Maharaja's
College
Ernakulam

A GOVERNMENT
AUTONOMOUS COLLEGE

Re-Accredited by NAAC with 'A Grade'
Affiliated to Mahatma Gandhi University
Centre of Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence

POST GRADUATE AND RESEARCH
DEPARTMENT OF CHEMISTRY

Estd. 1875

Post Graduate Curriculum and Syllabus
(Credit Semester System)

M. Sc. CHEMISTRY

For 2022 Admission Onwards

M.Sc. CHEMISTRY

FOREWORD

The Board of Studies in Chemistry take this opportunity to express our deep appreciation to all academicians and professionals who participated in the series of workshops organised by the Board for restructuring curriculum and syllabi of the PG courses in Chemistry-M.Sc Chemistry, M.Sc Analytical Chemistry, M.Sc Pharmaceutical Chemistry and M.Sc Applied Chemistry. We express our profound gratitude to the Honourable Vice-Chancellor, Pro-Vice Chancellor, Members of the Syndicate and Members of the Academic Council, Mahatma Gandhi University, for their sincere co-operation and guidance for completion of this work. Our special thanks are due to Chairman and members of the Governing Council, Chairman and members of the Academic Council, Maharaja's College, Ernakulam.

We also extend our gratitude to Prof. (Dr). K. Girish Kumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). Prathapachandra Kurup Professor and Head (Retd.) Department of Chemistry, Central University of Kerala, Padannakad, Dr. T. Narayanan, Associate Professor (Retd.), Maharaja's College, Ernakulam, and Dr. Benny Antony Arjuna Natural Extracts, Aluva who were entrusted with the responsibility as experts for the revision of the syllabus of different subjects. The Board of Studies in Chemistry expresses the whole hearted gratitude to all those who have helped in this endeavour.

The task of preparing the curricula and syllabi and bringing it out in the present form for all the four M.Sc courses was not simple but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS and the faculty members of the Department of Chemistry. I would like to express my sincere thanks to all my fellow members of BOS and the faculty members of the Department of Chemistry for all their help, cooperation, encouragement, active participation and useful suggestions for the completion of syllabus.

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REGULATIONS OF THE MAHARAJA’S COLLEGE
(Government Autonomous)
POST GRADUATE PROGRAMMES
UNDER CREDIT SEMESTER SYSTEM, 2022
(MC-PGP-CSS2022)

REGULATIONS OF THE POST GRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM, 2022
(MC-PGP-CSS2022)

1. SHORT TITLE

1.1. These Regulations shall be called Maharaja's College (Government Autonomous) Regulations(2022) governing Post Graduate Programmes under Credit Semester System (MC-PGP-CSS2022)

1.2. These Regulations shall come into force from the Academic Year 2022- 2023.

2. SCOPE

2.1. The regulation provided herein shall apply to all Post- graduate programmes from the academic year 2022-2023 admission.

2.2. The provisions herein supersede all the existing regulations for the regular post-graduate programmes conducted in Maharaja's College unless otherwise specified.

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 (MC-PGP- CSS2022).

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 minimum of 18 such academic weeks constitute 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 College Council to look into the matters relating to MC-PGP-CSS 2022 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 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 / viva-voce 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 thefinal 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 of 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 in the college.

3.17. **‘Department Council’** means the body of all teachers of a Department in aCollege.

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 an 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 students in a College. The external examiner shall be appointed by the University.

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

3.26. **‘Grace Grade Points'** means grade points awarded to course(s), in 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 points obtained in the course by the sum of the weights of the Course **(GPA = ΣWGP / ΣMW).**

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 Internalevaluation.

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. **MC-PGP-CSS2022 means Maharaja’s College (Government Autonomous) Regulations Governing Post Graduate programmes under Credit Semester System, 2022.**

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 assignments 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 proramme. 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 center 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 orfindings.

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

3.38. **'Semester'** means a term consisting of a minimum of 90 working days, inclusive of examinations, distributed over a minimum of 18 weeks of 5 working dayseach.

3.39. **'Seminar’** means a lecture given by the student on a selected topic and is 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 a 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’** 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. **‘University’** means Mahatma Gandhi University, Kottayam, Kerala.

3.43. **‘Weight’** is a numeric measure assigned to the assessment units of various components of a course of study.

3.44. **‘Weighted Grade Point’ (WGP)** is the grade point multiplied by weight. **(WGP** = GP × 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.

3.46. **‘Internship’** means gain a professional work experience

4. ACADEMIC COMMITTEE

4.1. There shall be an Academic Committee constituted by the Principal to manage and monitor the working of MC-PGP-CSS2022.

4.2. The Committee consists of

(a) Principal
(b) Vice-Principal
(c) Secretary, Academic Council
(d) The Controller of Examinations
(e) Two Teachers nominated from among the College Council

4.3. There shall be a subcommittee nominated by the Principal to look after the day-to-day affairs of the Regulations for Post Graduate Programmes under MC-PGP-CSS2022.

5. PROGRAMME STRUCTURE

- 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 / practicals etc.
- No regular student shall register for more than 25 credits and less than 16 credits per semester unless otherwise specified. The total minimum credits, required for completing a PG programme is 80.

5.1. Elective courses and Groups

5.1.1. There shall be at least two and not more than four elective groups(Group A, Group B, Group C, etc.) comprising of three courses each for a programme and these elective courses shall be included either in fourth semester or be distributed among third and fourth semesters. This clause is not applicable for programmes defined by the Expert Committees of Music and Performing Arts.

5.1.2. The number of elective courses assigned for study in a particular semester shall be the same across all elective groups for the programme concerned.

5.1.3. The colleges shall select any one of the elective groups for each programme as per the interest of the students, availability of faculty and academic infrastructure in the institution.

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

5.1.5. The elective groups selected by the College 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 by the college for the students who are admitted in a particular academic year shall not be changed.

5.2. Project work

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

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

5.2.3. 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.

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

5.2.5. 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.

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

5.2.7. 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.

5.3. Assignments: Every college going student shall submit at least one assignment as an internal component for each course.

5.4. Seminar Lecture: Every regular 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.

5.5. Test Papers (Internal): Every regular student shall undergo at least two class tests as an internal component for each course with a weightage of one each. The best two shall be taken for awarding the grade for class tests.

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

5.7. 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.

5.7.1. **Comprehensive Viva-Voce** shall cover questions from all courses in the programme.

5.7.2. 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 Principal.

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 MC-PGP-CSS2022 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 has registered for the programme shall complete the programme within a period of four years from the date of commencement of theprogramme.

8. ADMISSION

8.1. The admission to all regular PG programmes shall be through PG- CAP (Centralized Allotment Process) of the Maharaja’s College unless otherwise specified.

8.2. The eligibility criteria for admission to PG Programmes shall be published bythe Maharaja’s College along with the notification for admission.

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 recognized by 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 a particular 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 There shall be End Semester Examinations at the end of each semester.

11.2 Practical examinations shall be conducted by the College 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 subjected to the approval of the Academic Council of the College.

11.3 End-Semester Examinations: The examinations shall normally be conducted at the end of each semester for regular students.

11.4 There shall be one end-semester examination of 3 hours duration for each lecture based and practical courses.

11.5 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 12.15.

12.4 **Internal evaluation for Regular programme:** The internal evaluation shall be based on predetermined transparent system involving 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**

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

b) **For theory (ESE)** External Evaluation is based on the pattern of questions 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 the weightage of the components 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 the weightage of the components 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**)**

A two stage Internal evaluation to be followed for the fruitful completion of the project.

f) For Project (ECE) 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

Components	Internal (CE) Weight	External (ESE) Weight
Basic knowledge and Presentation skills	1	3
Topic of interest	1	3
Knowledge of core courses	3	9
Total	**5**	**15**

These basic components can be subdivided if necessary. Total as well as component weightage shall not be changed.

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 which shall be forwarded to the University through the Principal 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 University 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 preferably through Centralized Valuation.

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 College/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 beanswered
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 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**

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(pass)**
up to 1.99	**D**	**Deficient(Fail)**

12.19 No separate minimum is required for internal evaluation for a pass, but a minimum C 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 candidates who wish to improve the grade / grade point of the external examination 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**

semesters 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 practicals / 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 points of all courses taken by a student in the 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 $(S_j) = \Sigma\ (Ci \times G_i) / \Sigma(Ci$

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

Where 'Sj' is the j semester, 'Gi ' is the grade point scored by the Student in the ‘i' course 'q' is the credit of the ith course.

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

Cumulative Grade Point Average (CGPA) $= \Sigma(\ (Ci \times S_i) / \Sigma(Ci$

(CGPA= Total credit points awarded in all semesters /
Total credits of the programme)

Where 'Ci' is the credits for the ‘i' semester 'Si' is the SGPA for the ith 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 University under its seal shall issue to the students, a consolidated grade card on completion of the programme, which shall contain the following information.

- Name of College
- Title of the PG Programme.
- Name of the Semesters
- Name and Register Number of the student
- Code, Title, Credits and Max GPA (Internal, External & Total) of each course (theory& Practical), project, viva etc. in each semester.
- Internal, external and total grade, Grade Point (G), Letter Grade and Credit Point (P) in each course opted in the semester.
- The total credits and total credit points in each semester.
- Semester Grade Point Average (SGPA) and corresponding Grade in each semester
- Cumulative Grade Point Average (CGPA), Grade for the entire programme.
- Separate Grade card will be issued at the request of candidates and based on University Guidelines issued from time to time.
- 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 Vice- chancellor to monitor the internal evaluations conducted by institutions.

16. RANK CERTIFICATE

The College shall publish the list of top 10 candidates for each programme after the publication of the programme results. Rank certificate shall be issued to candidates who secure positions from 1st to 3rd in the list. Position certificate shall be issued to candidates on theirrequest.

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/position. Rank certificate and position certificate shall be signed by 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. 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.

19. CREDITS ALLOTTED FOR PROGRAMMES AND COURSES

19.1. Total credit for each programme shall be 80.

19.2. Semester-wise total credit can vary from 16 to 25

19.3. The minimum credit of a course is 2 and maximum credit is 5.

20. COMMON COURSE

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

21. COURSE CODES

The course codes assigned for all courses (core courses, elective courses, common courses etc.) shall be unique.

22. SCHEME OF THE SYLLABUS

Distribution of courses, course codes, type of the course, credits, teaching hours for a programme are given in the following table.

M.Sc. CHEMISTRY

	Course-code	Coursename	Type of the course	Teaching Hours Per Week	Total Hours	Credit	Weights		
							Internal	External	Total
Semester 1	PG1CHEC01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	core	4	72	4	5	30	35
	PG1CHEC02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	core	4	72	4	5	30	35
	PG1CHEC03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	core	4	72	4	5	30	35
	PG1CHEC04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	core	3	54	3	5	30	35
	PG2CHEP01	Inorganic Chemistry Practical–1	Practical	3	54	4	Evaluation at the end of fourth semester		
	PG2CHEP02	Organic Chemistry Practical-1	Practical	3	54				
	PG2CHEP03	Physical Chemistry Practical -1	Practical	4	72				
			Total	**25**	**450**	**19**			
Semester 2	PG2CHEC05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	core	4	72	4	5	30	35
	PG2CHEC06	Organic Chemistry- II (Reaction Mechanism)	core	4	72	4	5	30	35
	PG2CHEC07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	core	4	72	4	5	30	35
	PG2CHEC08	Physical chemistry- II (Molecular Spectroscopy)	core	3	54	4	5	30	35
	PG2CHEP01	Inorganic Chemistry Practical–1	Practical	3	54	4	5	15	20
	PG2CHEP02	Organic Chemistry Practical-1	Practical	3	54		5	15	20
	PG2CHEP03	Physical Chemistry Practical -1	Practical	4	72		5	15	20
			Total	**25**	**450**	**20**			
Semester 3	PG3CHEC09	Inorganic chemistry-III (Solid State Chemistry)	core	4	72	4	5	30	35
	PG3CHEC10	Organic chemistry- III (Organic Syntheses)	core	4	72	4	5	30	35

	PG3CHEC11	Physical chemistry- III (Chemical Kinetics, Surface Chemistry and Photochemistry)	core	4	72	4	5	30	35
	PG3CHEC12	Spectroscopic Methods in Chemistry	core	3	54	4	5	30	35
	PG4CHEP04	Inorganic Chemistry Practical–2	Practical	3	54	4	Evaluation at the end of fourth semester		
	PG4CHEP05	Organic Chemistry Practical-2	Practical	3	54				
	PG4CHEP06	Physical Chemistry Practical -2	Practical	4	72				
			Total	**25**	**450**	**20**			
Semester 4	PG4CHEE01	Elective –I Inorganic Chemistry - IV (Advanced Inorganic Chemistry)	Elective	5	90	3	5	30	35
	PG4CHEE02	Elective –II Organic Chemistry - IV (Advanced Organic Chemistry)	Elective	5	90	3	5	30	35
	PG4CHEE03	Elective –III Physical Chemistry- IV (Advanced Physical Chemistry)	Elective	5	90	3	5	30	35
	PG4CHEE04	Elective –IV Polymer Chemistry	Elective	5	90	3	5	30	35
	PG4CHEE05	Elective –V Analytical Chemistry	Elective	5	90	3	5	30	35
	PG4CHEP04	Inorganic Chemistry Practical–2	Practical	3	90	5	5	30	35
	PG4CHEP05	Organic Chemistry Practical-2	Practical	3	54		5	15	20
	PG4CHEP06	Physical Chemistry Practical -2	Practical	4	54		5	15	20
	PG4CHED01	Project	Core			5			
	PG4CHEV01	Comprehensive Viva -Voce	Core			2			
			Total	**25**	**450**	**21**			
			G. 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
Up to 1.99	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	20	A+	5	5	25
	21	-	-	-	-
	22	-	-	-	-
	23	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. *ie*., maximum 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	2	C	2	4	**WGP/Total weight = 59/15 = 3.93**
Project content & presentation	8	A+	5	40	
Project viva- voce	5	B	3	15	
Total	**15**			**59**	**B**

Project-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 1.5. Therefore Maximum Weighted Grade Point (WGP) is 75.

Components	Internal (CE) Weight	External (ESE) Weight
Basic knowledge and Presentation skills	1	3
Topic of interest	1	3
Knowledge of core courses	3	9
Total	**5**	**15**

Comprehensive viva voce-Internal-CE

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

These basic components can be subdivided if necessary

2. Evaluation - second stage - Consolidation of the Grade (GPA) of a Course PC-I.

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

Semester Grade Point Average (SGPA).

Course code	Title of 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 - fourth Stage - 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) and semester 4 (SGPA of semester 4) and a B grade in semester 3 (SGPA of semester 3). Then the 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				

Post Graduate Programme Outcome

At the completion of the Post Graduate Programme, the student will be able to accomplish the following

1. **Critical and creative thinking:**
    - Enables to evaluate information and its sources critically. .
    - Engage the imagination to explore new possibilities.
    - Formulate and articulate ideas.
    - Identify, evaluate and synthesize information (obtained through library, world-wide web, and other sources as appropriate) in a collaborative environment.
2. **Synergetic work culture and effective communication:**
    - Enables to develop a synergistic working relationship, which is essential for achieving a higher quantity and quality output.
    - Help to increase team productivity, enhanced individual performance and better customer engagement.
3. **Social Consciousness:**
    - Enables to understand one’s role , status, rights and responsibilities as a social being which is essential for the society
    - Helps to employ the knowledge and methodologies acquired to better understand economic, legal, and social issues and act effectively.
4. **Subject knowledge:**
    - Possess breadth and depth of knowledge within their discipline and more particularly within their chosen specialization.
    - They can articulate their interpretations with an awareness and curiosity for other people's perspectives.
5. **Lifelong learning:**
    - Recognize the need for, and have the preparation and ability to engage in independent and lifelong learning in the broadest context of technological change.
    - Understands his or her learning preferences and knows how to adapt them to maximize learning under different circumstances.
6. **Multidisciplinary approach:**
    - Brings pragmatism and flexibility, allowing students to carve their path.
    - Develop knowledge in a specific topic to instill in students the ability to assess information and apply it to real-life situations.

Programme Specific Outcome

PSO No.	**Expected Programme Specific Outcomes** ***Upon completion of this programme, the students will be able to:***	PO No.
1	Acquire thorough knowledge regarding the basic principles of chemistry and appreciate it in a broader multi-disciplinary context.	**1, 4, 6**
2	Apply their understanding in chemistry to address and design solutions in societal and environmental contexts and demonstrate the knowledge for sustainable development.	**3, 5**
3	Develop diverse skill sets and abilities to pursue variety of careers in academia, research, and industries.	**1, 6**
4	Apply appropriate techniques for the qualitative and quantitative analysis of chemicals and adopt safer life skills in a human friendly and eco-friendly way.	**3, 4, 5**
5	Develop objectivity, creativity, independent thinking and skills in communicating chemistry and related topics.	**1, 2, 3, 6**
6	Inculcate the spirit of research aptitude and to create and evaluate new ideas, research findings, methodologies and theoretical frameworks in a specialised field of study.	**4, 5, 6**
7	Operate advanced instruments and related soft-wares to execute in-depth analysis of chemical problems with a scientific outlook of being cautious about environmental aspects and impact in all frontiers of life.	**2, 3, 5**

SEMESTER I

<table>
<tr><td>Course code</td><td colspan="5">PG1CHEC01</td></tr>
<tr><td>Course</td><td colspan="5">INORGANIC CHEMISTRY- I
(COORDINATION AND BIOINORGANIC CHEMISTRY)</td></tr>
<tr><td>Degree</td><td colspan="5">M.Sc.</td></tr>
<tr><td>Branch</td><td colspan="5">CHEMISTRY</td></tr>
<tr><td>Year/Semester</td><td colspan="5">1/I</td></tr>
<tr><td>Type</td><td colspan="5">CORE</td></tr>
<tr><td>Credits</td><td>4</td><td>Hours/week</td><td>4</td><td>Total hours</td><td>72</td></tr>
</table>

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Classify the coordination compounds based on their structural aspects	**Understand**	**1, 2**
2	Interpret the structure and bonding in complexes based on CFT and MO model	**Apply**	**1, 2, 5, 6**
3	Analyse and predict the electronic spectra and magnetic properties of complexes.	**Analyse**	**1, 2, 5, 6**
4	Analyse the stereo chemical aspects of complexes	**Analyse**	**1, 2, 5, 6**
5	Explain and formulate the reaction mechanism of ligands substitution and redox reactions in complexes	**Create**	**1, 2, 5, 6**
6	Describe the role of metals ions in biological processes	**Understand**	**1, 2, 6**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Coordination Chemistry- Structural Aspects and Bonding**	**18**	**1, 2**
1.1	Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN, R_3P and Ar_3P.	4	
1.2	Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory,	14	

	evidence of covalency in the metal ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory- M.O energy level diagrams for octahedral and tetrahedral complexes with and without π-bonding, experimental evidences for π-bonding.		
2	**Spectral and Magnetic Properties of Metal Complexes**	**18**	**3**
2.1	Electronic Spectra of complexes- Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition- effect of spin orbit coupling and vibronic coupling.	5	
2.2	Interpretation of electronic spectra of complexes- Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and *β* (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.	5	
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. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism- inter and intra molecular interaction. Anomalous magnetic moments.	5	
2.4	Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments	3	
3	**Stereochemistry of Coordination Compounds**	**9**	**4**
3.1	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	5	

3.2	Linkage isomerism- electronic and steric factors affecting linkage isomerism. Symbiosis, hard and soft ligands, Prussian blue and related structures, Macrocycles- crown ethers.	4	
4	**Kinetics and Mechanism of Reactions in Metal Complexes**	**9**	**5**
4.1	Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.	3	
4.2	Kinetics and mechanism of octahedral substitution-water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).	3	
4.3	Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism	3	
5	**Bioinorganic Compounds**	**18**	**6, 7**
5.1	Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis, chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.	8	
5.2	Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems- ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Non-redox metalloenzymes- Carboxypeptidase A- structure and functions. Nitrogen fixation- nitrogenase, vitamin B_{12} and vitamin B_{12} coenzymes	8	
5.3	Metals in medicine- therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals (Cd, Hg, Cr and Pb).	2	

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Course code	**PG1CHEC01**				
Course	**INORGANIC CHEMISTRY- I (COORDINATION AND BIOINORGANIC CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	2	2	1	55
Module 3 (9 hrs)	2	1	0.5	32.5
Module 4 (9 hrs)	2	1	0.5	32.5
Module 5 (18 hrs)	2	2	1	55
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**

Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST SEMESTER
Programme: M.Sc. Chemistry
PG1CHEC01: INORGANIC CHEMISTRY- I (COORDINATION & BIOINORGANIC CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What is the significance of Dq values?
2. In MnF_2 and ZnF_2, there is no splitting of d orbitals ($\Delta o = 0$) Why?
3. What is the number of unpaired electrons in tetrahedral $[Ni(CO)_4]$ complex?
4. The ground state term symbol of central metal ion in $[Co(NH_3)_6]Cl_3$
5. What are hard and soft ligands? Give examples.
6. Give an example for an asymmetric synthesis catalysed by coordination compounds.
7. What do you mean by inert and labile complexes? How the inertness of a complex different from its thermodynamic stability.
8. What is trans effect? Arrange the following ligands in the increasing order of their lability a) CN^- b) NH_3 c) Cl^- d) OH^-
9. What are redox metalloenzymes?
10. Define ionophores.

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. For $[Cr(H_2O)_6]^{2+}$ ion, pairing energy is greater than crystal field splitting energy. Will it be a high spin or low spin complex?
12. Discuss the experimental evidences for the metal ligand π bonding in complexes.
13. What are the merits and demerits of Orgel diagram?
14. Explain the Gouy method for determining magnetic moment of complexes
15. What is linkage isomerism. Discuss the different factors affecting linkage isomerism.
16. Explain the Marcus theory for outer sphere mechanism with a suitable example.
17. Distinguish photosystem I and photosystem II.
18. Briefly explain sodium-potassium pump.

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. Apply the Molecular Orbital Theory for the complex $[Co(NH_3)_6)^{3+}$ and construct the molecular orbital energy level diagram.
20. What are Orgel diagrams? Draw the Orgel diagrams of d^1, d^2, d^3 and d^9 systems in both octahedral and tetrahedral fields.
21. (a) What is absolute configuration of a coordination compound. Discuss the note of CD and ORD in reading the absolute configuration of a complex.

    (b) Discuss the salient features and mechanism of outer sphere and inner sphere reactions with suitable examples.
22. Write short note on a) haemoglobin b) myoglobin c) hemocyanin d) hemerythrin e) hemovanadins

(2 × 5 =10)

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Course code	**PG1CHEC02**				
Course	**ORGANIC CHEMISTRY - I (STRUCTURE, REACTIVITY & STEREOCHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand the basic concepts in organic chemistry	**Understand**	**1, 2**
2	Recognize and apply the experimental tools of physical chemistry to study the mechanism of organic reactions	**Apply**	**1, 2, 5**
3	Illustrate the mechanisms involved in organic reactions.	**Apply**	**1, 2, 5, 6**
4	Analyse the three-dimensional structural aspects of molecules	**Analyse**	**1, 2, 5**
5	Demonstrate the relationship between energetics, reactivity with conformation of molecules.	**Apply**	**1, 2, 5**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Bonding and Aromaticity**	**9**	**1**
1.1	Review of basic concepts in organic chemistry: bonding, hybridization, MO theory and MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.	4	
1.2	Concept of aromaticity: delocalization of electrons - Huckel’s rule, criteria for aromaticity, examples of neutral and charged aromatic systems, azulenes, annulenes, mesoionic compounds. NMR as a tool for aromaticity. Antiaromatic and homoaromatic systems. Fullerenes, carbon nanotubes and graphene.	5	
2	**Investigation of Organic Reaction Mechanisms**	**9**	**2, 3**

2.1	Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Primary and secondary kinetic isotope effects.	4	
2.2	Introduction to carbon acids - pK_a of weak acids, kinetic and thermodynamic acidity. HSAB principle and its applications in organic reactions.	2	
2.3	Catalysis by acids, bases and nucleophiles with examples from acetal and cyanohydrin. Ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms. Phase transfer catalysis and its applications.	3	
3	**Review of Organic Reaction Mechanisms**	**18**	**3**
3.1	Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2), SN in bridge head systems, elimination (E_1 and E_2). Elimination vs substitution.	4	
3.2	A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E_1, E_2 and E_1CB) reactions. Stereochemical aspects of elimination reaction.	7	
3.3	Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).	2	
3.4	Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.	5	
4	**Stereochemistry of Organic Compounds**	**18**	**4**
4.1	Projection Formulae. Introduction to molecular symmetry and chirality: Examples from common objects to molecules. Axis, plane, center and alternating axis of symmetry.	3	
4.2	Stereoisomerism: definition based on symmetry and energy criteria, Configurational isomerism. Geometrical isomerism- nomenclature, methods of determination of geometrical isomers based on physical properties, NMR spectroscopy and chemical methods.	2	

4.3	Optical isomerism, nomenclature. Absolute configuration, R and S nomenclature using Cahn-Ingold-Prelog rules.	3	
4.4	Center of chirality: Molecules with C, N, S based chiral centers, molecules with a chiral center and C_n, molecules with more than one center of chirality, Definition of enantiomers, racemic modifications, diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.	3	
4.5	Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.	3	
4.6	Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.	3	
4.7	Chiral drugs	1	
5.0	**Conformational Analysis**	**18**	**5**
5.1	Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Bridged bicyclic systems- norbornane, camphor, bicyclo[2.2.2]octane.	9	
5.2	Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols, nucleophilic addition to carbonyl compounds (Cram's Rule). Chemical consequence of conformational equilibrium - Curtin Hammett principle.	9	

References

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4. H.O. House, Modern Synthetic Reactions, Organic Chemistry Monograph Series, Benjamin, 1965.
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Course code	**PG1CHEC02**				
Course	**ORGANIC CHEMISTRY - I (STRUCTURE, REACTIVITY & STEREOCHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (weightage/ Qn: 1)	**Section B (weightage/ Qn: 2)**	**Section C (weightage/ Qn: 5)**	**Total WGP**
Module 1 (9 hrs)	2	1	1/2	32.5
Module 2 (9 hrs)	2	1	1/2	32.5
Module 3 (18 hrs)	2	2	1	55
Module 4 (18 hrs)	2	2	1	55
Module 5 (18 hrs)	2	2	1	55
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

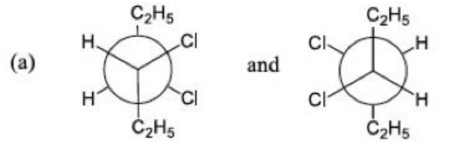
Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST SEMESTER
Programme: M.Sc. Chemistry
PG1CHEC02: ORGANIC CHEMISTRY- I
(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

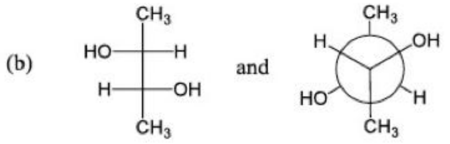
Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. Explain why *o-tert*-butylbenzoic acid is more acidic than the *para*-isomer.
2. Pyrene has 16-π electrons, yet it is considered as an aromatic compound. Why?
3. Write the mechanism of acetal formation.
4. Discuss microscopic reversibility with a suitable example.
5. How can you establish that the alkane hydrolysis of chloroform involves dichlorocarbene as the reactive intermediate?
6. Why an alcohol reacts with halide ion only in the presence of a strong acid? Give suitable example.
7. Label the following pairs of structures as homomers, enantiomers or diastereomers.





8. What are the conditions for chirality in biphenyls?
9. Draw the preferred conformation(s) of the following compounds:
   (a) 1-chloropropane (b) 2-chloroethanol.
10. Predict the most stable conformation of *cis*-1,4-di-*t*-butylcyclohexane. Explain.

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

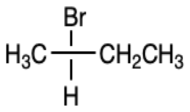
11. Discuss the aromaticity of azulenes and annulenes.
12. Discuss the different mechanisms of ester hydrolysis with experimental evidences.
13. Describe the effect of solvent on the rate of aliphatic nucleophilic substitution reactions.

14. (a) Although the -NH_2 group in aniline is *ortho*, *para*-directing, *m*-nitroaniline may be prepared by direct nitration of aniline in the presence of 98% H_2SO_4. Explain.

    (b) Explain why *p*-nitroaniline is prepared in the laboratory not by nitrating aniline directly but by nitrating acetanilide followed by hydrolysis.

    (c) Predict the major product in each of the following reactions and give your reasoning.

15. Given the following Fischer projections, indicate (a) stereochemical relationship between each other (b) assign configuration.

(1)

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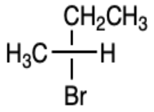
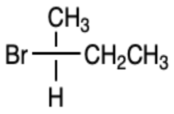
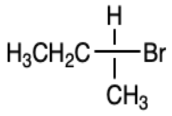
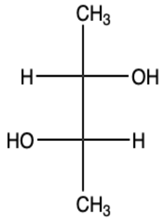
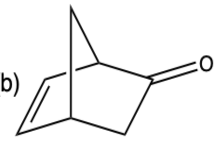
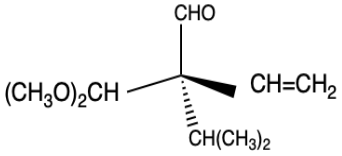

(3)

(4)


16. Assign the configuration of the following configurations:

(a)

(b)

(c)


17. Illustrate Curtin-Hammett principle with an example.
18. Discuss the conformations of (a) decalin (b) Adamantane.

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. a) What are hard acids and bases? State hard and soft acid-base principle.

    b) Derive Hammett equation and explain the physical significance of each term in the equation with examples.

20. a) Discuss the different mechanisms of ester hydrolysis with experimental evidences.

    b) Differentiate aromatic Addition-Elimination mechanism from Elimination-Addition mechanism with suitable examples.

21. a) Briefly discuss the axial, planar and helical chirality with examples.

    b) What is meant by prostereogenic centre? How can enantiotopic and diastereotopic faces be specified? Give examples.

22. a) Discuss the conformational analysis of cyclohexane.

    b) Draw the conformations of *cis* and *trans* isomer of *1, 2*-. *1, 3*- and *1,4*-dimethylcyclohexanes. Compare stabilities and optical properties of above compounds.

(2 × 5 = 10)

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Course code	**PG1CHEC03**				
Course	**THEORETICAL CHEMISTRY – I** **(QUANTUM CHEMISTRY AND GROUP THEORY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcome** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand the evolution quantum mechanics and basic concepts and terms related to quantum mechanics	**Understand**	**1, 2**
2	Apply appropriate quantum mechanical operators to predict spin and angular momenta	**Apply**	**1, 2, 5, 6**
3	Evaluate the methods of quantum mechanics to Translational/Rotational/Vibrational motions	**Apply**	**1, 2, 5, 6**
4	Apply quantum mechanics to single particle systems	**Apply**	**1, 2, 5, 6**
5	Predict the point group of molecules by analysing their symmetry operations and symmetry elements	**Apply**	**1, 2, 5, 6**
6	Construct character tables using rules derived from the great orthogonality theorem	**Create**	**1, 2, 5, 6**
7	Apply symmetry and group theory principles to predict the electronic/vibrational transitions in the molecules	**Evaluate**	**1, 2, 5, 6**

Module No.	Course Description	Hours	CO No.
1	**Formulation of Quantum Chemistry**	**18**	**1, 2**
1.1	Mathematical Concepts: Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions. Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships.	5	
1.2	Evolution of Quantum Mechanics: Failure of classical mechanics. The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation. The wave equation in Spherical polar coordinates	6	
1.3	Postulates of Quantum Mechanics: Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.	4	
1.4	Orbital and Spin angular momentum: Quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Ladder operator. Spherical harmonics as Eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmit, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.	3	
2	**Applications of Quantum Chemistry**	**18**	**3, 4**
2.1	Quantum Mechanics of Translational Motion: Particle in one-dimension with infinite potential walls, particle in a	4	

	three-dimensional box- separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.		
2.2	Quantum Mechanics of Vibrational Motion: One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. Rodrigue’s formula, Three-dimensional harmonic oscillator.	5	
2.3	Quantum Mechanics of Rotational Motion: Rotational motion: Particle on a ring, the Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)- separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Quantisation of energy and angular momentum. Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.	4	
2.4	Quantum Mechanics of Hydrogen-like Atoms: Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.	5	
3	**Molecular Symmetry and Group Theory**	**18**	**5**
3.1	Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.	8	
3.2	Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O as example).	7	

3.3	Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs. The Great Orthogonality Theorem (GOT).	3	
4	**Applications of Group Theory**	**18**	**6, 7**
4.1	Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.	6	
4.2	Applications of group theory in quantum mechanics, vanishing integrals, transition moment integral. Woodward – Hoffmann rules (cycloadditions and electrocyclic reactions).	5	
4.3	Vibrational & Raman spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules - selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O, Trans-N_2F_2 and NH3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra - determination of the number of active IR and Raman lines.	5	
4.4	Electronic spectra: selection rules for electronic transition, prediction of electronic transitions due to the carbonyl chromophore in formaldehyde by group theory.	2	

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3. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
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14. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.
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Course code	**PG1CHEC03**				
Course	**THEORETICAL CHEMISTRY – I (QUANTUM CHEMISTRY AND GROUP THEORY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	3	2	1	60
Module 3 (18 hrs)	3	2	1	60
Module 4 (18 hrs)	2	2	1	55
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST SEMESTER
Programme: M.Sc. Chemistry
PG1CHEC03 - THEORETICAL CHEMISTRY- I
(QUANTUM CHEMISTRY AND GROUP THEORY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What is a well-behaved function? Explain.
2. Explain ladder operators.
3. What are Hermite polynomials? Write down the Hermite polynomial for n = 2 and n = 3.
4. Write down Recursion formula. Explain its significance.
5. Plot the radial portions of the *4s, 4p, 4d* and *4f* hydrogen like wave functions.
6. Find the product of C_{2z} and $\sigma_{v\ (xz)}$ in C_{2v} point groups taking H_2O as example.
7. Obtain the matrix representation for a C_{2v} molecule with H_2O as example.
8. Explain the method of block diagonalisation.
9. What is direct product representation?
10. State Great Orthogonality Theorem.

(1 × 8 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Write a note on operators in quantum mechanics.
12. Explain the spin postulates.
13. Discuss the particle in one dimensional box with infinite potential walls.
14. Find the eigenvalues and Eigen functions of a particle on a ring.
15. What is meant by a point group? Write the properties of a group with C_{2V} point group as example.
16. Construct the group multiplication table of C_{3v} point group.
17. Determine the normal modes of trans-N_2F_2 molecule using internal coordinates.
18. Explain the Woodward-Hofmann method for the conversion of cyclobutene to 1,3- butadiene.

(6 × 2 = 12)

Section C
Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. (a) Explain the postulates of quantum mechanics. (Weight 3)

(b) Describe the construction of spin orbitals from orbital and spin functions. (Weight 2)

20. Setup the Schrodinger equation for hydrogen atom and separate the variables to obtain r, θ and ϕ equations. Write the general solution of these equations.
21. What are character tables? Construct the character table for C_{3v} point group. Discuss the significance of each area of the table.
22. Using group theory obtain the selection rules for vibrational transitions in IR and Raman spectroscopy. Examine the IR and Raman activities of the vibrations of H_2O molecule.

(2 × 5 = 10)

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Course code	**PG1CHEC04**				
Course	**PHYSICAL CHEMISTRY – I (KINETIC THEORY, CLASSICAL AND STATISTICAL THERMODYNAMICS)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**3**	**Hours/week**	**3**	**Total hours**	**54**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Describe the kinetic theory of gases, collision parameters and transport properties	**Understand**	**1, 2**
2	Understand the basic concepts of classical, statistical and irreversible thermodynamics	**Understand**	**1, 2, 5**
3	Calculate and predict thermodynamic and kinetic properties	**Apply**	**1, 2, 5**
4	Analyse the macroscopic properties of matter using classical and statistical thermodynamics	**Analyse**	**1, 2, 5, 6**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Gaseous state**	**9**	**1, 3**
1.1	Kinetic theory of gases, Derivation of Maxwell’s law of distribution of velocities, graphical representation, experimental verification of the law, derivation of average, root mean square and most probable velocity	4	
1.2	Collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states.	3	
1.3	Transport properties of gases: viscosity, thermal conductivity and diffusion. Determination of viscosity of gases, Influence of temperature and pressure on transport properties.	2	
2	**Classical Thermodynamics**	**18**	**2, 3, 4**
2.1	Mathematical foundations for thermodynamics-variables of	2	

	thermodynamics, equation for total differential, conversion formulas, exact differentials, definite integrals, reciprocity characteristics, homogeneous functions, Euler's theorem, Cyclic rule (non-evaluative)		
2.2	Brief review on the basic concepts in thermodynamics, First law of thermodynamics (work, heat, internal energy, enthalpy: definition), P-V diagram, reversible and irreversible transformations, Heat capacity, Joule-Thomson effect, Kirchoff equation	1	
2.3	Carnot cycle, Heat engine, Heat pump, Entropy, Second Law of thermodynamics, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state, Clausius inequality.	2	
2.4	Helmholtz Free energy, Gibbs Free energy, Four fundamental equations in thermodynamics, Maxwell relations and significance, temperature dependence of free energy, Gibbs-Helmholtz equation, applications of Gibbs-Helmholtz equation.	2	
2.5	Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy	1	
2.6	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	
2.7	Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions- free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.	3	
2.8	Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.	2	
2.9	Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies of solids, liquids and gases using third law, entropy changes in chemical reactions	2	
2.10	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, and three pairs of partially miscible liquids.	2	

3	**Irreversible Thermodynamics and Bioenergetics**	**9**	**2**
3.1	Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations, the principle of microscopic reversibility, the Onsager reciprocal relations, thermal osmosis and thermoelectric phenomena.	5	
3.2	Bioenergetics: Coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.	4	
4	**Statistical Thermodynamics**	**18**	**2, 3, 4**
4.1	Macroscopic and microscopic approach in science, permutation, probability, Stirling's approximation, macrostates and microstates, apriori probability and thermodynamic probability, Ensemble-types of ensembles.	4	
4.2	Boltzmann distribution law, partition function and its physical significance, relation between molecular partition function and molar partition function, distinguishable and indistinguishable particles, partition function and thermodynamic functions, separation of partition function- translational, rotational, vibrational, and electronic partition functions, Thermal de-Broglie wavelength.	6	
4.3	Calculation of thermodynamic functions and equilibrium constants, thermodynamic probability and entropy, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, residual entropy, heat capacity of gases - classical and quantum theories.	5	
4.4	Basics of statistical mechanics (Non-evaluative): Phase space and trajectory: Ergodic hypothesis, measure of ergodicity, Lioville theorem and lioville equation, Computer simulation methods in statistical mechanics: Monte Carlo and Molecular dynamics methods.	3	

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Course code	**PG1CHEC04**				
Course	**PHYSICAL CHEMISTRY – I (KINETIC THEORY, CLASSICAL AND STATISTICAL THERMODYNAMICS)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/I**				
Type	**CORE**				
Credits	**3**	**Hours/week**	**3**	**Total hours**	**54**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (9 hrs)	3	1	1	50
Module 2 (18 hrs)	3	3	1.5	82.5
Module 3 (9 hrs)	2	0	0.5	22.5
Module 4 (18 hrs)	2	4	1	75
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST SEMESTER
Programme: M.Sc. Chemistry
PG1CHEC04 - PHYSICAL CHEMISTRY- I (KINETIC THEORY, CLASSICAL AND STATISTICAL THERMODYNAMICS)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What are transport properties? How are they expressed using an equation?
2. The most probable velocity of O_2 at 25°C is 300 m/s. Calculate r.m.s and average velocity
3. Calculate the entropy change for a thousand-fold expansion of a mole of ideal gas, isothermally at 300K.
4. What are the applications of Gibbs Helmholtz equation?
5. Define mean free path and collision frequency. How do they vary with pressure and temperature?
6. What is meant by a) thermodynamic probability b) Principle of equal apriori probability
7. Derive the relationship between Internal energy(E) and Partition function
8. What is meant by uncompensated heat in a chemical process?
9. State and explain Onsager reciprocal relation.
10. What is fugacity and how it is calculated?

(1 × 8 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Derive the expression for collision frequency in a single gas.
12. State third law of thermodynamics. How can it be used to calculate the absolute entropy of liquids?
13. One mole of an ideal gas at 0^oC is allowed to expand isothermally from a pressure of 1.01×10^7 Nm^{-2} to 1.01×10^6 Nm^{-2}. Calculate w, q, ΔE and ΔH for a) reversible expansion b) gas is allowed to expand freely into vacuum.
14. Define excess thermodynamic function. Derive expression for H^E.
15. Calculate the translational partition function of hydrogen molecule confined to a volume of 100 cm^3 at 298 K. Also calculate the thermal de Broglie wavelength
16. What is partition function? Explain its significance
17. What are ensembles? How are they classified

18. Calculate the relative Boltzmann population of two energy levels at 25°C if the energy levels are separated by a) 1000 cm^{-1} b) 10 $kJmol^{-1}$

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight** 5)*

19. Derive average, RMS and most probable velocities from Maxwell's law of distribution of molecular velocities.
20. Draw phase diagram and explain the system of two salts that can form hydrates.
21. (a) Derive an expression for Fermi-Dirac statistics.
    (b) Give comparative account of the three statistics.
22. a) Explain Maxwell's relations in thermodynamics and their applications
    b) Explain the concept of coupled reactions with special reference to the role of ATP in bioenergetics

(2 × 5 = 10)

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SEMESTER II

Course code	**PG2CHEC05**				
Course	**INORGANIC CHEMISTRY- II (ORGANOMETALLIC & NUCLEAR CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcome** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Comprehend the concepts of organometallic chemistry including synthesis, reaction, structure and bonding.	**Understand**	**1, 2**
2	Compare different types of reactions in organometallic compounds	**Understand**	**1, 2**
3	Illustrate the industrially important organometallic catalytic reactions	**Apply**	**1, 2, 5, 6**
4	Appraise the importance of diverse class of organometallic polymers	**Understand**	**1, 2**
5	Predict the environmental aspects of organometallic compounds	**Apply**	**1, 2, 5**
6	Apprehend the types of nuclear reactions and their applications	**Understand**	**1, 2**
7	Understand the methods of radioactivity measurements	**Understand**	**1**
8	Exposition of the working principles of isotope dating, labelling diagnosis and radiation therapy	**Apply**	**1, 2, 5, 6**
9	Discuss the techniques of nuclear waste disposal and safety precautions	**Understand**	**1, 2, 5,7**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Organometallic Compounds- Synthesis, Structure and Bonding**	**18**	**1**
1.1	Organometallic compounds with linear π- donor ligands- olefins, acetylenes, dienes and allyl complexes-	4	

	synthesis, structure and bonding.		
1.2	Complexes with cyclic π-donors - metallocenes and cyclic arene complexes structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.	4	
1.3	Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters- LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade Mingos rules, cluster valence electrons.	10	
2	**Reactions and catalysis of Organometallic Compounds**	**18**	**2, 3**
2.1	Substitution reactions- nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.	5	
2.2	Addition and elimination reactions- 1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.	5	
2.3	Rearrangement reactions, redistribution reactions and fluxional isomerism	4	
2.4	Alkene hydrogenation, Tolman catalytic loop, Synthesis gas, Hydroformylation, Monsanto Acetic acid process, Wacker process, Zeigler Natta catalysis.	4	
3	**Organometallic Polymers**	**9**	**4**
3.1	Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain	3	
3.2	Condensation polymers based on ferrocene and on rigid rod polynes	2	
3.3	Polymers prepared by ring opening polymerization	2	
3.4	Organometallic dendrimers.	2	
4	**Biological applications and environmental aspects of organometallic compounds**	**9**	**5**
4.1	Medicine: Organometallics of group 1-5 elements-organo mercuric compounds in medicine-organo boron compounds in medicine -organo silicon compounds in medicine. Antitumor drugs	4	
4.2	Organometallics in industry	1	
4.3	Organometallic compounds in Agriculture	2	
4.4	Environmental aspects: cycling of inorganic and	2	

	organometallic compounds in the environment.		
5	**Nuclear Chemistry**	**18**	**6, 7, 8, 9**
5.1	Trans uranic elements (from atomic numbers 93 to 118), Synthesis of Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.	3	
5.2	The process of nuclear fission. Fission products and fission yield. Neutron capture cross section and critical size.	3	
5.3	Detection and measurement of Radioactivity. Wilson cloud chamber, Radiation dosimetry. Measurement of radiation doses. Principles of counting technique such as G.M counter, proportional, ionization and scintillation counters. Radiation chemistry of water and aqueous solutions- Ferrous and ceric sulphate dosimeters.	5	
5.4	Applications of radioisotopes: Chemical investigations- reaction mechanisms, isotope exchange reactions. Analytical Applications – radio chromatography, neutron activation analysis, prompt gamma neutron activation analysis, radiometric titrations, and neutron absorptiometry. Medical applications- thyroiditis, brain tumour location, positron annihilation tomography (PAS), defects in blood circulation, mechanism of bone fracture healing. Industrial Applications – thickness measurement and control, gamma radiography. Relevance of radiation chemistry in biology.	6	
5.5	Radiation safety precaution, nuclear waste disposal.	1	

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9. A.B.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn., Elsevier, 1984.
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Course code	**PG2CHEC05**				
Course	**INORGANIC CHEMISTRY- II (ORGANOMETALLIC & NUCLEAR CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

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	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	2	2	1	55
Module 3 (9 hrs)	2	1	0.5	32.5
Module 4 (9 hrs)	2	1	0.5	32.5
Module 5 (18 hrs)	2	2	1	55
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**

Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEC05 - INORGANIC CHEMISTRY- II (ORGANOMETALLIC & NUCLEAR CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What is isolobal concept? Explain with one example.
2. Give one typical method of synthesis of butadiene complex of transition metals.
3. Differentiate between oxidative addition and reductive elimination with examples.
4. Give examples of nucleophilic and electrophilic attack of coordinated ligands in organometallic compounds.
5. What are organo metallic polymers? How they are classified?
6. Write any two methods of preparations of rigid rod polyenes
7. Write a note on organomercuric compounds used in medicine.
8. Give one example each of organo boron and organo silicon compounds used in medicine.
9. What is nuclear reaction cross section?
10. Write a method for the synthesis of Plutonium. Which isotope is used as nuclear fuel?

(8 ×1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. What are metal carbynes? How these will be synthesized?
12. Discuss the structure and bonding of binuclear metal carbonyls taking $Mn_2(CO)_{10}$ and $Fe_2(CO)_9$ as examples.
13. Explain the mechanism of alkene hydrogenation reaction.
14. Briefly explain the mechanism of Zeigler Natta catalysis.
15. Briefly describe the convergent and divergent method of preparation of dendrimers.
16. Explain the organometallic compounds used in industry.
17. What is fission yield? Draw the fission yield curve of neutron induced fission of ^{235}U.

18. What do you understand by the term radiation dosimetry? Briefly describe the working of Frick's dosimeter

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight** 5)*

19. Explain the synthesis, structure and bonding involved in cyclic arene complexes taking ferrocene as example.
20. Explain in detail the hydroformylation reaction. Also explain the mechanism of Monsanto Acetic Acid process.
21. (a) Describe the preparation and properties of rigid rod polyenes

    (b) Explain in detail the cycling of inorganic and organometallic compounds in the environment.
22. (a) Describe the principle and working of (i) GM counter and (ii) Scintillation counter (b) Write the applications of radioisotopes in industry, medicine, autoradiography and radiopharmacology

(2 × 5 = 10)

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Course code	**PG2CHEC06**				
Course	**ORGANIC CHEMISTRY – II (REACTION MECHANISM)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes:** *Upon completion of this course the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand the involvement of reactive intermediates in different organic reactions	**Understand**	**1, 2**
2	Integrate various stereochemical, mechanistic and conformational aspects of different classes of organic reactions	**Analyse**	**1, 2, 5**
3	Predict the product distribution and stereochemistry of various organic reactions	**Apply**	**1, 2, 5, 6**
4	Illustrate mechanisms of different photochemical or photophysical transformations or organic reactions	**Evaluate**	**1, 2, 5**
5	Implement Woodward Hoffmann rules to solve problems related to different classes of concerted reactions.	**Create**	**1, 2, 5, 6, 7**

Module No.	**Course Description**	**Hours**	**CO No.**
1	**Chemistry of Carbocations**	**9**	**1, 2, 4**
1.1	Formation, structure and stability of carbocations. Classical and non-classical carbocation.	3	
1.2	C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi pinacol, Dienone-phenol and Benzilic acid rearrangements, Prins reaction, Demjanov rearrangement. Oxymercuration, halolactonisation.	6	

2	**Chemistry of Carbanions**	**18**	**1, 2, 3, 4**
2.1	Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates, Kinetic and thermodynamic enolates- alkylation and acylation of enolates. Chemistry of enamines, Stork-enamine reaction.	3	
2.2	Nucleophilic additions to carbonyls groups. Reactions involving carbanions mechanisms of Aldol condensation, Michael addition, Lithium and boron enolates in Michael and aldol reactions, Robinson annulation, Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.	9	
2.3	Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Cannizzaro reaction, addition of Grignard reagent, Mannich reaction, Acyloin condensation.	4	
2.4	Ylids: chemistry of phosphorous and sulphur ylides - Wittig and related reactions, Peterson olefination.	2	
3	**Carbenes, Nitrenes and Arynes**	**9**	**1, 2, 3, 4**
3.1	Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, Reimer-Tiemann reaction.	3	
3.2	Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.	4	
3.3	Arynes: generation, structure, stability and reactions. Orientation effect, amination of haloarenes.	2	
4	**Radical Reactions**	**9**	**1, 2, 3, 4**
4.1	Generation and detection of radical intermediates (EPR and Magnetic methods) and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements. Hydroperoxide: formation, rearrangement and reactions. Autoxidation	6	
4.2	Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.	3	

5	**Concerted reactions**	**18**	**1, 2, 3, 4, 5**
5.1	Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward-Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.	2	
5.2	Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2).Analysis of electrocyclic and cycloadditions by (i) FMO method (ii) - Orbital- correlation method and (iii) PMO method.	5	
5.3	Sigmatropic (1,3), (1,5) and (3,3), and with stereo chemical aspects. Analysis of sigmatropic reaction by FMO method	4	
5.4	Highlighting pericyclic reactions in organic synthesis such as Diels- Alder reactions and Ene reaction with stereochemical aspects, dipolar cycloaddition (introductory), Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements.	4	
5.5	Unimolecular pyrolytic elimination reactions, Cheletropic eliminations, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, (Cope reaction), acetates and xanthates (Chugaev reaction).	3	
6	**Organic Photochemistry**	**9**	**1, 2, 3, 4, 5**
6.1	Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.	4	
6.2	Photochemistry of carbonyl compounds, enes, dienes and arenes: Norrish reactions of cyclic and acyclic ketones, Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photochemistry of conjugated dienes (butadiene only), photochemistry of vision. Singlet oxygen generation and reactions	5	

References

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2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

3. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer Science & Business Media, 2007.
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5. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.
6. T.H. Lowry, K.H. Richardson, Mechanism and Theory in Organic Chemistry, Harper & Row, Publishers, Inc., New York, 1976.
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Course code	**PG2CHEC06**				
Course	**ORGANIC CHEMISTRY – II (REACTION MECHANISM)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (9 hrs)	1	1	0.5	27.5
Module 2 (18 hrs)	2	2	1	55
Module 3 (9 hrs)	2	1	0.5	32.5
Module 4 (9 hrs)	2	1	0.5	32.5
Module 5 (18 hrs)	2	2	1	55
Module 6 (9 hrs)	1	1	0.5	27.5
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**

Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEC06 : ORGANIC CHEMISTRY- II (REACTION MECHANISM)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries Weight 1)*

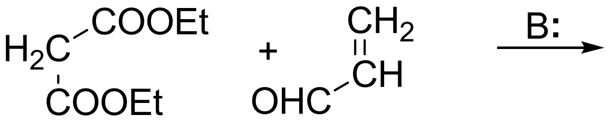
1. Distinguish between classical and non-classical carbocations
2. Explain Stork-enamine reaction
3. What are ylides? How it can be synthesized?
4. How nitrenes can be generated?
5. How will you distinguish triplet and single carbene experimentally?
6. Discuss Baldwin’s rule.
7. Explain autooxidation
8. Which are the symmetry elements involved in a pericyclic reaction and how is it related to the feasibility of a reaction?
9. What are chelotropic elimination?
10. What is photo sensitization and quenching?

(1 × 8 = 8)

Section B
Short Essay Questions

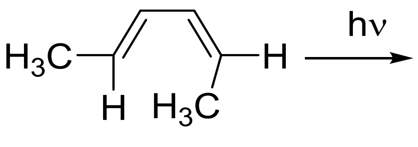
*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Explain dienone-phenol and benzilic acid rearrangements
12. Differentiate between kinetic and thermodynamic enolates with suitable examples.
13. Write the product(s) and mechanism of the following reaction.

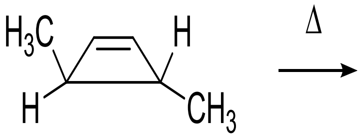


14. Write a note on the generation, structure, stability of arynes.
15. Give the product and specify its stereochemistry in the reactions given below.

a)



b)



16. Discuss Chugaeve elimination
17. Explain methods for generation and detection of free radicals.
18. Explain photochemistry of vision.

(2 × 6 = 12)

Section C

Long Essay Questions

(Answer any ***two*** *questions. Each question carries* ***Weight*** *5)*

19. Explain the following reactions:
    a) Prins reaction b) Demjanov rearrangement
    c) Barton deoxygenation c) McMurry coupling.
20. Discuss mechanism and applications of
    a) Aldol condensation b) Mannich reaction
    c) Robbinson annulation d) Clemmenson reduction
21. Analyse cycloaddition reactions on the basis of FMO, PMO and orbital correlation method.
22. Write a note on
    a) Norrish reactions of acyclic ketones b) Photo-Fries rearrangements
    c) Wolf rearrangement d) Beckmann rearrangement reaction

(5 × 2 = 10)

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Course code	**PG2CHEC07**				
Course	**THEORETICAL CHEMISTRY – II (CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	**Cognitive Level**	**PSO No.**
1	Apply quantum mechanical principles in solving both real and imaginary multi electron systems	**Apply**	**1, 2, 5, 6**
2	Understand the theories of chemical bonding and predict the nature of orbitals with the help of approximate methods	**Apply**	**1, 2, 5**
3	Understand group theoretical principles of molecular orbitals and hybridization	**Understand**	**1, 2**
4	Understand the quantum mechanical and non-quantum mechanical methods in computational chemistry for simulating/modeling various scientific problems.	**Analyse**	**1, 2, 5, 6, 7**
5	Compare various computational approaches such as HF (Hartree-Fock), semi-empirical, DFT (Density Functional Theory) and force field methods.	**Analyse**	**1, 2, 5, 6, 7**
6	Acquire skill in solving numerical problems	**Apply**	**1, 2, 5, 6, 7**

Module No.	**Course Description**	**Hours**	**CO No.**
1	**Approximate Methods in Quantum Mechanics**	**18**	**1, 6**
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	6	

	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.	6	
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.	6	
2	**Chemical Bonding**	**18**	**2, 6**
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.	4	
2.2	Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H2 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. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.	7	
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 order and free valency.	7	
3	**Applications of Group Theory in Chemical Bonding**	**9**	**3**
3.1	Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, and PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{3v}, C_{2h}, C_3 and D_{3h} groups. MO diagram for water and ammonia.	9	
4	**Computational Chemistry**	**18**	**4, 5**
4.1	Introduction: computational chemistry as a tool and its scope.	1	
4.2	Potential energy surface: stationary point, transition state or saddle point, local and global minima.	1	

4.3	Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterization from experiments of quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.	3	
4.4	Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.	3	
4.5	Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods- variational method, basic principles of Configuration Interaction (CI). Perturbational methods- basic principles of Møller Plesset Perturbation Theory.	3	
4.6	General introduction to semiempirical methods: basic principles and terminology.	2	
4.7	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).	3	
4.8	Model Chemistry-notation, effect on calculation time (cost).	1	
4.9	Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.	1	
5	**Computational Chemistry Calculations**	**9**	**4**
5.1	Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z- matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.	3	
5.2	Identifying a successful GAMESS/Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies,	3	

	Koopmans' theorem, electron affinities and atomic charges.		
5.3	Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.	3	

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2. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
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7. E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
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11. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.
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Course code	**PG2CHEC07**				
Course	**THEORETICAL CHEMISTRY – II (CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	3	2	1	60
Module 3 (9 hrs)	0	1	1	35
Module 4 (18 hrs)	4	3	0	50
Module 5 (9 hrs)	1	0	1	30
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEC07: THEORETICAL CHEMISTRY - II
(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What are slater determinants?
2. Explain Hellmann-Feynman theorem.
3. Explain Born-Oppenheimer approximation.
4. In-terms of molecular orbital (MO) theory, explain the non-existence of He_2.
5. Determine the molecular term symbol for the ground states of nitrogen and oxygen.
6. Explain AMBER.
7. What is CHARMM? Explain its use in molecular mechanics.
8. What is Koopman’s Theorem?
9. What are Kohn-Sham orbitals?
10. What are saddle points? Differentiate between local and global minimum.

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Illustrate variation theorem using the trial wave function x(a-x) for particle in a one-dimensional box.
12. Explain Hückel molecular orbital theory of Butadiene.
13. Using group theory, determine the hybridization in BF_3 molecule.
14. What are the important assumptions used in HFSCF method?
15. Write a short note on semiempirical methods highlighting the basic principles and terminology.
16. Compare MOT and VBT.
17. Explain the Kohn-Sham approach used in DFT?
18. Describe the basic principles of Møller Plesset Perturbation Theory.

(6 × 2 = 12)

Section C
Long Essay Questions

(Answer any ***two*** *questions. Each question carries* ***Weight 5****)*

19. How is GAMESS input file prepared? Illustrate with reference to water molecule?
20. Using group theory, derive the allowed electronic transitions in formaldehyde.
21. Explain Perturbation Method? Illustrate with Helium as Example
22. Explain molecular orbital theory and derive an expression for energy and wave function of Hydrogen molecule.

(2 × 5 = 10)

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Course code	**PG2CHEC08**				
Course	**PHYSICAL CHEMISTRY – II (MOLECULAR SPECTROSCOPY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**3**	**Total hours**	**54**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	**Cognitive Level**	**PSO No.**
1	Understand the fundamental concepts of spectroscopy	**Understand**	**1, 2**
2	Analyse rotational, vibrational and electronic spectroscopy, Raman and Mossbauer spectroscopy	**Analyse**	**1, 2, 5**
3	Apply quantum mechanics and group theory in spectroscopy.	**Evaluate**	**1, 2, 5, 6**
4	Solve problems based on the theory of various spectroscopic techniques	**Apply**	**1, 2, 5, 6, 7**
5	Compare principle and applications of NMR, EPR and NQR spectroscopic techniques.	**Analyse**	**1, 2, 5, 6**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Fundamentals of Spectroscopy**	**6**	**1, 4**
1.1	Brief review of Electromagnetic spectrum: nature of radiation, wave amplitude, angular frequency, phase, period, wavelength, wavenumber, wave vector, velocity of propagation, Black-body radiation, quantum theory of electromagnetic radiation, wave-particle duality.	2	
1.2	Radiation-matter interaction: basic concepts of absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering, absorption cross section, Einstein's coefficients, signal to noise ratio, natural line width, line broadening factors, Doppler broadening, time-dependent perturbation theory (no proof required) and its consequences in spectroscopy, transition moment integral,	4	

	symmetry and selection rules, intensity of spectral lines, influencing factors, Lamb dip spectrum, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels, radiative and non-radiative transitions, relaxation time.		
2	**Microwave Spectroscopy**	**6**	**1, 2, 4, 5**
2.1	Microwave spectroscopy:- Principal moments of inertia and classification of molecules (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of Jmax, effect of isotopic substitution, calculation of intermolecular distance, spectrum of rigid rotors, non-rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.	6	
3	**Infrared Spectroscopy**	**6**	**1, 2, 4, 5**
3.1	Infrared spectroscopy: Morse potential energy diagram, 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, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR, instrumentation.	6	
4	**Electronic, Mossbauer and Raman Spectroscopy**	**18**	**1, 2, 4, 5**
4.1	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.	6	
4.2	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	6	

	depolarized Raman lines, resonance raman scattering and resonance fluorescence.		
4.3	Different types of lasers- solid state lasers, Ti : Sapphire, Nd:YAG and semiconductor lasers, Continuous wave and pulsed lasers, gas lasers; helium-neon, argon ion and N_2 lasers, frequency doubling, applications of lasers in spectroscopy: Hyper Raman Spectroscopy, Stimulated Raman Spectroscopy, Coherent Anti-Stokes Raman Spectroscopy (CARS) (elementary idea only).	3	
4.4	Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift.	3	
5	**NMR Spectroscopy**	**18**	**1, 3, 5**
5.1	Theory of NMR Spectroscopy: Interaction between nuclear spin and applied magnetic field, important magnetically active nuclei, Nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, Chemical shift and its representation- δ scale of PMR, factors affecting chemical shift, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift - δ scale, Spin-spin coupling: Theory and illustration with AX system, exchange phenomenon, first order spectra, second order effects on spectra, spin systems (AB)	6	
5.2	Fourier Transformation (FT) NMR Spectroscopy: Instrumentation of NMR technique, effect of pulses, rotating frame reference, FID, FT technique, data acquisition and storage. Pulse sequences- Pulse width, spins and magnetisation vector. Solid state NMR-Applications. Magic Angle Spinning (MAS).	4	
5.3	An elementary study of NQR spectroscopy	2	
5.4	EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_\parallel$ and $g_\perp$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.	6	

References

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
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13. D.N. Sathyanarayana, Introduction To Magnetic Resonance Spectroscopy ESR, NMR, EQR, I.K. International Publishing House Pvt. Limited, 2009.

Course code	**PG2CHEC08**				
Course	**PHYSICAL CHEMISTRY – II (MOLECULAR SPECTROSCOPY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**1/II**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**3**	**Total hours**	**54**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (6 hrs)	2	1	0	20
Module 2 (6 hrs)	1	1	1	40
Module 3 (6 hrs)	1	2	1	50
Module 4 (18 hrs)	3	2	1	60
Module 5 (18 hrs)	3	2	1	60
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEC08: PHYSICAL CHEMISTRY - II (MOLECULAR SPECTROSCOPY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries weight **1**)*

1. What are the factors affecting the intensity of a spectral line?
2. Write a note on Born –Oppenheimer approximation
3. Classify the molecules based on their principal moment of inertia.
4. What are skeletal vibrations and functional group vibrations in IR spectroscopy?
5. What is Fermi resonance?
6. Give the basic theory of Birge Spooner method.
7. State and explain the rule of mutual exclusion with a suitable example.
8. What is the application of MAS NMR?
9. NMR is observed in RF region, while ESR in MW region. Why?
10. State and explain Mc Connell relation.

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Draw and explain the rotational- vibrational spectrum of a heteronuclear diatomic molecule.
12. What do you mean by spin- spin coupling? Explain using AX system as example. What are the characteristics of first order spectra?
13. Give the classical theory and quantum theory of Raman scattering.
14. Draw the NQR energy level splitting of any nucleus. How does NQR transitions affect NMR spectrum.
15. Explain the theory of vibrational spectroscopy of an anharmonic oscillator
16. In the rotational spectrum of CO, equidistant lines are 3.8 cm^{-1} apart. Calculate the bond length and the wave number of $J = 4 \rightarrow 5$ transition.
17. The spectroscopic bond dissociation energy of $^{35}Cl^{16}O$ radical is 1.9 eV. Calculate the equilibrium bond dissociation energy (which includes zero-point energy), if the fundamental frequency is 780 cm^{-1}.
18. Sketch the ^{13}C and ^{1}H NMR of ethanal showing spin –spin splitting giving approximate chemical shift values.

(6 × 2 = 12)

Section C
Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. Explain the basic principle and applications of ESR spectroscopy. Mention the significance of electron ‘g’ factor.
20. a) How do isotopic substitution and Zeeman effect affect the rotational spectrum of molecules.
    b) Explain the determination of inter nuclear distance of a rigid diatomic rotor
21. a) Explain the theory and application of Mossbauer spectroscopy with suitable examples.
    b) Explain the theory of lasers? Explain the application of lasers in Raman Spectroscopy
22. Explain the theory and instrumentation of FTIR spectroscopy. What are its advantages? What are overtones and combination bands in IR spectrum? What are the selection rules for vibrational spectroscopy?

(2 × 5 =10)

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SEMESTER I & II PRACTICALS

Course code	**PG2CHEP01**		
Course	**INORGANIC CHEMISTRY PRACTICAL – I**		
Degree	**M.Sc.**		
Branch	**CHEMISTRY**		
Year/Semester	**1/I & II**		
Type	**PRACTICAL**		
Hours/week	**3**	**Total hours**	**54 + 54 = 108**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Apply theoretical principles in the practical experiments.	**Appreciate**	**1, 2, 4, 6, 7**
2	Interpret the experimental results, draw conclusions, and communicate effectively through oral and written reports	**Evaluate**	**3, 4, 5, 6, 7**
3	Illustrate the separation, identification and confirmation of metal ions in a mixture of cations.	**Analyse**	**3, 4, 5, 6, 7**
4	Estimate analytes via volumetric titrations like argentometry, cerimetry and iodimetry	**Apply**	**3, 4, 5, 6, 7**
5	Perform colourimetric estimations	**Apply**	**3, 4, 5, 6, 7**
6	Synthesize and characterize coordination compounds by spectrometric methods	**Create**	**3, 4, 5, 6, 7**

Module No.	**Course description**	**Hours**	**CO No.**
1	**PART I**	**54**	**1, 2, 3**
1.1	Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - 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+}, Co^{2+}, Ni^{2+}, Ca^{2+},	54	

	Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+} , Na^{+} , K^{+}, NH_4^{+} (Interfering acid radicals are not to be present, Confirmation to be done by spot test, Minimum 8 mixtures are to be recorded).		
2	**PART II**	**18**	**1, 2, 4**
2.1	**Quantitative Estimations like** (a) Argentometric estimation of chlorides (b) Cerimetry – Fe(II) and nitrate (c) Potassium iodate – iodide estimation of Sn(II)	18	
3	**PART III**	**24**	**1, 2, 5**
3.1	Colorimetric estimation of Cr, Fe, Ni, Mn, Cu, NH_4^{+}, nitrate and phosphate ions.	24	
4	**PART IV**	**12**	**1, 2, 6**
4.1	Preparation and characterization complexes using IR, NMR and electronic spectra. (a) Tris (thiourea) copper (I) complex (b) Potassium tris (oxalate) aluminate (III) (c) Tetrammine copper (II) sulphate (d) Mercury tetra thiocyanato cobaltate (III)	12	

References

1. A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.
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3. V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.
4. M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn, McMillian, 1968.

QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST & SECOND SEMESTER
Programme : M.Sc. Chemistry
PG2CHEP01 - INORGANIC CHEMISTRY PRACTICAL – 1

Time: 6 hrs **Maximum Weight: 15**

PART A

1. Write down in 15 minutes the principle for the separation of group I to VI**.** **(Weight 1)**
2. Separate and identify the rare earth cations present in the given binary mixture**.** **(Weight 3)**
3. Write down in 15 minutes the theory and principle for the estimation of …………………… ion by colorimetric method**.** **(Weight 1)**
4. Estimate the mass of ferric ion in the whole of the given solution by colorimetric method. **(Weight 4)**
5. Write down in 15 minutes the theory and principle for the preparation of the metal complex ……………………. and its characterization by spectroscopic methods. **(Weight 1)**
6. Prepare the metal complex ……………………………… Dry and purify it by recrystallization. Determine the melting point of the metal complex. Display the crude and recrystallised samples. **(Weight 2)**

PART B: **Viva-voce** **(Weight 2)**

PART C: Evaluation of record **(Weight 1)**

Course code	**PG2CHEP02**		
Course	**ORGANIC CHEMISTRY PRACTICAL – I**		
Degree	**M.Sc.**		
Branch	**CHEMISTRY**		
Year/Semester	**1/I & II**		
Type	**PRACTICAL**		
Hours/week	**3**	**Total hours**	**54 + 54 = 108**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Apply theoretical principles in the practical experiments.	**Appreciate**	**2, 3, 4, 5, 6**
2	Interpret the experimental results, draw conclusions, and communicate effectively through oral and written reports	**Evaluate**	**2, 3, 4, 5, 6**
3	Familiarise with common methods for qualitative separation and purification of organic compounds	**Analyse**	**2, 3, 4, 5, 6**
4	Develop skills in separation and purification of binary mixtures of organic compounds	**Apply**	**2, 3, 4, 5, 6**
5	Acquire advanced knowledge in powerful set of tools for chemical drawing to enable scientific research.	**Create**	**2, 3, 4, 5, 6, 7**

Module No.	**Course description**	**Hours**	**CO No.**
1	**PART I**	**27**	**1, 2, 3**
1.1	General methods of separation and purification of organic compounds such as: (a) Solvent extraction (b) Soxhlet extraction (c) Fractional crystallization (d) TLC and Paper Chromatography (e) Column Chromatography (f) Membrane Dialysis	27	
2	**PART II**	**54**	**1, 2, 4**

2.1	Separation of organic binary mixtures:- Quantitative separation of a mixture of two components by solvent extraction	15	
2.2	Purification of the separated samples by distilling and crystallization.	10	
2.3	Determination of physical constants of separated and purified samples (No need of bifunctional compounds)	9	
2.4	Separation of organic mixtures by TLC and calculation of Rf values.	5	
2.5	Separation/purification of organic mixtures by column chromatography.	15	
3	**PART III**	**27**	**1, 2, 5**
3.1	Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, Symyx Draw and Chemsketch. (a) Cycloaddition of diene and dienophile (Diels-Alder reaction). (b) Oxidation of primary alcohol to aldehyde and then to acid. (c) Benzoin condensation. (d) Esterification of simple carboxylic acids. (e) Aldol condensation.	27	

References

1. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.
2. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
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4. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.
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QP code **Reg. No.**
Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FIRST & SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEP02 - ORGANIC CHEMISTRY PRACTICAL – 1

Time: 6 Hrs **Maximum Weight: 15**

PART A

1. Write the principle behind the separation/purification method .... **(Weight 1)**
2. Separate the given organic binary mixture quantitatively by chemical/physical method. Record the yield of the components, display the separated samples for inspection. **(Weight 5)**
3. Purify the separated organic components and find the B.P and M.P. **(Weight 1)**
4. Record the IR, UV-vis and NMR spectrum of the separated organic compounds. **(Weight 1)**
5. Separate the organic mixture by TLC and find the Rf value of the components**.** **(Weight 2)**
6. Draw the molecular structure and reaction scheme using Chem Draw/ ChemSketch (**Weight 2)**

PART B: **Viva-voce** **(Weight 2)**

PART C: Evaluation of record **(Weight 1)**

Course code	**PG2CHEP03**		
Course	**PHYSICAL CHEMISTRY PRACTICAL – I**		
Degree	**M.Sc.**		
Branch	**CHEMISTRY**		
Year/Semester	**1/I & II**		
Type	**PRACTICAL**		
Hours/week	**4**	**Total hours**	**72 + 72 =144**

CO No.	**Expected Course Outcomes:** *Upon completion of this course the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Apply the physical and applied chemistry principles to the practical laboratory experiments	**Apply**	**1, 4, 6**
2	Interpret the experimental results, draw conclusions, and communicate effectively through oral and written reports	**Analyse**	**5**
3	Develop skills in the scientific method of planning, designing, and conducting experiments	**Apply**	**4, 6**
4	Understand the safety requirements and lab skills to perform physico-chemical experiments	**Understand**	**4, 6**
5	Acquire the practical knowledge of composition determination from phase diagrams	**Analyse**	**4, 6**
6	Apply the chemistry software programs to model energy potentials and vibrational levels of molecules	**Apply**	**4, 6**

Module No.	**Course description**	**Hours**	**CO No.**
A	**Wet Lab experiments**	**72**	**1, 2, 3, 4**
A. I	**Adsorption**	**20**	
1	Verification of Freundlich adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.	4	
2	Verification of Freundlich adsorption isotherm: charcoal-oxalic acid system.	4	
3	Verification of Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.	4	

4	Verification of Langmuir adsorption isotherm: charcoal-oxalic acid system.	4	
5	Determination of the concentration of the given acid using the isotherms.	4	
A. II	**Phase diagrams**	**20**	**1, 2, 3, 4, 5**
1	Construction of phase diagrams of simple eutectics.	4	
2	Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.	4	
3	Effect of KCl on miscibility temperature	4	
	Effect of succinic acid on miscibility temperature	4	
4	Construction of phase diagrams of three component systems with one pair of partially miscible liquids.	4	
A. III	**Distribution law**	**12**	**1, 2, 3, 4**
1	Distribution coefficient of iodine between an organic solvent and water.	4	
2	Distribution coefficient of benzoic acid between benzene and water.	4	
3	Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$	4	
A. IV	**Surface tension**	**20**	**1, 2, 3, 4**
1	Determination of the surface tension of a liquid by		
	(a) Capillary rise method	4	
	(b) Drop number method	4	
	(c) Drop weight method	4	
2	Determination of parachor values.	4	
3	Determination of the composition of two liquids by surface tension measurements.	4	
B	**Computational Chemistry Experiments**	**72**	**1, 2, 6**
B. I	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	60	

	orbitals, dipole moments etc.		
B. II	Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.	12	

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.

QP code **Reg. No.**

Name:

Model Question Paper
M. Sc DEGREE (C.S.S.) PRACTICAL EXAMINATION
FIRST AND SECOND SEMESTER
Programme: M.Sc. Chemistry
PG2CHEP03: PHYSICAL CHEMISTRY PRACTICAL – I

Time: 6 Hrs. **Maximum Weight: 15**

PART A:

I. Physical Chemistry Experiments

1. Verify the Langmuir adsorption isotherm and hence determine the concentration of the given oxalic acid solution. **(Weight 7)**
2. Verify the Freundlich adsorption isotherm and hence determine the concentration of the given oxalic acid solution. **(Weight 7)**
3. Construct the solid-liquid equilibrium diagram for the system formed by two substances A and B and determine the eutectic temperature and eutectic composition of the system. Find out the composition of the given unknown mixture of A and B. **(Weight 7)**
4. (a) Melting points of two compounds A and B are ………°C and ………..°C respectively. The two compounds form a two component system with eutectic temperature, eutectic composition……..°C and …………% by mass of A respectively. Construct the phase diagram and determine the composition of the given mixture. **(Weight 4)**

   (b) Study the variation of miscibility temperature of phenol-water system by the addition of KCl and determine the concentration of the given KCl solution. **(Weight 3)**
5. Construct the isothermal ternary phase diagram of the ternary liquid system A-B-C and determine the composition of the given mixture D of B and C. **(Weight 7)**
6. Construct the isothermal ternary phase diagram of the ternary liquid system A-B-C and draw the tie line using the given mixture of A, B and C. **(Weight 7)**
7. Study the variation of surface tension of acetic acid with concentration and determine the concentration of the given acid. **(Weight 7)**
8. Study the variation of CST of phenol-water system by the addition of KCl and determine the concentration of the solution given KCl. **(Weight 7)**

II. Computational Chemistry Experiment **(Weight 5)**

Instructions: While creating the input file give your register number as title in the input builder. Take a print out of the input file and also take a print out of the last page of the FIREFLY output file showing 'Terminated Normally' message. Attach these to your main answer book.

a. Using FIREFLY determine the optimized geometrical parameters given below for ammonia/water/methane molecule and tabulate the result. Parameters to be determined: total energy (in eV), dipole moment, bond length, bond angle. Basis set to be used: STO – 3G/6 – 31G

b. Using FIREFLY determine the optimized geometrical parameters given below for Oxygen (triplet)/Oxygen / (singlet)/nitrogen /molecule and tabulate the result. Parameters to be determined: total energy (in eV), bond order, free valence, and bond length. Basis set to be used: STO – 3G /6 – 31G
c. Calculate the correlation energy in eV for hydrogen fluoride/lithium hydride using MP2 method with 6 – 31G (d) basis set.
d. Calculate the vibrational frequencies of ammonia/water/methane molecule at MP2 level using 6 – 31G (d) basis set and assign the frequencies as stretching, bending etc. Also find the dipole moment.
e. Calculate the vibrational frequency of hydrogen fluoride molecule at RHF level using STO – 3G/ 6 – 31G (d) basis set. Also find the dipole moment, bond length, and total energy (in eV)
f. Perform the population analysis for HF and H_2O molecules using RHF method and STO 3G basis set and find out and tabulate the Mulliken charge and Lowdin charge on each atom.
g. Identify HOMO and LUMO of H_2O/BH_3 (singlet) molecule using STO – 3G /6 – 31G basis sets and note down their energies in Joule.
h. Compute the ionization energy and electron affinity of ammonia/water/HF molecule based on Koopman's theorem using 6 – 31G(d) basis set. Also determine dipole moment and free valence.

PART B: **Viva-voce** **(Weight 2)**

PART C: Evaluation of record **(Weight 1)**

SEMESTER III

Course code	**PG3CHEC09**				
Course	**INORGANIC CHEMISTRY- III (SOLID STATE & MATERIAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand the advanced topics of solid state - structure, reactions and phase transition in solids.	**Understand**	**1, 2**
2	Interpret the electrical, magnetic and optical properties of solids	**Understand**	**1, 3, 5**
3	Comprehend the structure, synthesis and applications of inorganic rings chains and clusters	**Understand**	**1, 2, 5**
4	Summarise the biological importance of phosphate esters and phosphazenes.	**Evaluate**	**1, 2**
5	Distinguish the structural aspects of cages and cluster compounds of Boron	**Apply**	**1, 2**
6	Understand the synthesis characterization and applications of glass, ceramics, composites and clay products	**Understand**	**1, 2, 5**
7	Apprehend the properties different types of ceramic and refractory materials	**Apply**	**5, 6**

Module No.	Course description	Hours	CO No.
1	**Solid State Chemistry**	**18**	**1**
1.1	Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), AX_2 (Nickel Arsenide), ABX_3 (Perovskite, Ilmenite), Spinels, Inverse spinel structures.	6	
1.2	Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid- Type I reactions, Type II reactions.	3	
1.3	Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melt and vapour deposition technique.	9	
2	**Electrical, Magnetic and Optical Properties**	**18**	**2**
2.1	Free electron theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals	4	
2.2	Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.	3	
2.3	Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications ofoptical properties	2	
2.4	Super conductivity- Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates - YBaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.	9	
3	**Inorganic Chains, Rings, Cages and Clusters**	**18**	**3**
3.1	Chains - catenation, homo and heterocatenation. Silicate minerals. Structure of silicates common silicates, silicates	4	

	containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Zeolites synthesis, structure and applications.		
3.2	Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems.	4	
3.3	Ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds. Polythiazil-one dimensional conductors.	4	
3.4	Cages: synthesis, structure and bonding of cage like structures of phosphorous.	3	
3.5	Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains	3	
4	**Boron compounds**	**9**	**5**
4.1	Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides - styx numbers, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions	3	
4.2	Borazines–Structure and bonding of borazines and Borides	3	
4.3	Boron cage compounds- higher boranes, carboranes, metallo carboranes, Wade Mingos Lauher rules, Jemmis *mno* rule.	3	
5	**Chemistry of Materials**	**18**	**6**
5.1	Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers	9	
5.2	Ceramic structures - mechanical properties, clay products, refractories- characterizations, properties and applications.	9	

References

1. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
2. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
3. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
4. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
5. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
6. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
7. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
8. R.L. Dutta, A. Syamal, Elements of Magnetochemistry, Affiliated East-West Press, New Delhi, 1993.
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10. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, Wiley-Interscience,1999.
11. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
12. P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.
13. C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.

Course code	**PG3CHEC09**				
Course	**INORGANIC CHEMISTRY- III (SOLID STATE & MATERIAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	2	2	1	55
Module 3 (18 hrs)	2	2	1	55
Module 4 (9 hrs)	2	1	0.5	32.5
Module 5 (9 hrs)	2	1	0.5	32.5
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

Model Question paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
THIRD SEMESTER
Programme: M.Sc. Chemistry
PG3CHEC09: INORGANIC CHEMISTRY - III
(SOLID STATE AND MATERIAL CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. Explain briefly Fluorite structure.
2. Define the term plane defect.
3. Give any two applications of pyroelectric materials.
4. Differentiate intrinsic and extrinsic photo conductivities.
5. Polythiazil compounds are known as one dimensional conductor. Explain why?
6. Write any one method for the preparation of silicone.
7. State Wade rule.
8. How boranes are classified? Write one example for each category.
9. What are glass formers and glass modifiers?
10. What are safety glasses and fiber glasses?

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. How Bragg-William's theory explain the order – disorder transformations in solids?
12. Explain briefly the different methods used in crystal growth.
13. Write a note on Hall effect. Derive an expression for Hall coefficient.
14. How is BCS theory successful in explaining low temperature superconductivity?
15. Explain the structure and bonding of cage compounds of P-S and P-O taking five Examples from each.
16. Explain the synthesis, structure and applications of zeolites.
17. Discuss the structure and bonding in borazine
18. Briefly describe the sol-gel synthesis of nano materials with example.

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight** 5)*

19. Write a note on crystal structures and magnetic properties of **a)**. Perovskites **b)**. Rutile **c).** Inverse spinel.
20. Explain the conductivity of superconducting cuprates.
21. (a) Discuss the structure and bonding profile of B_4O_{10} with special reference to styx numbers (b) Write briefly on ceramics and refractory materials.
22. What are metal clusters? Explain their classification taking examples. Explain the structure and bonding of metal-metal multiple bonding in $(Re_2X_8)^{2-}$ complexes taking one example.

(2 × 5 = 10)

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Course code	**PG3CHEC10**				
Course	**ORGANIC CHEMISTRY – III (ORGANIC SYNTHESES)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Designing the synthetic pathways based on the retrosynthetic approach	**Understand**	**1, 2, 5,7**
2	Discuss the important reagents and their applications in organic syntheses	**Apply**	**1, 2, 3, 5**
3	Discuss various coupling reactions to build up a molecular framework	**Analyze**	**1, 3, 4, 5**
4	Illustrate the construction of carbocyclic and heterocyclic ring systems	**Create**	**1, 2, 4, 5, 6**
5	Illustrate the utility of protecting groups in peptide syntheses	**Apply**	**1, 2, 3, 5, 6**

Module No.	**Course Description**	**Hours**	**CO No.**
1	**Retrosynthetic Analysis**	**9**	**1**
1.1	Basic principles and terminology of retrosynthesis. Important strategies of retrosynthesis. Functional group interconversion. Umpolung. Synthesis of aromatic compounds. One group C-X disconnections of carbonyl derivatives and alkyl halides. Two group C-X disconnections-1,1-, 1,2- and 1,3-difunctionalised compounds. One group C-C disconnections of alcohols and carbonyl compounds. Two group C-C disconnections-1,2- and 1,3-difunctionalised compounds.	6	

1.2	Amine synthesis: Primary amine, other routes to amines using reduction, reagents for the synthon NH_2, Alkene synthesis- from alcohols and derivatives, Wittig reaction.	3	
2	**Organometallics**	**9**	**2**
2.1	Preparation and applications in organic synthesis of (i) Grignard Reagents, preparation and its applications (ii) Organo lithium compounds and addition to $-C=O$, $-COOH$ and $-CONR_2$ (iii) Lithium dialkyl cuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents, Glaser coupling and its modifications. (iv) Dialkyl cadmium compounds and (v) Benzenetricarbonyl chromium and reaction with carbanions.	9	
3	**Organic Synthesis via Oxidation and Reduction**	**18**	**2**
3.1	Survey of organic reagents and reactions in organic chemistry with special reference to oxidation. Metal based and non-metal based oxidations of (a) alcohols to carbonyls [(Chromium-John's oxidation, Collin's oxidation, Sarrett oxidation) Manganese, Aluminium and DMSO based reagents (Swern oxidation)] (b) alkenes to epoxides (peroxides/peracids 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 based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage: hydroboration- oxidation, Wacker oxidation, Selenium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.	10	
3.2	Survey of organic reagents and reactions in organic chemistry with special reference to reduction (a) Catalytic hydrogenation (Heterogeneous: Palladium, Platinum, Rhodium and Nickel, Homogeneous: Wilkinson) (b) Metal based reductions- Birch reduction, Pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $NaBH_4$, triacetoxyborohydride; $LiAlH_4$ and DIBAL-H, Meerwein-Pondorff-Verley reduction.	8	

	(d) Enzymatic reduction using Baker's yeast.		
4	**Modern Synthetic Methods and Reagents**	**18**	**2, 3**
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, Wohl-Ziegler reaction. Reagents such as NBS, DDQ, DCC.	14	
4.2	Introduction to multicomponent reactions- Three component reactions (Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (Huisgen 1,3-Dipolar Cycloaddition).	4	
5	**Construction of Carbocyclic and Heterocyclic Ring System**	**9**	**4**
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, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization. Construction of macrocyclic rings-ring closing metathesis (Grubb's catalyst)	6	
5.2	Structure and 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 (Paal Knorr), imidazole, pyrazole, thiazole, oxazole, (any one synthesis), quinoline (Skraup synthesis) and isoquinoline (Bischler-Napieralskii synthesis).	3	
6	**Protecting Group Chemistry**	**9**	**4, 5**
6.1	Introduction of the need of protecting groups in organic synthesis. Chemo and regio selective protection and deprotection. Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Illustration of protection and deprotection in synthesis.	3	

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).	5	
6.3	Role of trimethyl silyl group in organic synthesis.	1	

References

1. M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.
2. F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.
3. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Edn., Wiley, 2008.
4. V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.
5. I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & Sons, 2010.
6. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.
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8. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
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Course code	**PG3CHEC10**				
Course	**ORGANIC CHEMISTRY – III (ORGANIC SYNTHESES)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Part A (Weightage/ Qn: 1)	**Part B (Weightage/ Qn: 2)**	**Part C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (9 hrs)	2	1	0.5	32.5
Module 2 (9 hrs)	1	2	0	25
Module 3 (18 hrs)	2	2	1	55
Module 4 (18 hrs)	2	1.5	1	50
Module 5 (9 hrs)	2	0	1	35
Module 6 (9 hrs)	1	1.5	0.5	32.5
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**
Name:

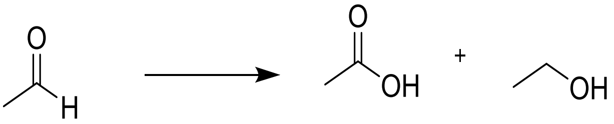
Model Question Paper
M Sc DEGREE (C.S.S) EXAMINATION
THIRD SEMESTER
Programme: M.Sc. Chemistry
PG3CHEC10 – ORGANIC CHEMISTRY – III
(ORGANIC SYNTHESES)

Time: 3 Hrs. **Maximum Weight: 30**

Section A
Short Answer Questions

(Answer any ***eight*** *questions. Each question carries* ***Weight 1)***

1. Explain the term Umpolung equivalent.
2. Give any two preparatory methods for alkyl lithium reagents
3. Give the mechanism of SeO_2 mediated allylic oxidation
4. Differentiate between synthon and synthetic equivalent
5. How do we synthesize oxetane and cyclobutane by photochemical methods?
6. Suggest reagent/s used for obtaining cis and trans diols from alkene
7. Give two preparatory methods for furan
8. Mention any two protection methods each for amino and hydroxyl functional groups.
9. How the following conversion is possible



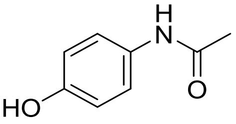
10. What is the role of DCC in esterification reaction?

(8 × 1= 8)

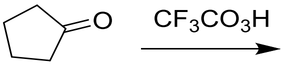
Section B
Short Essay Questions

(Answer any ***six*** *questions. Each question carries* ***Weight 2)***

11. Give a retro synthesis for the following molecule and suggest a synthetic strategy.

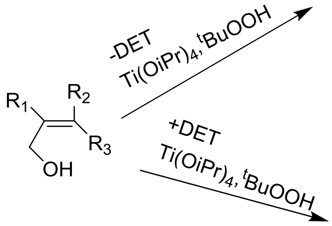


12. Compare the reactions of Gilman reagent and Alkyl lithium with enones
13. Write a note on Glaser coupling and its modifications
14. Predict the product of the reaction with a mechanism



15. Discuss a multicomponent reaction for the preparation of a bisamide
16. Differentiate the terms regioselective and chemoselective protection with suitable examples.

17. a) Explain the synthetic utility of trialkyl silyl groups b) Explain Baylis Hilman reaction
18. Predict the product/s and give the mechanism



(6 × 2 = 12)

Section C
Long Essay Questions

(Answer any 2 questions.** Each question carries **Weight 5)

19. Write a note on a) Sharpless asymmetric epoxidation b) Jacobsen epoxidation c) Shi epoxidation
20. Discuss any four metal mediated C-C coupling reactions with mechanism.
21. a) Demonstrate the utility of protecting groups in peptide synthesis b) Explain one group C-C disconnections
22. Discuss the following reactions with mechanism a) Pauson Khand reaction; b)Bischler-Napieralskii synthesis c) Bergman Cyclisation

(2 × 5 = 10)

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Course code	**PG3CHEC11**				
Course	**PHYSICAL CHEMISTRY- III (CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand the fundamental concept of the kinetics, surface chemistry and catalysis	**Understand**	**1, 2, 5**
2	Explain the thermodynamic parameters which are involved in the kinetics of a chemical reactions	**Analyze**	**1, 2, 5, 6**
3	Explain the effect of catalyst and its mechanism on the kinetics of a chemical reaction	**Analyze**	**1, 2**
4	Discuss various surface reactions and related characterization methods	**Evaluate**	**1, 2, 4, 6, 7**
5	Explain the fundamental concept of photochemistry	**Apply**	**1, 2**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Chemical Kinetics**	**18**	**1, 2, 3**
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 $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.	5	
1.2	Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory.	2	
1.3	chain reactions: free radical and chain reactions, steady state treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions,	4	

	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.		
1.4	Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.	3	
1.5	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, linear free energy relationship, kinetic isotope effect.	4	
2	**Surface Chemistry**	**18**	**1, 4**
2.1	Surface: Different types of surfaces, thermodynamics of surfaces, Gibb's adsorption equation and its verification, surface tension, surfactants and micelles, surface films, surface pressure and surface potential and their measurements and interpretation.	5	
2.2	Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, AFM, STM, ion scattering, SEM and TEM in the study of surfaces.	4	
2.3	Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory and derivation of isotherm, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.	5	
2.4	Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.	4	
3	**Catalysis**	**9**	**4, 5**
3.1	Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.	3	
3.2	Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis	2	

3.3	Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer-Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.	4	
4	**Colloids and Macromolecules**	**9**	**1**
4.1	Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.	4	
4.2	Macromolecules: Molecular mass- different averages, relation between different averages, calculation of different averages, methods of molecular mass determination- osmotic pressure, viscosity, sedimentation and light scattering methods.	5	
5	**Photochemistry**	**18**	**5**
5.1	Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.	6	
5.2	Principle of utilization of solar energy, solar cells and their working.	4	
5.3	Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, greenhouse effect, two photon absorption spectroscopy, lasers in photochemical kinetics.	8	

References

1. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row, 1987.
3. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
4. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
5. P.W. Atkins, Physical Chemistry, ELBS, 1994.
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7. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & sons, 1997.

8. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2th Edn., New Age International,1986.
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Course code	**PG3CHEC11**				
Course	**PHYSICAL CHEMISTRY- III (CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**4**	**Total hours**	**72**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Part A (Weightage/Qn: 1)	**Part B (Weightage/Qn: 2)**	**Part C (Weightage/Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	1	55
Module 2 (18 hrs)	2	2	1	55
Module 3 (9 hrs)	2	1	0.5	32.5
Module 4 (9 hrs)	2	1	0.5	32.5
Module 5 (18 hrs)	2	2	1	55
Total	**10**	**8**	**4**	**230**

QP code **Reg. No.**

Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
THIRD SEMESTER
Programme: M.Sc. Chemistry
PG3CHEC11: PHYSICAL CHEMISTRY III (CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. Mention the significance of $\Delta S^{\#}$.
2. What is Eyring equation?
3. Write Gibbs adsorption isotherm. Explain the terms involved
4. What are micelles?
5. What is Zeta potential?
6. Differentiate between number average and weight average molecular mass.
7. How the rate of enzyme catalysis varies with temperature?
8. Write the main difference between Langmuir Hinshelwood and Erly Riedel mechanism.
9. What is quantum yield?
10. What are excimers and exciplexes?

(8 × 1= 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Discuss the kinetics of H_2-Br_2 Reaction.
12. Explain ESR methods of studying fast reactions.
13. Explain the principle of Auger electron spectroscopy in the study of surfaces.
14. At $0^{o}C$ and 1 atm pressure, the volume of nitrogen gas required to cover a sample of silica gel, assuming Langmuir monolayer adsorption, is found to be 130 cm^3 g^{-1} of the gel. Calculate the surface area per gram of silica gel. [area occupied by a nitrogen molecule is 0.162 $(nm)^2$]
15. Write a note on Donnan membrane equilibrium, in case of charged polymers.
16. Explain in detail about Skrabel diagram.
17. Explain photosensitization and quenching.
18. What are E-type and P-type delayed fluorescence

(6 × 2 =12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight** 5)*

19. What are the factors determining reaction rates in solutions? Derive Bronsted-Bjerrum equation. Discuss primary and secondary kinetic salt effect
20. Derive BET adsorption isotherm. How it can be used to determine the surface area of the adsorbent.
21. (a) Derive the kinetics of proteolytic acid catalyse mechanism (b) How will you determine the molecular mass of polymers by viscosity methods?
22. Derive Stern-Volmer equation b) Write the mechanism for the photochemical dimerization of anthracene and derive its rate law.

(2 × 5 = 10)

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Course code	**PG3CHEC12**				
Course	**SPECTROSCOPIC METHODS IN CHEMISTRY**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**3**	**Total hours**	**54**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Describe the basic principles of UV-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectroscopy for the structure identification of organic compounds.	**Understand**	**1, 3, 4,**
2	Correlate the structure of molecule with UV-Visible and IR spectral data.	**Apply**	**1, 2, 4, 5**
3	Analyze and interpret first order NMR spectra.	**Analyse**	**1,2,4**
4	Analyze and interpret Mass spectral data of organic compounds.	**Analyse**	**2,3,4, 5**
5	Identify and elucidate structures of unknown organic compounds based on the data from UV-Vis, IR, Mass Spectrometry ^{1}HNMR and ^{13}CNMR spectroscopy.	**Apply**	**1,2,4 5**

Module No.	Course Description	Hours	CO No.
1	**Ultraviolet-Visible and Chiro optical Spectroscopy**	**9**	**1,2,5**
1.1	Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.	2	
1.2	Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.	2	
1.3	Problems based on the above topics.	2	
1.4	Chirooptical properties- Linear polarized effect, Circular polarized light, Elliptical polarized light, Optical rotation (specific rotation), Circular birefringence, CD, ORD, Application of ORD and CD curves - Functional group analysis, Determination of configuration and conformation, Position of functional groups ORD, CD, axial halo ketone rule, octant rule, Cotton effect.	3	
2	**Infrared Spectroscopy**	**9**	**1,2,5**
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.	3	
2.2	IR spectra of C=C bonds (olefins and arenes) and C=O bonds	3	
2.3	Problems on spectral interpretation with examples	3	
3	**Nuclear Magnetic Resonance Spectroscopy**	**18**	**1,3,5**
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, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.	3	
3.2	Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal’s triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling. NOE and cross polarization.	5	
3.3	Simplification of non-first order spectra to first order	3	

	spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling, ^{19}F and ^{31}P NMR.		
3.4	2D NMR and COSY, HOMOCOSY and HETEROCOSY	2	
3.5	Polarization transfer. Selective Population Inversion. DEPT. Sensitivity enhancement and spectral editing, MRI.	2	
3.6	Problems on spectral interpretation with examples.	3	
4	**Mass Spectrometry**	**9**	**1,4,5**
4.1	Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CI, MALDI, PD, Field Desorption Electrospray Ionization. Magnetic, TOF, quadrupole and ion cyclotron mass analyzers. MS^n technique. Fragmentation patterns- Stevenson's rule, Nitrogen rule, McLafferty rearrangement, Retro Diels-Alder reaction. Fragmentation patterns of polyenes, alkyl halides, alcohols, phenols, aldehydes, ketones, carboxylic acids and esters. HRMS, MS-MS, LC-MS, GC-MS.	6	
4.2	Determination of Hydrogen deficiency (DBE) Problems on spectral interpretation with examples.	3	
5	**Structure Elucidation Using Spectroscopic Techniques**	**9**	**1,2,3,4,5**
5.1	Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).	6	
5.2	Interpretation of the given UV-Vis, IR and NMR spectra.	3	

References

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.
2. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.
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11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.
12. Online spectral databases including RIO-DB.
13. P.S. Kalsi. Spectroscopy of Organic Compounds, 5th Edn., New Age International, 2004.

Course code	**PG3CHEC12**				
Course	**SPECTROSCOPIC METHODS IN CHEMISTRY**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/III**				
Type	**CORE**				
Credits	**4**	**Hours/week**	**3**	**Total hours**	**54**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Part A (Weightage/ Qn: 1)	**Part B (Weightage/ Qn: 2)**	**Part C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (9 hrs)	2	2	0.5	42.5
Module 2 (9 hrs)	2	1	0.5	32.5
Module 3 (9 hrs)	4	2	1.5	77.5
Module 4 (9 hrs)	2	2	0.5	42.5
Module 5 (18 hrs)	0	1	1	35
Total	**10**	**8**	**4**	**230**

QP code **Reg. No:**
Name :

Model Question paper
M.Sc. DEGREE (C.S.S) EXAMINATION
THIRD SEMESTER
Programme: M.Sc. Chemistry
PG3CHEC12 : SPECTROSCOPIC METHODS IN CHEMISTRY

Time: 3 Hrs **Maximum Weight: 30**

Section A

Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. Comment on the UV spectra of 2-methoxy pyridine and calculate the λ_{max}?
2. Absorption maximum of chloromethane, bromomethane and iodomethane are 172, 204, and 258 nm respectively. How can the trend of absorption be explained?
3. Arrange the following in the increasing order of carbonyl stretching frequencies: Acetaldehyde, acetone, Acetic acid, acetyl chloride, acetamide and ethyl acetate. Justify your answer.
4. Which spectroscopic technique is used to distinguish between intermolecular and intramolecular hydrogen bonding ?
5. What is NOE?
6. Give an account of quadrupole broadening and decoupling.
7. Give a brief idea about MALDI.
8. What is metastable peaks?
9. ^{1}H NMR spectrum of dimethyl formamide shows two signals at δ2.84 and 3.0 for methyl protons at room temperature but a single sharp line appears at high temperature. Explain.
10. Describe ABC and AMX type splitting with suitable examples.

(8 × 1 = 8)

Section B

Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

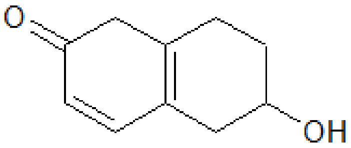
11. Explain 2D NMR spectroscopy? Distinguish between HOMOCOSY and HETEROCOSY?
12. What are the different methods used to simplify complex spectra?
13. How will you differentiate benzyl benzoate and phenyl benzoate using mass spectrum?
14. Explain how IR spectroscopy can be applied to predict the product formation at each step in the following reaction series.

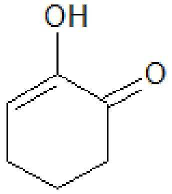
    Benzaldehyde → Benzoin → Benzil → Benzilic acid.
15. Can we use IR spectroscopy to distinguish between

    a) Acetaldehyde and acetone

    b) Butene and butadiene. Give a reason.
16. Write a note on Mclafferty rearrangement with suitable examples.
17. Write a note on a) Effect of solvent on the UV absorption maxima of ketones

    b) Axial halo ketone rule.
18. (a) Calculate the λ_{max} for the following compounds





    (b) Calculate the double bond equivalent (DBE) of the following molecules.

    i) $C_{10}H_8O_2$ ii) $C_{15}H_{13}Cl$

(6 × 2 = 12)

Section C

Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight** 5)*

19. An organic compound having molecular formula $C_9H_{10}O_2$, gave the following spectral data:

    UV : λ_{max} 274 nm ($\varepsilon = 2050$)

    IR : υ_{max} 3031, 2941, 1724, 1608, 1504, 1060 and 830 cm^{-1}.

    ^{1}HNMR : δ: (3H, s), 3.82 (3H, s) and 7.20-7.85 (4H,m)

    Ms (m/z): 150,145,119

    What is the probable structure of the compound?

20. (a) Bring out the major difference between off-resonance and broad band decoupling in ^{13}C NMR spectroscopy

    (b) Discuss the theory and applications of MRI.

21. (a) The mass spectrum of 4-hepatanone shows two ions at m/z 86 and 58. Account their formation. What other peaks can be expected in its mass spectrum.

    (b) Predict the structure of the compound (commercial sample) with the following spectral characteristics and justify your answer.

    MF: $C_4H_{10}O$

    IR: 3450 (broad), 2980, 1450, 1200, 1050cm^{-1}

    ^{1}HNMR: 1.5 (3H, t), 2.8 (2H, dq), 3.4 (1H, m), 4.5 (1H, s), 2.1 (3H, d).

    ^{13}C NMR: 22.6, 68.7, 32.0, 9.9 ppm.

    DEPT 45: 4 signals, DEPT 90 : 1 signal, DEPT 135: 3 +ve and 1 –ve signal

22. (a) What type of transition are observed in unsaturated carbonyl compounds? How absorption maximum and intensity are shifted when carbonyl group is not conjugated? Discuss the effect of solvent polarity on R band.

    (b) An organic compound C_8H_{18} records in its IR spectrum the following bands at 2960, 2845, 1480, 1440, 1385, 1370 cm^{-1} and several bands in the fingerprint region. Suggest the probable structure.

(2 × 5 = 10)

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SEMESTER IV

Course code	**PG4CHEE01**				
Course	**INORGANIC CHEMISTRY- IV (ADVANCED INORGANIC CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/ IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Apply the principles of group theory and symmetry to solve the problems of coordination complexes	**Apply**	**1, 2, 5, 6, 7**
2	Elucidate the structure of inorganic complexes using IR, Raman, ESR and Mossbauer spectroscopy	**Apply**	**1, 2, 3**
3	Identify and interpret the electronic spectra and magnetic properties of complexes.	**Apply**	**1, 2, 5**
4	Describe the principles of photochemistry in complexes	**Understand**	**1, 2**
5	Extend the principles of photochemistry to the coordination complexes	**Apply**	**1, 2, 5**
6	Understand the applications of photochemical properties complexes in the development of photo-devices	**Analyse**	**2 5, 6**
7	Understand the basic principles and synthesis of nano particles	**Understand**	**1, 2**
8	Apply the properties of nano particles in various fields of material sciences	**Apply**	**1, 2, 6**
9	Apprehend the basic principles of various analytical methods in various sampling and analysis techniques.	**Understand**	**1,2, 3, 4, 5**
10	Evaluate the techniques of analytical chemistry to monitor and quantify environmental pollution	**Evaluate**	**1,2, 3, 4, 5**

Module No.	Course description	Hours	CO No.
1	**Applications of Group Theory**	**36**	**1**
1.1	Transformation properties of atomic orbitals, hybridization schemes (σ-bonding only) for AB_3 (trigonal planar), AB_4 (tetrahedral and square planar), AB_5 (trigonal bipyramid) and AB_6 (octahedral) molecules. Derivation of SALCs (using projection operator method) and construction of MO diagram for σ-bonding in trigonal planar, tetrahedral, and octahedral molecules. SALCs and MO diagram for a complex with pi-bound ligands (eclipsed ferrocene as example).	18	1
1.2	Term symbols (R-S coupling scheme, derivation not required) for d^n systems. Splitting of one electron level (*s*, *p*, *d*, *f*, *g* and *h*) and free ion terms in T_d, D_{4h} and O_h ligand fields. Construction of correlation diagram for d^2 ion in T_d, and O_h ligand fields. Method of descending symmetry (for d^2 ion in O_h ligand field). Selection rules for d-d transitions. Electronic transition moment integral. Quick way of identifying vanishing integrals using character tables. Vibronic coupling in the electronic transitions of $[Co(NH_3)_6]^{3+}$complex. Prediction of IR and Raman active fundamentals in AB_4 (tetrahedral & square planar), AB_6 (octahedral) type complexes	18	
2	**Inorganic Spectroscopic Methods**	**9**	**2, 3**
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^-, $NO2^-$ and X^- (X=halogen).	5	
2.2	Electron Paramagnetic Resonance Spectroscopy: EPR of d*1* and d*9* transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.	3	
2.3	Mössbauer Spectroscopy: applications of Mössbauer spectroscopy in the study of Fe(III) complexes.	1	
3	**Inorganic Photochemistry**	**9**	**4, 5, 6**
3.1	Excited states, ligand field states, charge-transfer states and phosphorescence and fluorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications- synthesis and	6	

	catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds.		
3.2	Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction.	3	
4	**Nanomaterials**	**18**	**7, 8**
4.1	General introduction to nanomaterials and emergence of nanotechnology, Moore's law, Graphene (elementary idea only), synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum, techniques of synthesis-electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films-chemical vapour deposition and atomic layer deposition techniques.	9	
4.2	Diversity in nanosystems: self-assembled monolayers on gold-growth process and phase transitions. Gas phase clusters- formation, detection and analysis. Quantum dots-preparation, characterization and applications. Nanoshells-types of systems, characterization and application.	7	
4.3	Evolving interfaces of nanotechnology- nanobiology, nanosensors, nanomedicines	2	
5	**Analytical Methods**	**18**	**9, 10**
5.1	The basis and procedure of sampling-crushing and grinding, gross sampling. Sampling of solids, liquids, gas, particulate solids, metals and alloys. Preparation of a laboratory sample. Moisture in samples- essential and non-essential water, occluded water. Determination of water in samples- direct and indirect methods.	4	
5.2	Decompositions and dissolution-reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$ and HF. Microwave decompositions, combustion methods. Uses of fluxes like Na_2CO_3, Na_2O_2, KNO_3, $K_2S_2O_7$, NaOH, B_2O_3 and lithium meta borate.	5	
5.3	Elimination of interferences from samples by precipitation, electrolytic precipitation, separation by extraction and ion exchange separation.	4	
5.4	Analytical procedures involved in the environmental monitoring of water quality- BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: sampling and collection of air pollutants-SO_2, NO_2, NH_3, O_3, and PAM.	5	

References

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2. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Pub., 1985.
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Course code	**PG4CHEE01**				
Course	**INORGANIC CHEMISTRY- IV** **(ADVANCED INORGANIC CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

BLUE PRINT OF QUESTION PAPER

Module (Hrs.)	**Number of Questions**			
	Section A (weightage/ Qn: 1)	**Section B (weightage/ Qn: 2)**	**Section C (weightage/ Qn: 5)**	**Total WGP**
Module 1 (36 hrs)	2	4	1	75
Module 2 (9 hrs)	2	1	0.5	32.5
Module 3 (9 hrs)	2	1	0.5	32.5
Module 4 (18 hrs)	2	1	1	45
Module 5 (18 hrs)	2	1	1	45
Total	**10**	**8**	**4**	**230**

(Relevant character tables to be supplied with the question paper)

QP code **Reg. No.**

Name

Model Question Paper

M.Sc. DEGREE (C.S.S.) EXAMINATION
FOURTH SEMESTER
Programme: M.Sc. Chemistry
PG4CHEE01: INORGANIC CHEMISTRY - IV
(ADVANCED INORGANIC CHEMISTRY)

Time: 3 hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What is Laporte selection rule? How the Laporte rule is relaxed?
2. How does the character table provide a way of judging an overlap or transition integral is necessary zero?
3. State Kramer’s rule in EPR spectroscopy
4. What happens to the C=N stretching frequency in N-salicylidine aniline on complexation with metal ion? Give reasons.
5. Why Ruthenium complexes shows chemiluminasence during photo reaction?
6. Explain photochromism with example
7. What is Moore’s law.
8. What are nanosensors?
9. What are the different forms of water and explain each of them?
10. What are the different types of fluxes? Mention the uses of fluxes like Na_2CO_3, $K_2S_2O_7$ and lithium meta borate.

(8 × 1 = 8)

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Discuss the formation and shapes of SALCs for sigma bonding in an AB_4 tetrahedral molecule.
12. How does the spectral terms of d^2 system splits in an O_h environment.
13. Explain the method of descending symmetry.
14. Use group theory to predict the IR modes of AB_4 tetrahedral molecule.
15. Explain the changes that occur in IR spectra of aqua complexes coordination to metal.
16. What are the different types of photochemical reactions that occur in metal complexes?
17. What are quantum dots? How they are prepared. Discuss any two of its applications.

18. Write a short note on BOD, COD and DO.

(6 × 2 = 12)

Section C

Long Essay Questions

(Answer any ***two*** *questions. Each question carries* ***Weight 5****)*

19. Construct the MO energy diagram of ferrocene molecule (D_{5h} symmetry).
20. How Mossbauer Spectroscopy is useful in the study of Fe complexes? (b) Explain the photochemical reactions of Ru (II) and Ru(III) complexes.
21. Discuss the synthesis and properties of fullerenes and carbon nanotubes. (wt 3) (b) Write a short note on self-assembled monolayers. (wt 2)
22. Explain the elimination of interferences from samples by precipitation, electrolytic precipitation, separation by extraction and ion exchange separation.

(2 × 5 = 10)

***(relevant character tables to be supplied in the question paper)**

Course code	**PG4CHEE02**				
Course	**ORGANIC CHEMISTRY – IV (ADVANCED ORGANIC CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/ IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Explain the structural features of any given supramolecular system.	**Analyse**	**1, 2**
2	Analyse the type of possible interactions in any given host-guest assembly.	**Analyse**	**1, 2**
3	Utilize the studied supramolecular systems for applications for perfumery, medicines, drug delivery etc.	**Evaluate**	**2, 3**
4	Analyse the processes in organic chemistry from a green and sustainable perspective.	**Analyse**	**2, 3, 4**
5	Describe the various chromatographic techniques with their principles and applications.	**Apply**	**4, 6, 7**
6	Demonstrate strategies for the stereospecific/stereo selective organic transformations towards chiral target molecules and the strategies of asymmetric induction.	**Apply**	**2, 5**
7	Elucidate the structure and design synthesis of important natural products and biomolecules and, interpret their chemistry.	**Analyse**	**2, 3, 5, 6**
8	Analyse the mechanism of drug action, drug designing and mechanism of action of various categories of drugs.	**Analyse**	**2, 3, 6, 7**
9	Understand the chemistry of advanced polymeric materials.	**Understand**	**2, 3, 5, 6, 7**

Module No.	Course description	Hours	CO No.
1	**Molecular Recognition and Supramolecular Chemistry**	**18**	**1, 2, 3**
1.1	Concept of molecular recognition, host-guest complex formation, Lock and Key hypothesis, Preorganisation, forces involved in molecular recognition.	6	
1.2	Molecular receptors: General classification; crown ethers, cryptands, spherands, tweezers, cyclophanes, cyclodextrins, carcerands, calixarenes, carbon nanocapsules.	4	
1.3	Importance of molecular recognition in biological systems like DNA and protein. Controlled release phenomena.	4	
1.4	Applications of supramolecular complexes in perfumery and medicine. Targeted drug delivery.	4	
2	**Green Alternatives to Organic Synthesis**	**9**	**4**
2.1	Principles of Green Chemistry: basic concepts, atom economy, twelve principles of Green Chemistry.	2	
2.2	Green alternatives to Organic Synthesis: coenzyme catalyzed reactions- thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: pinacol-pinacolone and benzidine rearrangements. Electrophilic aromatic substitution reactions. Clay catalyzed synthesis. Green photochemical reactions.	4	
2.3	Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.	2	
2.4	General principles of microwave and ultrasound assisted organic synthesis.	1	
3	**Chromatographic techniques**	**9**	**5**
	Chromatographic techniques: Theory of chromatography: Rate theory and plate theory, Distribution of analytes between phases, Retention factor, selectivity factor, Band broadening and column efficiency, Resolution. Principle and applications of adsorption, partition, paper, thin layer and column chromatographic methods, Affinity and chiral columns, LC, HPLC, IEC, GC and GPC.		
4	**Stereoselective Transformations**	**9**	**6**
4.1	Asymmetric induction-chiral auxiliaries and chiral pool.	2	

4.2	Enantioselective catalytic hydrogenation developed by Noyori and Knowels.	2	
4.3	Asymmetric aldol condensation pioneered by Evans.	2	
4.4	Asymmetric Diels-Alder reactions.	2	
4.5	Enantioselective synthesis of Corey lactone.	1	
5	**Chemistry of Natural Products and Biomolecules – I**	**18**	**7**
5.1	Steroids: Classification and nomenclature of steroids. Stereochemistry of cholesterol. Biosynthesis of steroids-(cholesterol). Structure and semi-synthesis of steroid hormones- testosterone, progesterone and estrogens. Biomimetic synthesis of progesterone.	4	
5.2	Alkaloids: Classification of alkaloids. General methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine and quinine. Basic principles of the biosynthesis of alkaloids. Biosynthesis of morphine and papaverine. Biomimetic synthesis of sparteine.	6	
5.3	Terpenoids: Classification of terpenoids. Synthesis of camphor. Biosynthesis of terpenes (α-terpineol).	3	
5.4	Carbohydrates: Classification of carbohydrates. Biosynthesis of carbohydrates (glucose).	1	
5.5	Plant pigments: Anthocyanins and carotenoids. Structure and syntheses of cyanin, flavones, quercetine and β-carotene.	3	
5.6	Lipids: Classification of lipids.	1	
6	**Chemistry of Natural Products and Biomolecules – II**	**9**	**7**
6.1	Vitamins: Classification of vitamins. Structure of vitamins A, B_1, B_2, B_6 and C. Synthesis of vitamins A, B_1, B_2 and C.	2	
6.2	Amino acids, proteins and nucleic acids: Classification. Biosynthesis of phenylalanine. Structure of proteins and nucleic acids. Methods for primary structure determination of peptides and proteins. Replication of DNA, flow of genetic information, protein biosynthesis, transcription and translation, Genetic code, regulation of gene expression, DNA sequencing (elementary idea only). Human Genome Project. DNA profiling and the Polymerase Chain Reaction (PCR).	5	
6.3	Prostaglandins: Nomenclature. Synthesis of PGE_2 and $PGF_2\alpha$.	2	
7	**Medicinal Chemistry and Drug Designing**	**9**	**8**
7.1	Introduction to Drug design: Drug action, drug	4	

	selectivity, receptor proteins, drug receptor interaction, Drug-receptor theories- occupancy theory, rate theory, induced fit theory, activation-aggregation theory, drug metabolism- Phase I and Phase II pathways.		
7.2	Concept of combinatorial and parallel synthesis. Computer aided drug design. (a brief study).	2	
7.3	Important drugs used in the following classes with mechanism of action: Antibacterial agents (Penicillins, cephalosporins, tetracyclines, chloramphenicol, sulphonamides), antiviral agents (Acyclovir, remdesivir, baricitinib) and anticancer agents (alkylating agents-nitrogen mustards, methotrexate).	3	
8	**Advances in Polymer Chemistry**	**9**	**9**
8.1	Conducting polymers, polymers for NLO applications, temperature resistant and flame retardant polymers, polymers for medical applications.	4	
8.2	Dendrimers and dendritic polymers: terminology, classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers as organocatalysts.	5	

References

1. J.M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995.
2. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993.
3. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.
4. V.K. Ahluwalia, Green Chemistry, Ane Books, 2009.
5. T. Pradeep, Nano: The Essentials, Tata McGraw Hill, 2007.
6. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2004.
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8. R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, Blackie Academic and Professional, 1993.
9. J.M. Berg, J.L. Tymoczko, L. Stryer, Biochemistry, 6th Edn., W.H. Freeman,2010.
10. A.L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, 5th Edn., W.H. Freeman, 2008.
11. V.K. Ahluwalia, M. Chopra, Medicinal Chemistry, Ane Books, 2008.
12. V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS Press, 2007.

13. S.V. Bhat, B.A. Nagasampagi, M. Sivakumar, Chemistry of Natural Products, Springer Science & Business Media, 2005.
14. P. S. Kalsi, S. Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science, 2013.
15. T. Nogrady, D. F. Weaver, Medicinal Chemistry: A Molecular and Biochemical Approach, 3rd Edn., Oxford University Press Inc., 2005.
16. D. Sriram, P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
17. K. D. Tripathi, Essentials of Medical Pharmacology, 6th Edn., Jaypee, 2008.
18. P. Chandrasekhar, Conducting Polymers, Fundamentals and applications: A Practical Approach, Springer Science & Business Media, 2013.

Course code	**PG4CHEE02**				
Course	**ORGANIC CHEMISTRY – IV (ADVANCED ORGANIC CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/ IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	1	1	45
Module 2 (9 hrs)	1	1	0.5	27.5
Module 3 (9 hrs)	1	1	0	15
Module 4 (9 hrs)	1	1	0.5	27.5
Module 5 (18 hrs)	2	1	1	45
Module 6 (9 hrs)	1	1	0.5	27.5
Module 7 (9 hrs)	1	1	0.5	27.5
Module 8 (9 hrs)	1	1	0	15
Total	**10**	**8**	**4**	**230**

QP code **Reg. No:**
Name :

Model Question paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
Programme: M.Sc. Chemistry
PG4CHEE02: ORGANIC CHEMISTRY IV
(ADVANCED ORGANIC CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What are carcerands?
2. Discuss calixarenes. Give any one application.
3. Explain the green alternative reaction of benzoin condensation.
4. Briefly explain affinity and chiral columns.
5. Give the name and formula of the catalyst used in Noyori asymmetric hydrogenation.
6. Discuss the biosynthesis of papaverine.
7. Draw the structures of (i) morphine and (ii) cholesterol.
8. Give the structure of vitamin C. Name the disease due to its deficiency.
9. Analyse the MOA of sulpha drugs.
10. Illustrate the convergent synthesis of dendrimers. **(8 × 1 = 8)**

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Describe the following with their applications: a) tweezers and b) cyclophanes.
12. Illustrate the mechanism of green alternative benzidine rearrangement.
13. Describe the principle and applications of gel permeation chromatography.
14. Discuss the enantioselective synthesis of Corey lactone.
15. Outline the synthesis of (a) quercetine and (b) β-carotene.
16. Give a detailed account of polymerase chain reaction.
17. Explain the theories of drug-receptor interaction.
18. Explain hyper branched polymers. **(6 × 2 = 12)**

Section C
Long Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. Explain various types of non-covalent interactions with suitable examples.
20. (a) What are the twelve principles of green chemistry?
    (b) Discuss asymmetric Diels-Alder reaction.
21. Illustrate the structure elucidation and synthesis of quinine.
22. (a) Discuss the various pathways of drug metabolism.
    (b) Explain the terms (a) Replication of DNA and (b) Human Genome Project.

(2 × 5 = 10)

Course code	**PG4CHEE03**				
Course code	**PHYSICAL CHEMISTRY – IV** **(ADVANCED PHYSICAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/ IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

CO No.	Expected Course Outcomes *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Categorize the point groups and characterize different solid and liquid crystals	**Analyse**	**1, 2**
2	Describe and understand various theories of ions in solution and solve problems on electrochemical cell parameters.	**Analyse**	**1, 2**
3	Identify and interpret the electrode double layer and solve problems on current and overpotential under given condition	**Evaluate**	**1**
4	Analyze the various quantum statistics and theories on heat capacity of solids	**Analyse**	**1**
5	Apply various electro-analytical techniques in qualitative and quantitative analysis.	**Apply**	**1, 2, 3, 4, 5**
6	Explain the methods of electron diffraction, atomic spectroscopic techniques and fluorescence sensing.	**Apply**	**2, 3, 4, 5**

Module No.	Course description	Hours	CO No.
1	**Crystallography**	**18**	**1**
1.1	Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.	14	
1.2	Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.	3	
1.3	Liquid crystals: mesomorphic state, types, examples and applications of liquid crystals.	1	
2	**Electrochemistry**	**18**	**2**
2.1	Conductance measurements, results of conductance measurements, ionic mobilities, influence of pressure and temperature on conductance of ions, Walden equations, abnormal ionic conductance.	2	
2.2	Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, 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.	14	
2.3	Electrochemical cells, concentration cells with and without transference and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties.	2	
3	**Electrode Double layer**	**9**	**3**
3.1	Electrode double layer, electrode-electrolyte interface, different models of double layer-Helmholtz compact layer model, Guoy-Chapman model, Stern model, theory of	**4**	

	multilayer capacity, electrocapillary, Lippmann equation, membrane potential.		
3.2	Fuel cells, classification based on working temperature, chemistry of fuel cells, H2 – O2 fuel cells.	1	
3.3	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, rate constants.	4	
4	**Quantum Statistics**	**9**	**4**
4.1	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, application in electron gas, thermionic emission. Comparison of three statistics- Maxwell Boltzmann, Bose Einstein and Fermi - Dirac Statistics.	6	
4.2	Heat capacity of solids- Dulong and Petit's law, the vibrational properties of solids, Einsteins theory- derivation and its limitations. Debye theory – derivation and its limitations.	3	
5	**Electroanalytical Techniques**	**18**	**5**
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, the dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition method, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.	6	
5.2	Amperometric titrations: General principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, titration procedure, merits and demerits of amperometric titrations.	6	
5.3	Coulometry: Coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, applications of coulometric titrations-neutralization titrations, complex formation	6	

	titrations, redox titrations. Advantages of coulometry.		
6	**Diffraction Methods, Atomic Spectroscopic Techniques and Fluorescence Spectroscopy**	**18**	**6**
6.1	Electron diffraction of gases. Wierl's equation. Neutron diffraction method. Comparison of X-ray, electron and neutron diffraction methods.	3	
6.2	Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.	4	
6.3	Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.	3	
6.4	Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation.	3	
6.5	Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorophores: long life time metal-ligand complexes.	5	

References

1. J.M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995.
2. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993.
3. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.
4. V.K. Ahluwalia, Green Chemistry, Ane Books, 2009.
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8. R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, Blackie Academic and Professional, 1993.
9. J.M. Berg, J.L. Tymoczko, L. Stryer, Biochemistry, 6th Edn., W.H. Freeman,2010.
10. A.L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, 5th Edn., W.H. Freeman, 2008.
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14. P. S. Kalsi, S. Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science, 2013.
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16. D. Sriram, P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
17. K. D. Tripathi, Essentials of Medical Pharmacology, 6th Edn., Jaypee, 2008.
18. P. Chandrasekhar, Conducting Polymers, Fundamentals and applications: A Practical Approach, Springer Science & Business Media, 2013.

Course code	**PG4CHEE03**				
Course	**PHYSICAL CHEMISTRY – IV (ADVANCED PHYSICAL CHEMISTRY)**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/ IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

BLUE PRINT OF QUESTION PAPER

	Number of Questions			
	Section A (Weightage/ Qn: 1)	**Section B (Weightage/ Qn: 2)**	**Section C (Weightage/ Qn: 5)**	**Total WGP**
Module 1 (18 hrs)	2	2	0.5	42.5
Module 2 (18 hrs)	2	1	1	45
Module 3 (9 hrs)	1	2	0	25
Module 4 (9 hrs)	1	0	1	30
Module 5 (18 hrs)	2	1	1	45
Module 6 (18 hrs)	2	2	0.5	42.5
Total	**10**	**8**	**4**	**230**

QP Code **Reg. No.**

Name

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FOURTH SEMESTER
M.Sc. Chemistry
PG4CHEE03: PHYSICAL CHEMISTRY – IV
(ADVANCED PHYSICAL CHEMISTRY)

Time: 3 Hrs **Maximum Weight: 30**

Section A
Short Answer Questions

*(Answer any **eight** questions. Each question carries **Weight 1**)*

1. What are Miller indices ? Explain.
2. What are liquid crystals? Give one example.
3. What is Debye – Falkenhagen effect?
4. What are the restoring forces acting on the ions in the electrolyte?
5. What are fuel cells? Explain with an example.
6. Distinguish between bosons and fermions with examples
7. What is the role of supporting electrolyte in voltammetry?
8. Write note on silver coulometer
9. What are the types of sources of light used in fluorescence spectroscopy?
10. Write a note on collisional quenching **(8 × 1 = 8)**

Section B
Short Essay Questions

*(Answer any **six** questions. Each question carries **Weight 2**)*

11. Compare the structure of KCl & NaCl
12. Explain single crystal X-ray diffraction technique.
13. Discuss the validity of DHO equation for aqueous and non-aqueous solutions
14. Explain $H_2 – O_2$ fuel cell.
15. Explain the different models of electrical double layers.
16. What are the merits and demerits of amperometric titrations?
17. Give the importance of Wierl’s equation in diffraction studies.?
18. Explain the principle and instrumentation of AAS. **(6 × 2 = 12)**

Section C
Essay Questions

*(Answer any **two** questions. Each question carries **Weight 5**)*

19. a) What is structural factor, scattering factor and Fourier synthesis?
b) Compare electron, neutron and x-ray diffraction methods.
20. Derive Debye- Huckel limiting law
21. Derive Debye theory of heat capacity of solids. How does it differ from Einstein’s theory?
22. Give a brief account of polarographic analysis. **(2 × 5 = 10)**

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Course code	**PG4CHEE04**				
Course	**POLYMER CHEMISTRY**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

CO No.	**Expected Course Outcomes:** *Upon completion of this course the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Describe the basic concepts and terms related to polymer chemistry and identify different monomers present in common commercial polymers	**Remember**	**1, 2**
2	Compare different methods for determination of molecular weight and solve problems related to molecular weight determination	**Apply**	**1, 2, 4**
3	Illustrate different mechanisms and techniques of polymerisation	**Evaluate**	**1, 2, 5**
4	Establishes theoretical basis for the structure – property relationship of polymers	**Analyse**	**1, 2, 5**
5	Understand structural and stereochemical aspects of the polymers and their characterisation techniques	**Understand**	**1, 2, 4**
6	Appreciate the diverse application potential of different polymeric materials in day-to-day life	**Evaluate**	**1, 2, 5**
7	Understand the properties, classification, preparation, characterisation and applications dendrimers	**Understand**	**1, 2**

Module No.	Course Description	Hours	CO No.
1	**Introduction to Polymer Science**	**9**	**1, 2, 5**
.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. Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces.	3	
1.2	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.	3	
1.3	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 6, 12, 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.	3	
2	**Fundamentals of Polymerization**	**18**	**3**
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.	3	
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.	4	
2.3	Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization,	3	

	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	3	
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	3	
2.6	Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).	2	
3	**Properties of Polymers**	**18**	**4, 5**
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.	6	
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.	6	
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.	6	
4	**Stereochemistry and Conformation of Polymers**	**9**	**5**
4.1	Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional	9	

	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.		
5	**Morphology and Order in Crystalline Polymers**	**9**	**4, 5**
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.	4	
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.	5	
6	**Advances in Polymers**	**9**	**6, 7**
6.1	Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications	6	
6.2	Carbon fibres. Synthesis, characterization and applications of carbon nanofibers. properties, applications	**3**	
7	**Dendrimers and Dendritic Polymers**	**18**	**3, 4, 5, 6, 7**
7.1	Basic concepts and terminology: Dendrons, star shaped and star bust polymers, dendrimer formation and generations, various types of dendrimers.	**3**	
7.2	Synthesis of dendrimers-convergent and divergent approaches, methods and mechanism. Properties of dendrimers- polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.	**5**	
7.3	Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies (MALDI and TOF).	**6**	

7.4	Dendritic macromolecules: hypergrafted and hyperbranched polymers-definition and classification, synthesis-methods and mechanism, characterization,	4	

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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.
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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.
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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.

Course code	**PG4CHEE05**				
Course	**ANALYTICAL CHEMISTRY**				
Degree	**M.Sc.**				
Branch	**CHEMISTRY**				
Year/Semester	**2/IV**				
Type	**ELECTIVE**				
Credits	**3**	**Hours/week**	**5**	**Total hours**	**90**

CO No.	**Expected Course Outcomes:** *Upon completion of this course the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Explain the theoretical principles of selected methods within electroanalytical, spectrometric/ spectrophotometric /mass spectrometry methods/ various separation techniques including chromatography, and main components of analytical instruments	**Understand**	**1,2,4,6**
2	Independently integrate concepts and techniques in instrumental analysis and correlate to relevant applications.	**Analyze**	**1,2,4,5**
3	Integrate a fundamental understanding of the underlining physical principles as they relate to specific instrumentation used for atomic, molecular, and mass spectrometry, magnetic resonance spectrometry and chromatography.	**Apply**	**1, 2, 5**
4	Apply the theory and operational principles of analytical methods in environment pollution monitoring and quality control	**Evaluate**	**1,2,5,6**
5	Plan sampling and understand how different sampling methods and instrumental analytical methods can be used in analysis	**Evaluate**	**1,2,5,6**
6	Distinguish between qualitative and quantitative measurements and be able to effectively compare and critically select methods for elemental and molecular analyses.	**Create**	**1,2,5,6**
7	Apply analytical principle for the purification and preservation of aquatic resources	**Apply**	**1,2,4,5,6**

Module No.	Course Description	Hours	CO No.
1	**Instrumental Methods**	**36**	**1, 2, 3, 6**
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.	**6**	
1.2	Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio hardware and software methods.	**2**	
1.3	Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.	**6**	
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.	**6**	
1.5	Molecular fluorescence and fluorometers: photoluminescence and concentration electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.	**5**	
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.	**4**	
1.7	Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.	**4**	
1.8	NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.	**3**	
2	**Sampling**	**18**	**4, 5**
2.1	The basis and procedure of sampling, sampling	**9**	

	statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non-essential water, absorbed and occluded water, determination of water (direct and indirect methods).		
2.2	Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.	**9**	
3	**Applied Analysis**	**9**	**1,2,4,6**
3.1	Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.	**3**	
3.2	Soil-moisture, salinity, colloids, cation and anion exchange capacity.	**2**	
3.3	Air pollution monitoring sampling, collection of air pollutants-SO2, NO2, NH3, O3 and SPM.	**2**	
3.4	Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.	**2**	
4	**Capillary Electrophoresis and Capillary Electro Chromatography**	**9**	**1, 2, 3**
4.1	Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection (indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.	**6**	
4.2	Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.	**3**	
5	**Process instrumentation**	**9**	**1, 2, 3**
5.1	Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N	**9**	

	analysers.		
6	**Aquatic Resources**	**9**	**1, 2, 7**
6.1	Aquatic resources: renewable and non-renewable resources, estimation, primary productivity and factors affecting it, regional variations.	**2**	
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.	**4**	
6.3	Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.	**3**	

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.
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5. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
6. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
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13. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.

SEMESTER III & IV PRACTICALS

Course code	**PG4CHEP04**		
Course	**INORGANIC CHEMISTRY PRACTICAL – II**		
Degree	**M.Sc.**		
Branch	**CHEMISTRY**		
Year/Semester	**2/III & IV**		
Type	**PRACTICAL**		
Hours/week	**3**	**Total hours**	**54 + 54 = 108**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Illustrate the separation and estimation of two metal ions in a binary mixture by volumetric and gravimetric methods.	**Apply**	**1, 3, 4**
2	Analyse the constituent metals in alloys	**Analyse**	**1, 3, 4, 5**
3	Analyse the constituent metals in ores	**Analyse**	**1, 3, 4, 5**

Module No.	**Course description**	**Hours**	**CO No.**
1	**PART I**	**60**	**1**
1.1	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.	**60**	**1**
2	**PART II**	**48**	**2, 3**
2.1	Analysis of one of the alloys of brass, bronze and solder.	24	
2.2	Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.	24	

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.

QP code **Reg. No.**

Name:

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
FOURTH SEMESTER
Programme: M.Sc. Chemistry
PG4CHEP04: INORGANIC CHEMISTRY PRACTICAL – II

Time: 6 Hrs **Maximum Weight: 15**

PART A

1. Write a brief procedure for the analysis of alloy.................. **(Weight 1)**
2. Write briefly the procedure for the estimation of .... and ....in the given mixture. **(Weight 1)**
3. Determine the amount of .... and .... in the whole of the given mixture. **(Weight 10)**

PART B: Viva-Voce **(Weight 2)**

PART C: Evaluation of record **(Weight 1)**

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Course code	**PG4CHEP05**		
Course	**ORGANIC CHEMISTRY PRACTICAL - II**		
Degree	**M.Sc.**		
Branch	**CHEMISRY**		
Year/Semester	**2/III & IV**		
Type	**PRACTICAL**		
Hours/week	**3**	**Total hours**	**54 + 54 = 108**

CO No.	**Expected Course Outcomes** ***Upon completion of this course, the students will be able to*:**	Cognitive Level	PSO No.
1	To know the various strategies for the assessment of organic compounds	**Analyse**	**1, 2, 3, 4**
2	Foster innovative laboratory skills for the multistep synthesis of various organic compounds	**Apply**	**1, 2, 3, 4**
3	Synthesize organic compounds in an ecological cordial manner	**Apply**	**1, 2, 3,4**
4	Procure progressive skills for the spectroscopic identification of organic compounds	**Analyse**	**1,2,3,4,7**
5	Understand the various principles involved in the synthesis, separation, characterization and applications of various organic compounds	**Understand**	**1,2,3,4, 7**

Module No.	Course Description	Hours	CO. No.
1	**PART I**	**18**	**1**
1.1	Volumetric estimation of 1) Aniline 2) Phenol 3) glucose 4) Salicylic Acid 5) Iodine value and 6) saponification value of oil	9	
1.2	Spectrophotometric/colorimetric estimation of 1) Aniline 2) Glucose 3) Cholesterol 4) ascorbic acid 5) Streptomycin and 6) Aspirin.	9	
2	**PART II**	**40**	**2, 5**
2.1	Preparation of compounds by two stages 1. Acetanilide – p-nitroacetanilide – p-nitroaniline	40	

	2. Methyl benzoate – m-nitromethylbenzoate – m-nitrobenzoic acid 3. Acetanilide – p-bromoacetanilide – p-bromoaniline 4. Phenol – salicylaldehyde – coumarin 5. Benzophenone – benzophenone oxime – benzanilide 6. Aniline – 2,4,6-tribromoaniline – 1,3,5-tribromoaniline 7. Benzaldehyde-benzoin-benzilic acid 8. Aniline-sulphanilic acid-methylorange 9. O-Toluidine-o-methyl acetanilide-N-acetyl anthranilic acid 10. Aniline-acetanilide-p-nitroacetanilide		
3.0	**PART III**	**40**	**3,5**
3.1	Preparation involving green alternatives of chemical methods. **1.** 1,1-bis -2-naphthol from 2-naphthol **2.** Benzopinacol from benzophenone **3.** Benzopinacolone from Benzopinacol **4.** o-Methyl acetanilide from o-toludine **5.** Acetanilide from aniline	25	
3.2	Microwave assisted organic synthesis. **1.** Benzoic acid from ethyl benzoate **2.** Benzoic acid from benzyl alcohol **3.** Ethyl-3-nitrobenzoate from 3-nitrobenzoic acid **4.** 2-hydroxychalcone from salicylaldehyde **5.** Anthracene-maleic anhydride adduct	15	
4.0	**PART IV**	**10**	**4**
4.1	Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.	10	

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 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, 1979.
5. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

6. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.
7. R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th Edn., Wiley, 2015.
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9. J. B. Cohen, Practical Organic Chemistry, McGraw Hill.
10. C.E Bella and D.F Taber, Organic Chemistry laboratory, Thomson.
11. P.F Shalz, J. Chem. Education, 1996, 173, 267.
12. P.D.L Lampman and Chriz, Introduction to Organic Laboratory techniques, College publishing.

QP code **Name:**

Reg. No:

Model Question Paper

M.Sc. DEGREE (C.S.S.) EXAMINATION
THIRD & FOURTH SEMESTER
Programme: M.Sc. Chemistry
PG4CHEP05 ORGANIC CHEMISTRY PRACTICAL-II

Time: 6 Hrs **Maximum Weight: 15**

PART A

1. Write the theory for the two-step synthesis of ……………. From……… (**Weight 1**)
2. Synthesize …………….from ……………… by a two-step synthetic strategy. Isolate and purify the product at each step and exhibit for inspection. Re-crystallize the final product and display for evaluation. (**Weight 4)**

Or

3. Write the theory and principle for the estimation of……………. (**Weight 1)**
4. Estimate the weight of Aniline/Phenol/Glucose in the given solution.(**Weight 4)**

(Either combination of 1&2 or 3&4 could be given)

5. Write the theory for the microwave assisted organic synthesis of ………… from……… (**Weight 1)**
6. Synthesize……………from………by a microwave assisted organic synthetic method. Isolate and purify the product and exhibit for evaluation. (**Weight 1)**
7. Synthesise ……………….. from ……………..using a green protocol **(Weight 2)**
8. Predict the IR, ^{1}H NMR and ^{13}C NMR spectral values of the products in each of the synthesis carried out in Qn No.2 (Two compounds), Qn No. 6 & 7 (**Weight 3)**

PART B: Viva Voce **(Weight 2)**

PART C: Evaluation of record **(Weight 1)**

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Course code	**PG4CHEP06**		
Course	**PHYSICAL CHEMISTRY PRACTICAL- II**		
Degree	**M.Sc.**		
Branch	**CHEMISTRY**		
Year/Semester	**2/IV**		
Type	**PRACTICAL**		
Hours/week	**4**	**Total hours**	**72 + 72 = 144**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
1	Understand and correlate theoretical principles involved in different experiments	**Analyse**	**1, 2, 3, 4, 5, 7**
2	Develop skill in performing physical chemistry experiments related to chemical kinetics, viscometry, Polarimetry, Refractometry, Conductometry and Potentiometry.	**Application**	**1, 2, 3, 4, 5, 7**
3	Evaluate the applications of different physical chemistry experiments (chemical kinetics, viscometry, Polarimetry, Refractometry, Conductometry and Potentiometry) in determination concentration of analytes	**Evaluate**	**1, 2, 3, 4, 5, 7**
4	Verify Onsager theorems and determine different parameters	**Apply**	**1, 2, 3, 4, 5, 7**

Module No.	**Course description**	**Hours**	**CO No.**
1	**Chemical Kinetics**	**24**	**1, 2, 3**
1.1	Determination of the rate constant of the acid / alkaline hydrolysis of ester.	4	
1.2	Determination of Arrhenius parameters.	4	
1.3	Kinetics of reaction between $K_2S_2O_8$ and KI	8	
1.4	Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI	4	
1.5	Iodination of acetone in acid medium.	4	
2	**Polarimetry**	**16**	**1, 2, 3, 4**

2.1	Kinetics of the inversion of sucrose in presence of HCl.	4	
2.2	Determination of the concentration of a sugar solution.	4	
2.3	Determination of the concentration of HCl.	4	
2.4	Determination of the relative strength of acids.	4	
3	**Refractometry**	**20**	**1, 2, 3**
3.1	Identification of pure organic liquids and oils.	4	
3.2	Determination of molar refractions of pure liquids.	4	
3.3	Determination of concentration of solutions (KCl-water, glycerol-water).	4	
3.4	Determination of molar refraction of solids.	4	
3.5	Study of complex formation between potassium iodide and mercuric iodide	4	
4	**Viscosity**	**16**	**1, 2, 3, 4**
4.1	Determination of viscosity of pure liquids.	4	
4.2	Verification of Kendall's equation.	4	
4.3	Determination of the composition of binary liquid mixtures (alcohol-water, benzene-nitrobenzene).	4	
4.4	Determination of the molecular weight of a polymer (polystyrene in toluene).	4	
5	**Conductivity measurements**	**36**	**1, 2, 3, 4**
5.1	Verification of Onsager equation.	8	
5.2	Determination of the degree of ionization of weak electrolytes.	4	
5.3	Determination of pKa values of organic acids.	4	
5.4	Determination of solubility of sparingly soluble salts.	4	
5.5	Titration of a mixture of acids against a strong base.	8	
5.6	Titration of a dibasic acid against a strong base.	8	
6	**Potentiometry**	32	**1, 2, 3**
6.1	Determination of single electrode potentials (Cu and Zn).	8	
6.2	Application of Henderson equation.	4	
6.3	Potentiometric Titrations.	4	
6.4	Determination of end point of a titration using Gran Plot.	8	
6.5	Determination of the concentration of a mixture of Cl^- and I^- ions.	8	

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.

QP code **Reg. No:**
Name :

Model Question Paper
M.Sc. DEGREE (C.S.S.) EXAMINATION
THIRD & FOURTH SEMESTER
Programme: M.Sc. Chemistry
PG4CHEP06: PHYSICAL CHEMISTRY PRACTICAL-II

Time: 6 Hrs **Maximum weight: 15**

PART A: Physical chemistry Experiments

Instructions: Select each question from ***PART A-I** and **Part A-II*** **Or** select a question from ***PART A-III*** so as to get total ***Weight 11***

PART A-I *(Each questions carries **Weight 4**)*

1. Determine the concentration of given sugar solution polarimetrically
2. Find the velocity constant for the hydrolysis of the given ester in the presence of the given acid/alkali.
3. Obtain the concentration of the given KCl solution by RI measurements. Determine the viscosities of pure sample of liquids A or B
4. Determine the strength of given weak acid using conductometric titration. (Standard of NaOH solution is given)
5. Determine the concentrations of the given NaOH solution by potentiometric titration. You are provided with A.R oxalic acid crystals

PART A-II *(Each questions carries **Weight 7**)*

6. Using refractive index measurements, determine the concentration of the given potassium iodide solution by complexing it with HgI_2.
7. Obtain the concentration of the given KCl solution by refractive index measurements and determine the molar refractivity of solid KCl
8. Determine the viscosities of six mixtures of liquids A and B and graphically represent the variation of viscosity with composition. Hence determine the composition of the given mixture C of A and B.
9. Determine the viscosities of pure sample of liquids A or B and verify the Kendall’s equation.
10. Standardize the given NaOH solution and estimate the amount of acetic acid and hydrochloric acid in the whole of the given solution by conductometric titrations. You are provided with A.R oxalic acid crystals.
11. Standardize the given NaOH solution using conductometric titration. You are provided with A.R Oxalic acid crystals.
12. Verify Debye - Huckel - Onsagar equation and determine the values of the Onsagar constants for the given strong electrolytes graphically.

13. Determine the degree of dissociation of weak monobasic acid in the given solution of concentration 01M. Calculate the pKa value of the acid λ_{H+} = 348 and λ_{AC-} = 52.
14. Study the variation of single electrode potential of Zinc/Copper electrode with change in concentration of $ZnSO_4$/$CuSO_4$ and determine the concentration of the given $ZnSO_4$/$CuSO_4$ solution potentiometrically
15. Standardize the given NaOH solution and hydrochloric acid solution by potentiometric titrations. You are provided with A.R oxalic acid crystals.
16. Determine end point from first derivative plots of potentiometric titration and determine the concentration of HCl and acetic acid in the mixture. You are provided with standard NaOH solution.
17. Determine potentiometrically the volume of the given NaOH solution that should be added to 20 ml of the weak acid solution so as to make the pH of the mixture equal to p^{Ka} + log 3. Also calculate the pH of the mixture at this stage (given $K_a = 1.75 \times 10^{-5}$).

PART A-III *(Each question carries* ***Weight 11****)*

18. Determine the velocity constants for the hydrolysis of the given ester in presence of the acid ‘A’ of known concentration and acid ‘B’ of unknown concentration. Using graphical values of the rate constants, determine the concentration of B**.**
19. Obtain the rate constant for the hydrolysis of the given ester in the presence of the given acid and also determine the Arrhenius parameters.
20. Verify the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.
21. Determine polarimetrically, the specific reaction rate constants for the inversion of cane sugar in each of the given solutions of HCl (A) of known concentration and unknown concentration (B). Using graphical values of the rate constants, determine the concentration of HCl (B).
22. Determine the concentrations of iodide and chloride ions in the given solution potentiometrically by titrating against $AgNO_3$ solution. Standardize the $AgNO_3$ solution potentiometrically by titrating against standard KCl solution.

II. Write the procedure for the experiment(s) selected from **PART- A**

(Weight 1)

PART B: Viva-voce **(Weight 2)**

PART C: Evaluation of Record **(Weight 1)**

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Course code	**PG4CHED01**
Course	**PROJECT**
Degree	**M.Sc.**
Branch	**CHEMISTRY**
Year/Semester	**2/IV**
Type	**CORE**
Credits	**5**

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	**Cognitive Level**	**PSO No.**
CO1	Identify and hypothesise an advanced level research problem.	**Create**	**1,2,3,4,5**
CO2	Design experiments and validate the hypothesis of an advanced level research problem.	**Create**	**1,2,3,4,5**

Course code	**PG4CHEV01**
Course	**VIVA**
Degree	**M.Sc.**
Branch	**CHEMISTRY**
Year/Semester	**2/IV**
Type	**CORE**
Credits	**2**

There will be a comprehensive viva at the end of the programme, which covers questions from all courses in the programme as per the syllabus.

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