]
12. Explain the Stern Gerlach experiment for the spin discovery.
13. Find <Px> for particle in one dimensional box.
14. Compare a classical harmonic oscillator and quantum mechanical oscillator
15. Evaluate and sketch $H_{(1)}$ and $H_{(2)}$ for a harmonic oscillator.
16. What is meant by block diagonalisation?
17. Explain the properties of screw axis?
18. Assign point groups to each of the following and specify the corresponding symmetry elements? a) IF_7 b) naphthalene c) cis-dichloroethylene d) PCl_3 e) Ethylene

Section C (Answer any **2** questions. Each question carries a weight 5)

19. Set up the Schrodinger equation and find eigen values and eigen function for a particle moving in a ring.
20. Outline the essential postulates of quantum mechanics.
21. a) State the GOT and discuss the rules regarding irreducible representations.
    b) Derive the character table for C_3 point group.
22. a) Explain the selection rules for Raman and electronic spectroscopy.
    b) Determine the vibrational modes of ammonia molecule

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- I Semester
PG20CH104 - PHYSICAL CHEMISTRY - I
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. What is Nernst theorem?
2. Differentiate between flux and force in phenomenological relations
3. What is collision frequency?
4. Write a note on chemical potential
5 Define Partial Molar Properties
6. Explain the term 'fugacity'. How is it related to pressure?
7. Derive Gibbs-Duhem equation
8. How can we determine fugacity from α ?
9. State third law of thermodynamics. Explain its importance
10. What are thermodynamic excess functions? Give the experimental determination of excess Volume.

SECTION B

(Answer any **6** questions. Each question carries a weight 2)

11. Derive Maxwell distribution law.
12. How can the partial molar volume be determined experimentally?
13. Derive Gibbs- Helmholtz equation. What are its applications?
14. Derive thermodynamic equations of state
15. Calculate the entropy change for the transformation of solid iodine to iodine vapours at 1 atmosphere and 455 K. ΔH_f = 16 KJ mol^{-1} at the melting point 113^0C and ΔH_v = 28 KJ mol^{-1} at the boiling point 185^0C. The molar heat capacities are $I_2(s)$ = 15 JK^{-1} mol^{-1} and $I_2(l)$ = 82 JK^{-1} mol^{-1}
16. Calculate the translational partition function of a molecule of oxygen gas at 1 atm and 298K moving in a vessel of volume 24.4 dm^3
17. 4 dm^3 of methane and 1dm^3 of argon each at 1 atm and 27^0C are mixed isothermally in a vessel of 3 dm^3 capacity. Find ΔG_{mix}, ΔS_{mix} and ΔH_{mix}. Assume that gases behave ideally.
18. Calculate the translational entropy of gaseous iodine at 298K and 1 atm.

Section C (Answer any **2** questions. Each question carries weight of 5)

19. Sketch and describe the phase diagrams of the following three component systems
    (a) Ternary solutions with common ions
    (b) Hydrate formation
    (c) Compound formation
20. Derive Maxwell's thermodynamic relationship

21. (a) Compare Bose-Einstein and Fermi- Dirac statics
    (b) Derive Bose- Einstein statistics
22. (a) Derive Sackur- Tetrode equation applicable to monatomic gas
    (b) Derive expression for free energy and partition function

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- II Semester

PG20CH205 - INORGANIC CHEMISTRY- II
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries weight of 1)

1. Sketch the fluorite structure and comment on its relation to fcc structure
2. Distinguish between wurtzite and zinc blende structures.
3. What is meant by nuclear reaction cross section? Give an expression for obtaining the nuclear reaction cross section.
4. Differentiate between spinels and inverse spinels. Give typical examples.
5. Comment on the hardness of boron nitride with respect to its structure
6. Diamond is an insulator, Si is a semi conductor, Ge is a better semi conductor, Sn is a conductor & lead is a metallic conductor. Discuss
7. What is piezoelectric effect & inverse piezoelectric effect?
8. What are condensed phosphates?
9. What is Meissner effect? How type I super conductivity differ from type II superconductivity
10. State Vegard's law . Give its significance?

Section B (Answer any **6** questions. Each question carries weight of 2)

11. Write a brief note on sintering.
12. What are solid state reactions? Explain the various factors affecting it.
13. Discuss the applications of radioactivity giving special reference to industry and agriculture.
14. What are phase transitions? Give the kinetics of phase transitions.
15. Write a note on high temperature super conductors
16. Explain the BCS theory for the mechanism of low temperature super conductivity.
17. Explain the applications of Wade's rule for carboranes and metalloboranes
18. How are $(SN)_x$ Prepared ? Explain the 1 D metallic character of $(SN)_x$

Section C (Answer any **2** questions. Each question carries weight of 5)

19. Write briefly on:
    a. Preparation of single crystals.
    b. Order disorder transitions
20. Write notes on a) relevance of radiation chemistry in biology b) principle and working of scintillation counters
21. (a)Discuss the band theory of transition metal oxides.
    (b)Discuss the antiferromagnetism in transition metal complexes.
22. (a) Discuss on isopolyvanadates and isopolymolydates

(b) Explain Hall Effect with any two applications.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- II Semester

PG20CH206 - ORGANIC CHEMISTRY-II
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. How nitrenes are prepared? Discuss their properties.
2. Discuss autooxidation with an example
3. What are Benzynes? Discuss its structure and stability.
4. Explain Hammond postulate with an example.
5. What are the applications of Taft equation in ester hydrolysis
6. What is regioselectivity? Exemplify.
7. Mechanistically indicate Benzil-Benzilic acid rearrangement
8. Write a note on classical and non classical carbocations.
9. What is chelotropic reaction with an example
10. Explain Wittig rearrangement in pericyclic reaction.

Section B (Answer any **6** questions. Each question carries weight of 2)

11. Discuss the structure, formation and reactions of carbene.
12. Using a suitable example illustrate SN^2Ar mechanism.
13. Write a note on Barton reaction and Mc Murry Coupling.
14. Explain Shapiro reaction and Juliya elimination.
15. Explain 4+2 cycloaddition by FMO method.
16. Describe Neighboring Group participation.
17. Explain Hammett equation. Using a suitable example explain how the nature of the transition state is inferred.
18. Discuss the applications of kinetic isotopic effect in determining reaction mechanisms.

Section C (Answer any **2** questions. Each question carries weight of 5)

19. Give a brief notes on Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement
20. Explain (1) Claisen, rearrangements (2) Sommelet – Hauser reaction (3) Ene reaction (4) Pyrolytic elimination reactions.
21. Discuss the mechanisms of (a) Woodward and Prevost hydroxylation (b) acyloin condensation (c) Heck reaction (d) Peterson olefination.
22. Discuss different mechanisms of esterification and ester hydrolysis

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- II Semester

PG20CH207-THEORETICAL CHEMISTRY-II
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Explain the independent particle model.
2. What is Hellmann-Feynman theorem?
3. Compare GTO and STO.
4. Explain free valence with an example.
5. Derive the term symbols for C and He
6. Discuss about CHARMM and AMBER.
7. Discuss Woodward Hoffmann rules.
8. Calculate the number of basis functions on each atom for a 6-31G(d,p) basis set calculation of H_2O.
9. Explain the notation MP2/6-31G(d,p) and HF/6-31G.
10. Write a note on potential energy surface emphasizing stationary point and asymptotes.

Section B (Answer any **6** questions. Each question carries a weight 2)

11. Apply perturbation method to He atom.
12. Use HMO theory to determine the energies and wave functions of the pi electron system in ehylene.
13. Write a note on HFSCF Theory.
14. Draw the MO diagram of LiH molecule.
15. Briefly explain Koopman's Theorem.
16. Describe any two computational methods that include electron correlation.
17. Determine the SALC of C_{2h} point group.
18. Write a note on the various classes of basis sets.

Section C (Answer any **2** questions. Each question carries a weight 5)

19. Taking H_2 as an example compare and contrast VB and MO theory.
20. Explain briefly the various methods in Semi Empirical Calculations.
21. State and prove the variation theorem. Apply it to particle in a 1-D box using the trial function x(a-x).
22. Compare molecular mechanics method with DFT method

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- II Semester
PG20CH208-PHYSICAL CHEMISTRY-II
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. State Born Oppenheimer approximation
2. Derive an expression for $J_{max}$for the rigid rotor.
3. What is the effect of substituting a hydrogen atom by a deuterium atom in hydrogen molecule on rotational constant B?
4. Explain Fermi resonance.
5. Discuss the applications of microwave spectroscopy in chemical analysis.
6. Write McConnel equation and explain the terms.
7. Explain Kramer's degeneracy.
8. Calculate the resonance frequency of hydrogen nucleus in an applied field of 2.4 T if β_N = 5.05 x 10^{-27} JT^{-1} and g = 5.585.
9. Draw the EPR spectrum of methyl free radical.
10. Explain the principle of NQR spectroscopy.

Section B

(Answer any **6** questions. Each question carries a weight 2)

11. Explain the various factors influencing the intensity of spectral lines.
12. Explain the classical theory of Raman spectrum
13. Discuss FT techniques in spectroscopy and explain its advantages.
14. Explain Karplus relationship.
15. The rotational spectrum of $^{79}Br^{19}F$ shows a series of equidistant lines separated by 0.71433 cm^{-1}. Calculate the rotational constant, moment of inertia and Br-F bond length.
16. The fundamental and first overtone transition of $^{14}N^{16}O$ arecentred at 1876.06 cm^{-1} and 3724.20 cm^{-1} respectively. Calculate the force constant, zero point energy, anharmonicity constant and equilibrium vibration frequency of the molecule.
17. Predict the EPR spectrum of the following radicals (a) CF_2H, (b) $^{13}CF_2H$ and (c) $(C_{10}H_8)^-$
18. Calculate the relative population N_{upper}/N_{lower} if ΔE = 7 x 10^{-26} J in a 2.3487 T field and 6 x 10^{-24} J in a 0.33 T field for nuclei and electrons respectively.

Section C

(Answer any **2** questions. Each question carries a weight of 5)

19. Discuss any three methods used for simplification of second order NMR spectra.
20. Outline the principle of Mossbauer spectroscopy. Explain the application of this technique in the study of Fe(II) and Fe(III) cyanides.
21. Discuss
    a) Relaxation methods in NMR spectroscopy

b) Nuclear Overhauser Effect.

22. Discuss
    a) Applications of Raman spectroscopy
    b) Resonance Raman scattering and resonance fluorescence.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- III Semester
PG20CH309 – INORGANIC CHEMISTRY- III
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. What is Zeises's salt? How is it synthesised ?
2. Explain the action of cisplatin.
3. What do you mean by essential trace elements? What are the essential and beneficial metals?
4. What is meant by FBR? What are its advantages?
5. Explain fluxionality with two examples.
6. Discuss the oxidative addition reaction in organometallic chemistry with one example .
7. Dinitrogen complexes are very rare even though N_2 is isoelectronic with CO , which forms a number of complexes. Give reasons
8. Calculate the EAN of $[Ir\ Br_2\ CH_3\ PPh_3]$
9. Ethylene is commonly chosen to illustrate homogeneous hydrogenation with Wilkinson's catalyst but the process is very slow. Explain Why?
10. Calculate the number of M – M bonds in $(\eta^4\ C_4H_4)_2\ Fe_2\ (CO)_3$

Section B (Answer any **6** questions. Each question carries weight of 2)

11. What are iron sulphur proteins? How are they classified? State their important functions.
12. Write briefly on the forces inside an atomic nucleus.
13. Explain the role of photosystems I and II in photosynthesis.
14. Explain with relevant equations, radiolysis of water?
15. Explain the use of IR spectroscopy in distinguishing the different bonding modes of CO in metal carbonyl complexes
16. Explain insertion reaction in organometallic compounds with suitable examples.
17. Explain the bonding in metal - butadiene complexes using M.O diagram.
18. What are metal carbenes ? How will you synthesise Fischer & Schrock carbenes

Section C (Answer any **2** questions. Each question carries weight of 5)

19. Write briefly on (a)Olefin metathesis (b) Carboxy peptidase and its function

20. Explain the oxygen transport process by hemoglobin. Compare the oxygen binding process in Hb and Mb.
21. (a) Give the catalytic cycle for the conversion of propene to butyraldehyde using the catalyst $HRh(CO)_4$ (b) Explain Wade-Mingos rules with suitable examples.
22. Write a note on (a) platinum POP (b) Explain Monsanto acetic acid process.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- III Semester
PG20CH310 -ORGANIC CHEMISTRY-III
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Give one method each for the synthesis of (a) Pyrrole (b) Oxazole (c) Thiazole.
2. Explain Umpolung?
3. Explain the carbodiimide method of peptide bond formation?
4. Give one example each for manganese and lead based oxidation of alkenes to carbonyl compounds.
5. What is DIBAL-H? Give any two applications of DIBAL-H.
6. What is Nef reaction? Explain its mechanism.
7. What is allylic oxidation? Give an example.
8. Give an example of Preterson olefination.
9. Explain the basic principle of retrosynthesis
10. Write a note on Stille reaction.

Section B (Answer any **6** questions. Each question carries a weight of 2)

11. Explain the method of construction of macrocyclic rings by ring closing metathesis?
12. Write note on different methods of protection of (i) carbonyl group (ii) hydroxyl group?
13. Explain the mechanism of a) Ullmann Coupling b) Wohl-Zeigler reaction
14. Discuss the method of synthesis of epoxide from alkenes. Explain the mechanism of (a) Sharpless asymmetric epoxidation and (b) Shi epoxidation.
15. Write a note on Click reaction.
16. Write down the mechanism of (i) Pauson-Khand reaction (ii) Mitsunobu reaction.
17. Explain the role of trimethyl silyl group in organic synthesis?
18. Write a note on (i) Nazarov cyclisation (ii) Bergman cyclization.

Section C (Answer any **2** questions. Each question carries a weight of 5)

19. Write an essay on metal mediated C-C and C-X coupling reactions with special reference to (a) Suzuki coupling (b) Heck reaction (c) Suzuki-Miyaura coupling (d) Glaser coupling and (e) Nozaki-Hiyama reaction.
20. a) Compare the Prevost and Woodward hydroxylations.
    b) Explain briefly the synthetic utility of Wacker process in organic synthesis
21. (i) Explain the role of different hydride transfer reagents in organic reduction reactions.
    (ii)Write an essay on the role of protection, and deprotection in peptide synthesis. Illustrate with examples with special reference to SPPS method. Explain the mechanism.

22. How the following heterocyclic compounds are synthesized (a) Imidazole (b) Thiazole (c) Oxazole (d) Thiophene

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- III Semester
PG20CH311 - PHYSICAL CHEMISTRY-III
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Define Michaelis – Menten constant. How is it determined?
2. Explain with an example how NMR can be used in the study of fast reaction.
3. What is primary kinetic salt effect?
4. Write down the steps in a chain reaction and explain the terms initiation, propagation and termination.
5. Describe the effect of pH and temperature on catalysis.
6. What is membrane potential? How it is developed?
7. Write the Langmuir adsorption isotherm and indicate its limitations
8. Distinguish between excimers and exciplexes
9. Explain green house effect.
10. What is meant by photo stationary state? Discuss with reference to formation of ozone in the atmosphere.

SECTION B

(Answer any **6** questions. Each question carries a weight 2)

11. Describe Lindemann's theory of unimolecular reactions.
12. Describe Rice – Herzfeld mechanism with thermal decomposition of acetaldehyde
13. Discuss the use of Auger Electron spectroscopy in the study of surface
14. Briefly discuss on Langmuir Hinshelwood Mechanism of adsorption.
15. A second order reaction has a rate constant k = 2.5 x 10^{-3} L $mol^{-1}S^{-1}$ at 25^0C. Its energy of activation is 48 KJ $mol^{-1.}$ Calculate $\Delta S^{\#}$ for the reaction, assuming that the reaction takes place in solution.
16. The adsorption of a gas is described by Langmuir isotherm with K=0.75KPa^{-1} at 25^0C. Calculate the pressure at which fractional surface coverage is 0.5
17. In a photochemical reaction A -→2B +C the quantum efficiency with 500 nm light is 2.1x10^{-2} mol $Einstein^{-1}$. After exposure of 300 m mol of A to the light 2.28 m mol of B was formed. How many photons were absorbed by A?
18. In an experiment to measure quantum efficiency of a photochemical reaction, the absorbing substance was exposed to 490 nm light from a 100 W source for 45 minutes. The intensity of transmitted light was 40 % of the intensity o f the incident light. As a result of irradiation, 0 .344 mol of the absorbing substance decomposed. Determine the quantum efficiency.

Section C

(Answer any **2** question. Each question carries a weight of 5)

19. (a) Distinguish between glory scattering and rainbow scattering
    (b) Describe the factors affecting reactions in solution

20. How would you determine surface area of a solid using BET isotherm? Explain.
21. a) Distinguish between E-type and P-type delayed fluorescence.
    b) Discuss the working of solar cells.
22. a)Derive Stern- Volmer equation.
    b) Discuss the kinetics of anthracene dimerisation.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- III Semester
PG20CH312 – ORGANIC CHEMISTRY-IV
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight 1)

1. Explain MALDI-TOF.
2. Explain Mc Lafferty rearrangement.
3. Calculate DBE of the following molecules:-
   (a) $C_{10}H_8O_2$
   (b) $C_{15}H_{13}Cl$
4. Write down the total number of signals obtainable in the PMR spectra of the following molecules:-
   (a) 2R,3R-2,3-Di bromopentane
   (b) Mesotartaric acid
   (c) Fumaric acid
5. Describe the splitting pattern in the PMR spectra of 2R-3S-2,3-Dibromopentane
6. Distinguish between $\Pi \rightarrow \Pi$ and $n \rightarrow \Pi$ transitions in UV spectroscopy.
7. Distinguish between hypochromic effect and hyperchromic effect in UV spectroscopy
8. What are the selection rules in UV spectroscopy?
9. How intramolecular hydrogen bonding is distinguished from intermolecular hydrogen bonding using IR spectra?
10. Explain why the relative intensities of the peaks in a quartet are 1:3:3:1.

Section B (Answer any **6** questions. Each carries a weight of 2)

11. Explain Nitrogen rule.
12. Explain Karplus curve. How is it helpful in determining the conformation?
13. Show how NMR measurements are of use in deciding the aromaticity of compounds?
14. Explain solvent effect in UV- visible spectroscopy.
15. Explain the effect of auxochromic substitution in UV spectroscopy
16. (a) Give molecular formulas of hydrocarbon cations with m/z values of **(i) 29 (ii) 51(iii) 91**
    (c) Give a combination of C, H and N to account for m/z values of **(i) 29 (ii) 57**
17. Explain the principle of 2D NMR. State its advantages over normal NMR.
18. Write briefly on the theory and applications of MRI.

Section C (Answer any **2** questions. Each question carries a weight 5)

19. Explain HRMS.
20. (a) Describe the effect of steric hindrance on coplanarity in UV spectroscopy
    (b) Explain bathochromic shift and hypsochromic shift
21. Discuss the different methods to simplify complex spectra.
22. An organic compound with molecular formula $C_8H_8O_3$ give the following spectroscopic data.

MS: m/z = 152 (49 %), 121 (29%), 120 (100%), 92 (54%)

IR: r main = 3205 broad, 1675 (s), 1307 (s), 1253(s) and 1220(s) cm^{-1}
^{1}H NMR ($CDCl_3$): d 3.92 (s, 3H) , 6.85 (t , 1H , J=8Hz) , 7.00 (d ,1H , J=8Hz), 7.44 (t ,1H , J=8Hz), 7.83 (d, 1H, J = 8Hz) 10.8(s, 1H)
^{13}C NMR ($CDCl_3$): d 52.1, 112.7 (s), 117.7 (d) , 117.2(d), 130.1(d) , 135.7 (d), 162.0(s), 170.7(s)
Deduce the structure and interpret the spectra.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- IV Semester
PG20CH413 –ADVANCED INORGANIC CHEMISTRY
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight of 1)

1. What are vanishing integrals?
2. How will you distinguish between a thiocyanato and isothiocyanato metal complex using IR spectroscopy?
3. Give the characters of the reducible representation for d orbital wave function in a square planar field**.**
4. Give the pictorial representation of the linear combination of a_{1g} and a_{2u} LGO's cyclopentadienyl ring with Fe^{2+} orbitals
5. What is meant by GILCs? Give any two applications of GILCs.
6. Give any four applications of nanomaterials as sensors
7. Differentiate between electroplating and electrophoretic deposition
8. Explain the role of X ray Diffraction technique in the structure elucidation of nanomaterials.
9. Explain electron transfer process in ruthenium complexes.
10. What is meant by Photo induced electron collection? Explain with an example.

SECTION B
(Answer any **6** questions. Each carries a weight of 2**)**

11. Discuss the transformation properties of orbitals using examples
12. Write an account on the application of Mossbauer spectroscopy to the study of Fe complexes**.**
13. What is meant by correlation diagram? Construct the correlation diagram of d^2 by the method of descending symmetry
14. Write a note on the synthesis and applications of quantum dots
15. Explain synthesis, structure and applications of zeolites
16. Write a note on the applications of nanotechnology in biology.
17. Discuss the electron relay mechanism for water photolysis
18. Write a note on dye sensitized photochemical solar cell.

SECTION C
(Answer any **2** questions. Each carries a weight 5**)**

19. Construct a MO energy level diagram for an octahedral complex involving pi bonding ligands.
20. Explain the application of character table to IR and RAMAN spectroscopy
21. Write notes on a) Synthesis and applications of metal nanoparticles b) lithography
22. (a)What are the different types of photochemical reactions that occur in metal complexes? (b)How is knowledge of absorption spectra useful in studying their photochemistry?

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS) Degree Examination- IV Semester
PG20CH414 –ADVANCED ORGANIC CHEMISTRY
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight of 1)

1. What is meant by metabolites?
2. What are Agonism and Antagonism?
3. Write down the mechanism of benzoin condensation. Discuss the green alternative of benzoin condensation and its advantages.
4. What are the important features of Jacobsen's catalyst?
5. What is meant by polymerase chain reaction?
6. Give one important chemical used as anti-bacterial drugs? Explain with structures.
7. Briefly explain NLO polymers. What are hyper branched polymers?
8. Write briefly on the different types of scientific publications.
9. 12. Briefly discuss asymmetric Diels-Alder reactions.
10. What are the forces involved in molecular recognition?

Section B (Answer **6** questions. Each question carries a weight of 2)

11. What are the applications of Supra Molecular Chemistry?
12. Explain the importance of molecular recognition in DNA?
13. Write a note on cholesterol lowering agents.
14. What is asymmetric induction? Explain the importance of chiral auxiliaries.
15. Write a note on PGE2 and PGF2α.
16. Briefly discuss the important drugs used for Cancer and AIDS.
17. Discuss the action and applications of temperature resistant and flame resistant polymers.
18. Write on various types of chemical literature.

Section C (Answer any **2** questions. Each question carries a weight of 5)

19. What are molecular receptors? Explain the structure, functions, and applications of (a) cyclodextrins (b) crown ethers (c) cryptands (d) calixarenes and e) carbon nanocapsules as receptors.
20. (a)What are the principles of 'Green Chemistry'? (b) Explain the importance of 'Green solvents' in organic synthesis.
21. Write notes on (a) polymerase chain reaction (b) DNA sequencing and (c) human genome project.
22. What are 'Dendrimers'? Explain the classification, synthesis and applications of dendrimers.

MAR ATHANASIUS COLLEGE (AUTONOMOUS), KOTHAMANGALAM
M.Sc. Chemistry (PGCSS)Degree Examination- IV Semester
PG20CH415 –ADVANCED PHYSICAL CHEMISTRY
MODEL QUESTION PAPER

Time: 3 hrs Max. Weight**:** 30

Section A (Answer any **8** questions. Each question carries a weight of 1)

1. Describe Wein effect.
2. What is meant by Debye – Falkenhagen effect?
3. What is osmotic coefficient?
4. Write a note on electro capillarity and Lippmann equation.
5. What are the advantages of DME?
6. Why the dissolved oxygen removed in polarographic measurements?
7. Differentiate between reduction potential and decomposition potential
8. Compare and contrast electron diffraction and neutron diffraction methods.
9. Explain the mechanism of fluorescence sensing.
10. Write a short note on flame emission spectroscopy.

Section B

(Answer any **6** questions. Each question carries a weight 2)

11. Write a note on Tafel equation and its significance.
12. Describe the principle of atomic emission spectroscopy and explain its advantages.
13. Describe the rotating crystal method
14. What is meant by dead stop end point in amperometric analysis?
15. Iron (II) oxide, FeO, crystal has a cubic structure and each edge of the unit cell is 500 pm. Taking density of the oxide as 4000 kg m^{-3}, calculate the number of Fe^{2+} and O^{2-} ions present in each unit cell
16. Calculate the separation of (123) and (246) planes of an orthorhombic unit cell with a= 0.82nm, b= 0.94nm and c= 0.75nm.
17. For the cell Hg, Hg_2Cl_2(s), KCl (0.07m)/KCl (0.03m), Hg_2Cl_2(s), Hg, write the overall cell reaction and calculate the emf if transference number of K^+ is 0.48
18. Calculate the ionic strength of the following solutions (a) a solution containing 0.2 molal KCl and 0.1 molal K_2SO_4 (b) 0.5 molal aluminium sulphate solution.

Section C (Answer any **2** questions. Each question carries a weight of 5)

19. Derive Debye - Huckel limiting law and discuss its various forms.
20. (a) Discuss the applications and advantages of polarography
    (b) Write a note on cyclic voltametry.
21. Explain the principle, instrumentation and application of atomic absorption Spectroscopy.
22. Derive Debye – Huckel- Onsager equation. Discuss its validity for aqueous and non- aqueous solutions.