Syllabus and Regulations

for

2-Year, 4-Semester M. Sc. Course in

CHEMISTRY

Scottish Church College
Kolkata

Affiliated to

University of Calcutta

July 2013

Syllabus and Regulations for
Two-Year (Four Semester) M. Sc. Course in Chemistry at
Scottish Church College, Kolkata
Affiliated to the
University of Calcutta

1. The examination for the degree of Master of Science (M. Sc.) shall consist of four semesters: Semester-I, Semester-II, Semester-III, - and Semester-IV. Each semester examination will be held after the completion of all the papers for that particular semester and before the next semester begins, commencing on such dates and time as will be decided by the College authority and will be duly notified. Total duration of the course is two years [hereafter, "Course" refers to M. Sc. Course in Chemistry and "Paper" refers to the individual papers of 75/80/85/90/100 marks divided into two halves: Group-A: Theoretical (50-marks) and Group-B: Practical: (25/30/35/40/50 marks)]. The duration of the semester shall ordinarily be as follows:

Semester	**Duration**
Semester-I	July to December
Semester-II	January to June
Semester-III	July to December
Semester-IV	January to June

Course Structure

2. The course will consist of 12 papers of 75/80/85/90/100-marks (Group-A: Theoretical-50 Marks and Group-B: Practical- 25/30/35/40/50-Marks) each. The examiners shall forward assessment in respect of every candidate to the Principal / Controller of Examination / Coordinator P. G. Courses (as the case may be) for tabulation of the results.

3.(a) The entire course of 1000 marks has been divided in to 12 papers of 75/80/85/90/100/ marks of which 6 papers (Papers: I-VI, included in Semesters I-II) (Total: 500-marks) are **compulsory common (General) papers** and 6 papers (Papers: VII-XII, included in Semester-III & IV), (Total: 500-marks), are **optional or Special papers** in **Inorganic Chemistry** / **Organic Chemistry** / **Physical Chemistry**, any **one** of which is allotted to a candidate during the third and fourth semesters.

(b) Special papers shall be allotted to the students on the basis of the merit of their performance in the M Sc. Semester-I and II examinations taken together.

(c) Each paper is composed of a theoretical component (Group-A: 50 marks) and a practical component (Group-B: 25/30/35/40/50-marks). The structure and curricula of the revised syllabus for the M. Sc. Course in Chemistry (Semester system) applicable from the academic session 2013-2014 is stated below:

Course Structure							
Semester	**Duration**	**Marks**			**Credit**	**Course Type**	**Examination**
		Theoretical	**Practical**	**Total**			
I	July-Dec.	150	100	**250**	**25**	General (G)	January
II	Jan-June	150	100	**250**	**25**	General (G)	June
III	July-Dec.	150	100	**250**	**25**	Special (S)	January
IV	Jan-June	150	100	**250**	**25**	Special (S)	June
Total	**2 Years**	**600**	**400**	**1000**	**100**		

Special (Optional) Papers(S):

Inorganic Chemistry (IS) / Organic Chemistry (OS) / Physical Chemistry (PS).

Paper-wise Marks and Credit Distribution

Semester-I; General Papers (G) -250 Marks: 25 Credits

Papers Course ID	Subjects	Group-A (Theoretical)		Group-B (Practical)	
		Marks	Credits	Marks	Credits
Paper-I **CHEM(G)-11**	Inorganic Chemistry.	50	5	30	3
Paper-II **CHEM(G)-12**	Organic Chemistry.	50	5	30	3
Paper-III **CHEM(G)-13**	Physical Chemistry.	50	5	30 + (CAC-1) 10	4

CAC=1: Computer Applications in Chemistry- 1

Semester-II: General Papers (G) -250 Marks: 25 Credits

Papers Course ID	Subjects	Group-A (Theoretical)		Group-B (Practical)	
		Marks	Credits	Marks	Credits
Paper-IV **CHEM(G)-21**	Inorganic Chemistry.	50	5	30	3
Paper-V **CHEM(G)-22**	Organic Chemistry.	50	5	30	3
Paper-VI **CHEM(G)-23**	Physical Chemistry.	50	5	30 (CAC-2) 10	4

CAC: Computer Applications in Chemistry

Semester-III: Special Papers(S):250 Marks: 25 Credits
(IS): Inorganic Special / (OS): Organic Special / (PS): Physical Special

Papers Course ID	Subjects	Group-A (Theoretical)		Group-B (Spl. Practical)	
		Marks	Credits	Marks	Credits
Paper-VII **CHEM(IS/OS/PS)-31**	Special Theo.-1	50	5	35	3.5
Paper-VII **CHEM(IS/OS/PS)-32**	Special Theo.-1	50	5	35	3.5
Paper-VIII **CHEM(IS/OS/PS)-33**	Special Theo.-1	50	5	30	3.0

Semester-IV: Special Papers(S):250 Marks: 25 Credits
(IS): Inorganic Special / (OS): Organic Special / (PS): Physical Special

Papers Course ID	Subjects	Group-A (Theoretical)		Group-B (Spl. Practical)	
		Marks	Credits	Marks	Credits
Paper-X **CHEM(IS/OS/PS)-41**	Special Theo.-1	50	5	25	2.5
Paper-XI **CHEM(IS/OS/PS)-42**	Special Theo.-1	50	5	Grand Viva 25	2.5
Paper-XII **CHEM(IS/OS/PS)-43**	Special Theo.-1	50	5	Project 30 & Seminar 20	5

Theoretical Courses

5. (i). The theoretical part of 50 marks of a paper shall be composed of three course units of 18/ 16/ 16 marks and each such course unit shall be covered by lecture periods totaling about 1000 minutes i.e., 22-24 lectures of 45 minutes duration.

(ii). The duration of examination of theoretical part of 50 marks of a paper shall be 2 hours. Two questions shall be set from **each** course **unit**, of which **one** question has to be answered.

(iii). Questions will be set by internal teachers and guest faculties, which will be moderated by a set of moderators for each paper. The set of moderators, as recommended by the P.G. Board of Studies, should include at least one internal and one external moderator.

(iv). For the theoretical portion of each paper, questions shall be set and the scripts examined by a set of at least two examiners appointed from among the teachers of the department offering the respective courses, including the guest teachers (if any) appointed by the appropriate authority of the College, on recommendation of the P. G. Board of Studies in Chemistry.

Practical Courses

6.(i). The Practical part of a paper shall consist of the following components: Experimental, Laboratory Records, Viva-voce, Internal Assessment and Lab-Quiz (as the case may be).

(ii). The duration of laboratory session for a practical course shall be 90-120 hours and the duration of examination of such a practical course shall be 6 hours.

(iii). For the practical portion of each paper, the examination shall be conducted, and scripts evaluated, by the internal examiners, appointed from the teachers (including guest teachers) of the department, as recommended by the P. G. Board of Studies.

(iv). There shall be no terminal examination for the Computer Application in Chemistry courses in semester I and II, (CAC-1, CAC-2), the entire marks (10/15) for each part shall be awarded by the concerned teacher(s) through continuous assessment.

(v). Grand Viva-Voce examination at the end of 4^{th}. Semester [Paper-XI-(Group-B) Practical, Unit-1, (25 marks)] shall be conducted by a Board of Examiners consisting of External and Internal examiners. This examination shall principally test an examinee's knowledge of the practical course.

(vi). Project work and Seminar presentation [Paper-XII-(Group-B) Practical, Unit-1(30 marks) and Unit-2(20 marks)] to be carried out by the candidates individually in the 4^{th}. Semester may be composed of the following components: experimental / theoretical / review. The project report has to be submitted by the respective candidates (in triplicate) in the form of dissertations. The dissertation part (30 marks) and the seminar part (20 marks) shall be evaluated by a Board of Examiners consisting of external and internal examiners, including guest teachers, as approved by the Board of Studies.

Course Curricula

Semester-I

General Papers

Paper- I: CHEM(G)-11: Inorganic Chemistry General-1(80 Marks)

Group-A Theoretical : (50 Marks)		Group-B : Practical (30 Marks)	
Unit-1 (18M)	**Symmetry,Group Theory and Bonding**	Unit-1 (20M)	Quantitative Inorganic Analysis
Unit-2 (16M)	**Coordination Chemistry I**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Chemistry of Elements I**	Unit-3 (5M)	Lab. Records including Internal Assessment

Paper- II: CHEM(G)-12: Organic Chemistry General-1(80 Marks)

Group-A Theoretical : (50 Marks)		Group-B : Practical (30 Marks)	
Unit-1 (18M)	**Bonding in Organic Compounds**	Unit-1 (20M)	Qualitative Organic Analysis 1
Unit-2 (16M)	**Stereochemistry and Conformational Analysis**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Hetereocyclic Chemistry 1**	Unit-3 (5M)	Lab. Records including Internal Assessment

Paper- III: CHEM(G)-13: Physical Chemistry General-1 (90 Marks)

Group-A: Theoretical (50 Marks)		Group-B : Practical (40 Marks)	
Unit-1 (18M)	**Quantum Mechanics**	Unit-1 (15M)	Physical Chemistry Experiments
Unit-2 (16M)	**Atomic Spectroscopy**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Surface Phenomena**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment
		Unit-5 (10M)	CAC-1

CAC: Computer Applications in Chemistry

Semester-II

General Papers

Paper- IV: CHEM(G)-21: Inorganic Chemistry General-2(80 Marks)

Group-A : Theoretical (50 Marks)		Group-B : Practical (30 Marks)	
Unit-1 (16M)	**Statistical error, Electrochemical analyses, Radiochemical and Environmental analysis**	Unit-1 (20M)	Semi-Micro Qualitative Inorganic Analysis
Unit-2 (16M)	**Bioinorganic Chemistry 1**	Unit-2 (5M)	Viva-voce
Unit-3 (18M)	**Organometallic Chemistry 1**	Unit-3 (5M)	Lab. Records including Internal Assessment

Paper- V: CHEM(G)-22:Organic Chemistry General-2(80 Marks)

Group-A : Theoretical (50 Marks)		Group-B: Practical (30 Marks)	
Unit-1 (18M)	**Pericyclic Reactions 1**	Unit-1 (20M)	Quantitative Organic Analysis
Unit-2 (16M)	**Synthetic Methodology and Polymerization Reaction**s	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Natural Products 1**	Unit-3 (5M)	Lab. Records including Internal Assessment

Paper- VI: CHEM(G)-23: Physical Chemistry General-2(90 Marks)

Group-A :Theoretical (50 Marks)		Group-B : Practical (40 Marks)	
Unit-1 (18M)	**Statistical Thermodynamics**	Unit-1 (15M)	Experiment
Unit-2 (16M)	**Chemical Kinetics**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Molecular Spectroscopy**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment
		Unit-5 (10M)	CAC-2

CAC: Computer Applications in Chemistry

Semester-III

Special Papers

Inorganic Chemistry / Organic Chemistry / Physical Chemistry

Inorganic Chemistry Special

Paper- VII: CHEM(IS)-31: (85 Marks) : Special Paper-IS-1

Group-A: Special Theoretical-1 (50 Marks) *(Common with Physical Special)*		Group-B Special Practical (35 Marks) Synthesis and Characterization of Complex Materials	
Unit-1 (18M)	**Group theory and its Applications in Spectroscopy**	Unit-1 (20M)	Analysis of Complex Materials
Unit-2 (16M)	**Advanced Organometallic Chemistry**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Nuclear Chemistry**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal. Assessment

Paper- VIII: CHEM(IS)-32: (85 Marks) : Special Paper-IS-2

Group-A: Special Theoretical-2 (50 Marks)		Group-B Special Practical (35 Marks) Analysis of Complex Materials	
Unit-1 (18M)	**Chemistry of Elemnets 2: Comparative Accounts**	Unit-1 (20 M)	Experiment
Unit-2 (16M)	**Inorganic Rings, Cages and Clusters**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Inorganic Reaction Mechanism**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Paper- IX: CHEM(IS)-33 (80 Marks) : Special Paper IS-3

Group-A Special Theoretical-3 (50 Marks)		Group-B Special Practical (30 Marks) Spectroscopic Studies of Model Compounds	
Unit-1 (18M)	**Spectroscopy 1:NMR, EPR .**	Unit-1(15M)	Experiment
Unit-2 (16M)	**Spectroscopy2:ORD/CD,NQR, Mossbauer**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Spectroscopy 3 I.R., Raman, Mass, PES, ESCA**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Semester-III

Organic Chemistry Special

Paper- VII: CHEM(OS)-41 (85Marks): Special Paper OS-1

Group-A: Theoretical (50 Marks)		Group-B : Practical (35 Marks)	
Unit-1 (18M)	**Spectroscopy**	Unit-1 (20M)	Multi-step Organic Synthesis
Unit-2 (16M)	**Techniques of Chemical Separation**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Green Chemistry and Nanoscience**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Paper- VIII: CHEM(OS)-42 (85 Marks): Special Paper OS-2

Group-A: Theoretical (50 Marks)		Group-B : Practical (35 Marks)	
Unit-1 (18M)	**Organometallic Chemistry of Transitional Elements**	Unit-1 (20M)	Qualitative Organic Analysis 2
Unit-2 (16M)	**Synthetic Methodology 2**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Advanced Pericyclic Reactions**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Paper- IX: CHEM(OS)-43 :(80 Marks) : Special Paper OS-3

Group-A :Theoretical (50 Marks)		Group-B : Practical (30 Marks)	
Unit-1 (18M)	**Bioorganic Chemistry**	Unit-1(15M)	Chromatographic Separation Techniques and Spectroscopic Studies of Model Compounds
Unit-2 (16M)	**Supramolecular Chemistry**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Chemistry of Natural Products 2 (Terpenoids and Carotenoids, Alkaloids,Coumarins and Flavonoids, Steroids, Porphyrins, Prostaglandins)**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Semester-III

Physical Chemistry Special

Paper- VII: CHEM(PS)-41 (85 Marks) : Special Paper PS-1

Group-A: Theoretical (50 Marks)		Group-B : Practical (35 Marks)	
Unit-1 (18M)	**Equilibrium Statistical Mechanics and Non-Equilibrium Thermodynamics**	Unit-1 (20M)	Experiment
Unit-2 (16M)	**Advanced Quantum Mechanics-I**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Mathematical Methods in Chemistry**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Paper- VIII: CHEM(PS)-32: (85Marks) : Special Paper PS-2

Group-A: Theoretical (50 Marks)		Group-B : Practical (35 Marks)	
Unit-1 (18M)	**Advanced Quantum Mechanics-II**	Unit-1 (20M)	Experiment
Unit-2 (16M)	**Photochemistry-I**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Polymers**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Paper- IX: CHEM(PS)-33 :(80 Marks) : Special Paper PS-3

Group-A :Theoretical (50 Marks)		Group-B : Practical (30 Marks) Computer Applications in Chemistry	
Unit-1 (18M)	**Advanced Quantum Mechanics-III**	Unit-1 (15M)	Programming
Unit-2 (16M)	**Group Theory-I**	Unit-2 (5M)	Viva-voce
Unit-3 (16M)	**Electrochemistry**	Unit-3 (5M)	Lab. Records
		Unit-4 (5M)	Internal Assessment

Semester-IV

Special Papers

Inorganic Chemistry / Organic Chemistry / Physical Chemistry

Inorganic Chemistry Special

Paper- X: CHEM(IS)-41: (75 Marks) : Special Paper IS-4

Group-A: Special Theoretical-1 (50 Marks)		Group-B Special Practical (25 Marks) Analysis of Complex Materials	
Unit-1 (18M)	**Group theory and its Applications in Bonding**	Unit-1 (15M)	Advanced Physico-chemical Experiments
Unit-2 (16M)	**Advanced Bioinorganic Chemistry**	Unit-2 (5M)	Lab. Records
Unit-3 (16M)	**Structure and Properties of Solids**	Unit-3 (5M)	Internal. Assessment

Paper- XI: CHEM(IS)-42: (75 Marks) : Special Paper IS-5

Group-A: Special Theoretical-2 (50 Marks)		Group-B : Practical (25 Marks)	
Unit-1 (18M)	**Synthetic methodology for transition and non-transition metal compounds**	Unit 1 (25 Marks)	Grand Viva-Voce Including All Semester Practical Courses
Unit-2 (16M)	**Magnetochemistry**		
Unit-3 (16M)	**Complex Equilibria**		

Paper- XII: CHEM(IS)-43 (100 Marks) : Special Paper IS-6

Group-A Special Theoretical-3 (50 Marks)		Group-B Special Practical (50 Marks)	
Unit-1 (18M)	**Analytical techniques: Isolation, Characterization and Structure Detremination**	Unit-1(30M)	Project Dissertation
Unit-2 (16M)	**Supramolecular Chemsirty**	Unit-2(20M)	Seminar
Unit-3 (16M)	**Chemistry of Elements 3**		

Semester-IV

Organic Chemistry Special

Paper- X: CHEM(OS)-41 (75Marks): Special Paper OS-4

Group-A: Theoretical (50 Marks)		Group-B : Practical (25 Marks)	
Unit-1 (18M)	**Photo Organic Chemistry and Free Radical Reactions**	Unit-1 (15M)	Separation, Purification and Identification of Organic Compounds in Binary Mixture
Unit-2 (16M)	**Advanced Spectroscopy**	Unit-2 (5M)	Lab. Records
Unit-3 (16M)	**Advanced Stereochemistry**	Unit-3 (5M)	Internal Assessment

Paper- XI: CHEM(OS)-42 (75 Marks): Special Paper OS-5

Group-A: Theoretical (50 Marks)		Group-B : Practical (25 Marks)	
Unit-1 (18M)	**Advanced Organic Synthesis**	Unit 1 (25 Marks)	Grand Viva-Voce Including All Semester Practical Courses
Unit-2 (16M)	**Oxidation and Reduction of Functional Groups**		
Unit-3 (16M)	**Dynamic Aspects of Stereochemistry**		

Paper- XII: CHEM(OS)-43 :(100 Marks) : Special Paper OS-6

Group-A :Theoretical (50 Marks)		Group-B : Practical (50 Marks)	
Unit-1 (18M)	**Heterocyclic Chemistry 2**	Unit-1(30M)	Project Dissertation
Unit-2 (16M)	**Chemistry of Natural Products 3 (Biogenesis and Biosynthesis)**	Unit-2(20M)	Seminar
Unit-3 (16M)	**Medicinal Chemistry**		

Semester-IV

Physical Chemistry Special

Paper- X: CHEM(PS)-41 (75 Marks) : Special Paper PS-4

Group-A: Theoretical (50 Marks)		Group-B : Practical (25 Marks) Computer Applications in Chemistry	
Unit-1 (18M)	**Quantum Statistics**	Unit-1 (15M)	Programming
Unit-2 (16M)	**Molecular Interactions**	Unit-2 (5M)	Lab Records
Unit-3 (16M)	**Solid State Chemistry**	Unit-3 (5M)	Internal Assessment

Paper- XI: CHEM(PS)-42: (75Marks) : Special Paper PS-5

Group-A: Theoretical (50 Marks)		Group-B : Practical (25 Marks)	
Unit-1 (18M)	**Group Theory-II**	Unit-1 (25M)	Grand Viva-Voce including All Semester Practical Courses
Unit-2 (16M)	**Photochemistry-II**		
Unit-3 (16M)	**Advanced Molecular Spectroscopy-I**		

Paper- XII: CHEM(PS)-43 :(100 Marks) : Special Paper PS-6

Group-A :Theoretical (50 Marks)		Group-B : Practical (50 Marks)	
Unit-1 (18M)	**Non-Equilibrium Statistical Mechanics and Reaction Dynamics**	Unit-1 (30M)	Project Dissertation
Unit-2 (16M)	**Advanced Molecular Spectroscopy-II**	Unit-2 (20M)	Seminar
Unit-3 (16M)	**Biophysical Chemistry**		

Eligibility of admission

7. A candidate who has passed the B. Sc. examination in Chemistry (as Honours in Chemistry for CU, and major or as one of the special subjects for other universities or UGC recognized institutions) along with **Mathematics** and ***any one*** of the **Physics, *or* Computer Science** as his/her elective subjects and secured a **minimum of 50% marks** (**45% marks for the reserved category**) in aggregate is eligible to apply for admission to the two-year four-semester M. Sc. Course in Chemistry.

8. Candidate from any other university or UGC recognized institution passed in any other course should bring an equivalence certificate from Calcutta University before admission.

Eligibility for appearing in a Semester Examination

9. A candidate will be eligible to appear in a semester examination provided he/ she has attended at least 75% of the lectures delivered and laboratory sessions conducted in that particular semester , after his / her admission to the course.

Candidate whose attendance is less than 75% would have to repeat the semester.

10. All candidates who have secured the required percentage of attendance as defined in Regulation-9 shall be called **regular candidates**.

Evaluation:

11. (a). A 6 (six) point grade system shall be followed for the purpose, details of which are laid down hereunder:

Numerical Grade Point	Grade	Remarks
10.00-8.00	**A++**	**Outstanding**
7.99-7.00	**A+**	**Excellent**
6.99-6.00	**A**	**Good**
5.99-5.50	**B**	**Fair**
5.49-4.00	**C**	**Average**
3.99-3.50	**D**	**Below Average**
3.49-0.00	**E**	**Unsuccessful**

(b). The following multiplication table shall be used for calculation of the exact grade points:

Marks Between (excluding the end points)	**Multiplication Factors**
100-80	**0.1**
79-70	**0.1**
69-60	**0.1**
59-55	**0.1**
54-40	**0.1**
39-35	**0.1**
34-00	**0.1**

(c). Award of Grades

Example-1: If a candidate secures 63% marks in a particular paper, his/her grade point for the paper will be: $(6.00 + 0.1 \times 3) = 6.3$

Example-2: If a candidate scores 64% in theory and 68% in practical in a 8-credit course (Theoretical- 5 credits + Practical -3 credits = Total 8-credits), then his/her grade point for the course will be as follows:

$$\text{Grade Point} = \frac{[\,5 \times (\,6.0 + 0.1 \times 4) + 3 \times (\,6.5 + 0.1 \times 3)\,]}{(5 + 3)} = 6.55$$

Example-3: If a candidate scores 68% in theory and 64% in practical in a 8-credit course (Theoretical- 5 credits + Practical -3 credits = Total 8-credits), then his/her grade point for the course will be as follows:

$$\text{Grade Point} = \frac{[\,5 \times (\,6.5 + 0.1 \times 3) + 3 \times (\,6.0 + 0.1 \times 4)\,]}{(5 + 3)} = 6.65$$

(i). The Semester Grade Point Average (SGPA) will be just the average of the grade points obtained in all the papers (Group-A and Group-B of a paper taken separately) of a particular semester. If the numerical grade points obtained by a candidate are denoted by C_i (here, i = 1 to 3, as there are 3 papers in each semester), the SGPA will simply be equal to $\Sigma C_i / 3$ usually, as all the papers are of equal weightage.

(ii). Cumulative Grade Point Average (CGPA) over four semesters shall be calculated by working out the simple average of the SGPA for individual semesters.

(iii). On the basis of CGPA obtained by a candidate over four semesters, Grade and Class will be awarded as follows:

CGPA	Grade	Remarks	Class /Division
10.00-8.00	A++	Outstanding	I (First Class)
7.99-7.00	A+	Excellent	I (First Class)
6.99-6.00	A	Good	I (First Class)
5.99-5.50	B	Fair	II (Second Class)
5.49-5.00	C	Average	II (Second Class)
4.99-4.00	D	Below Average	II (Second Class)
3.99-0.00	E	Unsuccessful	X (Fail)

(iv). Both SGPA and CGPA shall be rounded off to the second place of decimal and the rounded off value will be shown as such on the mark sheet.

(v). The mark sheet issued at the end of each semester shall include both the Grade point Average (GPA) and the total marks obtained in each paper, as well as SGPA and the total marks obtained in that semester. The final mark sheet for the 4^{th} semester shall also include the CGPA and the total marks obtained out of 1000 along with Grade and Class.

12. (a). If a candidate gets E in one or more paper(s), he/she shall be deemed to have failed in that / those paper(s) only and he /she shall be required to appear at the subsequent examination for that paper / those papers in a subsequent semester examination.

(b). A candidate can appear a maximum number of two times (excluding, but *immediately after,* his/her regular appearance) to clear a particular paper or to clear a particular semester (for those who fail in aggregate), failing which he/she shall be dropped from the Rolls of the College / University.

13 . A candidate failing in all the courses (papers) in a semester examination shall have to repeat the entire semester examination.

14. A candidate must secure at least 35% marks in each theoretical paper and at least 40% marks in each practical paper and a minimum aggregate of 40% (taking theoretical & practical marks separately) in any semester to qualify for the semester.

Candidates scoring 40% or more but below 60% marks in the aggregate, shall be declared to have passed the examination and have been placed in the second class. Those scoring 60% or more marks in the aggregate, shall be declared to have passed the examination and have been placed in the first class. Class secured by a candidate shall be shown in the final mark sheet of 4^{th} semester examination.

A candidate who has not cleared two consecutive semesters will not be promoted to the next semester.

15. If a candidate gets E grade in one or more papers in a semester examination, his / her SGPA for that semester shall be temporarily withheld and Grade Point Withheld (GPW) shall be marked in place of SGPA on his/her mark sheet. Fresh mark sheet with duly calculated CGPA shall be issued to him/her when the candidate (grade D or above) clears the paper/ papers subsequently within the stipulated time frame.

16. If a candidate has one or more back papers (including those who fail in aggregate) in any semester, then his/her CGPA shall remain incomplete (INC) till he/ she clears all those back papers. The CGPA of such a candidate shall be marked "INC" on the mark sheet. Fresh mark sheet with duly calculated CGPA shall be issued only after he/she clears all those back papers subsequently within the stipulated time frame.

17. To be eligible for the award of ranks in order of merit, a candidate must pass all the four semester examinations at the first chance (as a regular candidate). The final merit list shall be prepared on the basis of CGPA (including all the four semesters) provided, however, that the candidates taking exanimation of back papers shall be excluded from such merit list.

18. Separate mark sheets in prescribed formats given below shall be issued to the candidates for Semester-I, Semester-II, Semester-III and Semester-IV examinations.

Semester-I Mark Sheet

Code: SCCK-CU/CHEM/SEM-1/No….. University Monogram Serial No…….

University of Calcutta

M. Sc. **First** Semester Examination-2013

The following is the statement of marks obtained by **……(*Name of the candidate*)……..,**
Roll: SCCK/CHEM/SEM-1/No.2010-00XX Registration No. …….of 20… – 20…, appearing from ***Scottish Church College, Kolkata*** at the M.Sc. First Semester Examination-2013
(held in January, 2014).

Paper (Course ID)	Course Curricula(G)	Marks obtained Theo.	Pr.	Credit	GPA	SGPA	Grade Remarks
Paper-I CHEM(G)-11	**Inorganic Chemistry** (Group-A): Theoretical (F..M.50) (Group-B):Practical (F. M. 30)						
Paper-II CHEM(G)-12	**Organic Chemistry** (Group-A):Theoretical (F. M.50) (Group-B):Practical (F.M.30)						
Paper-III CHEM(G)-13	**Physical Chemistry** (Group-A):Theoretical (F.M.50) (Group-B):Practical (F.M. 40)						

GPA: Grade Point Average, SGPA: Semester Grade Point Average, GPW: Grade Point Withheld, INC: Incomplete

G: General Papers, * Minimum marks to be obtained: 35% in each course and 40% in aggregate.

SGPA	10.00-8.00	7.99-7.00	6.99-6.00	5.99-5.50	5.49-4.00	3.99-3.50	3.49-0.00
Grade	A++	A^+	A	B	C	D	E
Remarks	Outstanding	Excellent	Good	Fair	Average	Below Average	Unsuccessful

Monogram of College

Principal Controller of Examination

Class

Course Details

Semester-I

Paper-I: CHEM (G)-11: Inorganic Chemistry (General) (80-Marks)

Group-A: Theoretical (50-Marks)

Unit I: Symmetry and Group Theory : (18 Marks) (24 Lectures)

Symmetry as a universal theme, Symmetry Elements and Symmetry operations, Group theory: Definitions and theories, Multiple symmetry Operations, Multiplication Tables, Point groups, identification of point groups, Symmetry operations of the Platonic solids and Stereographic projection, Symmetry properties of Orbitals [**12 lectures**]

Valebcy Theories- Quantum chemical Approach

Huckel approximation applied to H_2^+ and H_2 type systems, comparative study of the application of VB and MO methods to diatomic (homo and hetero) species; MO of polyatomic molecules; Walsh diagram, configuration interaction, orbital construction for H_n type systems, [**12 lectures**]

Unit II: Coordination Chemistry I : (16 Marks) [22 Lectures]

Crystal field theory, crystal field diagram, Experimental evidences of the metal ligand overlap, Nephelauxetic effect. ligand field theory, molecular orbital theory and angular overlap model; Splitting of d-orbitals in linear triangular, tetrahedral, square planer, trigonal bipyramidal, square pyramidal and octahedral fields of similar and dissimilar ligands, crystal filed stabilization energies in weak filed and strong field, octahedral site preference energy, tetragonal distortion and Jahn-Teller effect of Crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stability of complexes (Irving-Williams order). Interpretation of the general features of the electronic absorption spectra, including the charge transfer spectra of the transition metal complexes in aqueous solutions. Spin-orbit coupling constant and interelectronic repulsion parameters in complex ion terms-vs-free ion terms, vibronic coupling, intensity stealing, band broadening, spectrochemical series, nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric effect on energy levels, magnetic properties, quenching of orbital moment and spin only formula. Different types of magnetic materials

Unit III: Chemistry of Elements I: (16 Marks) [22 Lectures]

Introduction to the metal atom clusters present. The blue oxides of Mo-W: the tungsten bronze: sulphides of Mo. Iso- and hetero-poly acids and salts of Mo,W. Platinum Group Metals: oxidation state, valence preference toward π-donor and π-acceptor ligands. Dinitroigen complexes of Ru in the context of nitrogen fixation. Nitrosyl complexes of ruthenium in the perspective of structure and bonding. *cis-trans* complexes of Pt, uses of Pt metals in medicine and catalyst, *Some historically important compounds:* Creutz-Taube compound, Vaska's compound, Magnus' green salt, Vauqelin's pink salt, Krogmann salt etc.

Paper-I: CHEM(G)-11: (Group-B) -30 Marks
Course Duration: 90 Hours
Quantitative Inorganic Analysis

Quantitative estimations based on spectrophotometry, ion-exchange separation, acid-base , complexometric and argentimetric titrations.

Model Experiments

1.Spectrophotometric Estimations:

(a). Estimation of single components: (at least two)
(i). Fe^{III} as $[Fe^{III}(SCN)^{2+}]$ complex
(ii). Mn as MnO_4^-
(iii). Phosphate as phosphomolybdate blue complex
(iv). (Ti^{IV}/V^{v}) as H_2O_2 complex.

(b). Estimation of two components in binary mixtures: (at least one)
(i). Fe^{III} and Fe^{II} in mixture as $[Fe^{II}(1,10\text{-phenanthroline})_3^{2+}]$ complex
(ii). $Cr_2O_7^{2-}$ and MnO_4^- in mixture
(iii). Ti^{IV} and V^{v} in mixture as their H_2O_2 complexes
(iv). Cu^{II} and Zn^{II} as their PAR complexes.

2.Estimations based on ion-exchange separation , acid-base, complexometric and argentimetric titrations.

(a) Estimation of two components in binary mixtures: (at least two)
(i). $Co^{II} + Ni^{II}$
(ii). $Zn^{II} + Cd^{II}$
(iii). $Zn^{II} + Mg^{II}$
(iv). $Cl^- + Br^-$.

(b). Analysis of ternary / quaternary mixtures: (at least one)

(i). $K^+ : H^+ : SO_4^{2-}$ ratio in $KHSO_4$
(ii). H^+, Na^+, Mg^{2+} and Zn^{2+} in mixture
(iii). Al^{3+}, Fe^{3+}, Co^{2+} and Ni^{2+} in mixture.

Examination: Any one experiment or a part of it has to be completed in six (6) hours.

Marks Distribution:

Experiment -20, Viva-voce-05, Lab. Records incli\uding Internal Assessment-05. Total=30.

Paper II: CHEM(G)-12: Organic Chemistry (80 Marks)

Group –A Theoretical (50 Marks)

Unit I :Bonding in Organic Compounds : (18 Marks) [24 lectures]

Qualitative M.O. treatment to acyclic and cyclic conjugated systems. Huckel's theory-application to ethylene, allylsystem, butadiene, cyclopropenylsystem, cyclobutadiene and benzene. Concept of aromaticity in benzenoid, and non benzenoid systems. Alternant and non-alternant hydrocarbons. Aromaticity in annulenes, hetero-annulenes and fullerenes (C_{60}). Examples of anti-aromaticity and homo aromaticity. Graphical method- Frost diagram. Hammett Equation and its modification.

Unit II : Stereochemistry and Conformational Analysis : (16 Marks) [22 lectures]

Acyclic systems upto 4 chiral centres, compounds with asymmetric carbons in the branched chain, symmetry, point groups, Klyne Prelog conformational terminology. Axial chirality, plannar chirality configuration and nomenclature, correlation with centrodisymmetric compounds, conformation of cyclic systems- advanced aspects of cyclohexane system, cyclohexene, cyclohexanone, decalin and hydrindane systems. Different methods for analysis of conformational free energy, Winstein-Holness equation and Curtin-Hammett principle.

Unit III: Heterocyclic Chemistry I : (16 Marks) [22 lectures]

Systematic nomenclature (Hantzch-Widman system) for monocycle and fused heterocycles. General approach to heterocyclic synthesis-cyclisation and cycloaddition routes.

Heterocycles in organic synthesis-masked functionalities, umpolung, Stork annulation reaction. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

Paper-II: CHEM(G)-12: (Group-B)- 30 Marks
Course Duration: 90 Hours

Qualitative Organic Analysis 1

Identification of single solid organic compounds by chemical tests and preparation of a suitable solid derivative after consulting literature.

Tests include-

a) Determination of m.p. of solid sample
b) Detection of special Elements (Nitrogen, Halogens, Sulphur)
c) Solubility in solvents at room temperature and classification
d) Preliminary tests
e) Test for functional group/s [aromatic 1°,2°,3° amino, anilido-, nitro-, amido-, phenolic –OH, carboxylic acid, carbonyl (keto, aldehydo), ester-, unsaturation, hydrocarbon]
f) Literature survey
g) Preparation of at least one solid derivative including recrystallisation.
h) Determination of m.p. of derivative.

At least six unknown samples to be performed during lab session.

Examination: Identification of an organic compound (solid) under the above headlines, submission of recrystallised derivative and reporting the results in six (6) hours.

Marks Distribution:

Experiment -20, Viva-voce-05, Lab. Records including Internal Assessment-05. Total=30.

Paper-III: CHEM (G)-13: Physical Chemistry (90-Marks)
Group-A: Theoretical (50-Marks)

Unit I : Quantum Mechanics : (18 Marks) [24 lectures]

Time independent Schrödinger equation. Properties of the Hermitian operator, canonical commutation relations, Ehrenfest theorem.

Applications: Particle-in-a-box (1-, 2-, 3- dimensional), different potential functions and barrier problems, degeneracy, density of states.

Simple harmonic oscillator: Ladder operator, properties of the eigenfunctions.

Rigid rotor: Angular momentum operator, spherical harmonics.

Hydrogen atom: Details of the solution, shapes of the orbitals.

Unit II : Atomic Spectroscopy : (16 Marks) [22 lectures]

Wilson-Sommerfeld quantization rules and quantum numbers and applications to various problems. Orbital- and spin- angular momentum. Stern-Gerlach experiment. Atomic states. Term symbols. L-S and j-j coupling for one- and two-electron systems.

Zeeman and Paschen-Beck effect.

Unit III : Surface Phenomena : (16 Marks) [22 lectures]

Thermodynamics of surfaces, adsorption phenomena (mono- and multi-layer). Langmuir and B.E.T. isotherms.

Classification and properties of surfactants. Hydrophobic interactions. Micellization.

Thermodynamics of micellization, ‘phase separation’ and ‘mass action’ models. Emulsion and ‘reverse micelles’. Effect of micellization on the rate of chemical reactions.

Characterization of the surface of a solid by different experimental techniques, including spectroscopy. Langmuir-Blodgett films.

Paper-III: CHEM(G)-13: (Group-B) - 40-Marks
Course Duration: 120 Hours

Physical Chemistry Experiments -30 Marks
Course Duration: 90 Hours
Physical Chemistry Experiments
Semester I

Experiments involving (i) analytical procedures related to kinetics and equilibrium (ii) polarimetry (iii) conductometry (iv) potentiometry (v) pH-metry (vi) colorimetry, (vii) surface phenomena (viii) viscosity.

Examination:

In the examination one experiment or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the records including theory, experimental data, data processing and result are to be submitted within six (6) hours.

Marks Distribution:

Experiment-15, Viva-voce-05, Lab.Records-05, Internal Assessment-05, Total = 30.

Computer Applications in Chemistry (CAC-1): 10-Marks
Course Duration: 30 Hours

To be evaluated internally by continuous assessment

Data handling. Number system with different bases – binary, octal, decimal, hexadecimal.

The architecture of the computer and its working.

Introduction to Fortran programming. Application to problems in chemistry.

Semester-II

Paper-IV: CHEM(G)-21: Inorganic Chemistry (80-Marks)
Group-A: Theoretical (50-Marks)

Unit I: Statistical Error, Electrochemical Analyses, Environmental Analyses
(18 Marks) [24 lectures]

Errors in quantitative analyses, types of errors, handling of systematic errors, random errors, random walk phenomenon, Normal and Gaussian distribution and its properties, standard deviation, normal distribution of mean, confidence limits of the mean, propagation of random errors, presentation of results. Method of reporting computed data.

Voltammetry, Cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, elctrogravimetry.

Toxic inorganic substances. Health hazards of SPM [Suspended (inorganic) Particulate Matter], IPM [Inhaleable (inorganic) Particulate Matter]. Methods of determination of SPM (High Volume Sampler) and IPM (Cascade Impactor). Heavy metal toxicities. Mechanism of toxicity. Pesticides, metallo-organic compounds and their toxicity. Application of some analytical methods to determine toxic species.

Unit II: Bioinorganic Chemistry: (16Marks) [22 lectures]

Reversible oxygenation in life process O_2-uptake proteins, myoglobin, hemoglobin, hemeerythrin, hemocyanin and model systems, electron transport proteins, Fe-S proteins, ferridoxin, rubredoxin andmodel systems, respiratory electron transport chains: cytochromes, photosynthetic electron transport chain, chlorophyll, PS-I and PS-II, Biological nitrogen fixation (Nitrogenase) and abiological nitrogen fixation

Metal dependent diseases Wilsons, Alzheimer, vitamin B_{12} and B_{12}-enzyme, Metal complexes in therapeutic use of chelated and non chelated compounds, Chelation therapy

Unit III: Organometallic Chemisty: (16 Marks) [22 lectures]

The 18- electron rule for organometallic compounds of transition metals: Classification based on 18-electron rule: complexes of two, three, four, five six, seven, eight-electron pi-ligands: nomenclature. Exceptions to 18 electron rule: the 16-electron rule. Isolobal and isoelectronic relationship of complexes, Agostic interaction

Metal-carbon-bonded compounds (compounds of the sigma electron ligands), Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and cyclopentadienyl complexes structure and bonding in η^2- ethylene and η^3- allylic compounds with typical examples, structure and bonding of $K[PtC_4H_4Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$, $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$
Elementary idea about homoleptic and non-homoleptic compounds: synthesis, reactivity, oxidative addition and reductive elimination reaction: insertion reactions and elimination; electrophilic and nucleophilic reactions; instability (decomposition pathway) and stabilization. Metallacycles.

Paper-IV : CHEM(G)-21: (Group-B): 30-Marks
Course Duration: 90 Hours

Semi-Micro Qualitative Inorganic Analysis

Semi-Micro Qualitative Inorganic Analysis of Complex Inorganic Mixtures containing not more than six (6) inorganic radicals from the lists ***(a), (b), (c),*** and ***(d),***of which two (2) radicals must be derived from the rare elements ***(d)***, and the mixture should not contain more than one insoluble material from the lists ***(c),*** and ***(d),*** :

(a). Cation Radicals derived from:
Ag, Hg, Pb, Bi, Cd, Cu, As, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, Na, K and NH_4^+ ion.

(b).Anion Radicals:
F^-, Cl^-, Br^-, I^-, BrO_3^-, IO_3^-, SCN^-, S^{2-}, $S_2O_3^{2-}$,SO_3^{2-}, SO_4^{2-}, NO_2^-, NO_3^-, PO_4^{3-}, AsO_3^{3-}, AsO_4^{3-}, BO_3^{3-}, H_3BO_3, SiO^{2-},CrO_4^{2-}, $Cr_2O_7^{2-}$, $[Fe(CN)_6^{4-}]$, $[Fe(CN)_6^{3-}]$.

(c). Insoluble Materials:
$PbSO_4$, $BaSO_4$, $SrSO_4$, $PbCrO_4$, CaF_2, SiO_2 and various silicates, SnO_2, Al_2O_3, Fe_2O_3, Cr_2O_3, AgCl, AgBr, AgI.

(d). Cation radicals, anion radicals and insoluble materials derived from the following rare Elements: V, Mo, W, U, Ti, Zr, Ce, Th and Be.

Experiment-1: Known tests for detection of radicals derived from rare elements.
Experiment-2: Treatment of known insoluble materials.
Experiment-3: Analysis of unknown inorganic mixtures containing six radicals including two radicals derived from the rare elements (at least 4-5 samples)

Examination:

One sample (6 radicals) has to be analyzed by a candidate by semi-micro tests and the records of the analysis shall be submitted in 6 hours time for evaluation.

Marks Distribution:

Experiment-20, Viva-voce-05, Lab Records including Internal Assessment -05. Total =30.

Paper-V: CHEM(G)-22: Organic Chemistry: (80- Marks)
Group-A: Theoretical (50-Marks)

Unit I: Pericyclic Reactions I : (18 Marks) [24 lectures]

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Theory of pericyclic reactions(i) Frontier Molecular Orbital (FMO) approach, (ii) Concept of aromaticity of transition states (Huckel/Mobius systems).

The Woodward-Hoffmann selection rules and general rules. Scope, reactivity and stereochemical features of electrocyclic reactions (4e,6e, neutral systems), cycloaddition reactions thermal and photochemical ([4+2] and [2+2]) systems with special reference to Diels Alder reaction. Sigmatropic rearrangements ([1,3] and [1,5] H shifts, [3,3] rearrangements with special reference to Cope, Claisen and aza-Cope rearrangements.

Unit II : Synthetic Methodology and Polymerisation Reactions
(16 Marks) [22 lectures]

Synthetic methodology : Hydroboration reaction and synthetic application of its applications organobroranes. Reactions of organoboranes, isomerisation of organoboranes, formation of carbon-carbon bonds, formation of aldehydes, ketones, trialkylcarbinols, reactions of alkenylboranes and trialkylalkynyl borates, free-radical reactions of organoborane.

Polimerisation Reactions: monomers, dimmers and oligomers, polymerization by- carbonyl substitution reactions, electrophilic aromatic substitution reactions, S_N2 reactions, nucleophilic attack on isocyanates; polymerizations of alkenes, co-polymerisation, crossed-linked polymers, biodegradable polymers and plastics.

.

Unit III : Natural Products I : 16 Marks (16 Marks) [22 lectures]

Alkaloids : Structural types; structure elucidation, reactions and synthesis of representative examples (nicotine, atropine, coniine and papaverine)

Terpenoids : Isoprene rule, structure elucidation and synthesis of representative examples of acylic, monocylic and bicyclic monoterpens. Structural types; general introduction to sesqui di- and tri- terpenoids.

Paper-V : (Group-B): 30-Marks : Course Duration: 90 Hours

Short Organic Synthesis

1.Oxidation of benzylic carbon by prior protection of $-NH_2$ group in the nucleus followed by deprotection: 4-Aminotoluene ⟶ 4-Aminobenzoic acid

2.Preparation of imide followed by Hofmann degradation:

Phthalic anhydride ⟶ Anthranilic acid

3.Reductive removal of aromatic amino group by prior diazotization followed by Sandmeyer reaction:

Anthranilic acid ⟶ o-Chlorobenzoic acid.

4.Nitration of aromatic ester followed by hydrolysis:

Methylbenzoate ⟶ 3-Nitrobenzoic acid

5.Oxidation of α–hydroxyketone to diketone followed by rearrangement:

Benzoin ⟶ Benzilic acid.

6. 1,4-Dihydropyridine ring generation:

Ethyl acetoacetate ⟶ 2,6-Dimethyl-3,5-dicarbethoxy-1,4-dihydropyridine.

7.Partial reduction of aromatic dinitro compound:

m-Dinitrobenzene ⟶ m-Nitroaniline.

8.Benzoylation of amino group in presence of carboxylic acid group:

Glycine ⟶ Hippuric acid.

9.Reduction of a hydroxycarboxylic acid with HI and red P:

Benzilic acid. ⟶ Diphenylacetic acid.

At least five experiments to be performed in class.

Examination: One experiment or apart of it has to be carried out and the product has to be purified by recrystallisation. The yield of the crude product and m.p. of the recrystallised product are to be noted. Both crude and recrystallised products are to be submitted.

Marks distribution :

Experiment- 20, viva-voce- 05, Internal assessment including Laboratory Records-05.

Paper-VI: CHEM(G)-23: Physical Chemistry: (90-Marks)

Group-A: Theoretical (50-Marks)

Unit I: Statistical Thermodynamics (18 Marks) [24 lectures]

Thermodynamic probability and entropy. Maxwell-Boltzmann statistics. Justification of the laws of thermodynamics.

Translational, rotational, vibrational and electronic partition functions of diatomic molecules. Calculation of the thermodynamic functions including 'chemical potential', equilibrium constants and the 'Saha Ionization' formula. Sackur-Tetrode equation.

Salient features of Bose-Einstein and Fermi-Dirac statistics.

Unit II: Chemical Kinetics: **(16 Marks) [22 lectures]**

Thermal and photochemical reactions. Chain reactions and 'explosion limit'. 'Absolute reaction rate' theory and its comparison with 'collision' theory. Eyring and Arrhenius's equations. Reactions in solutions involving ions: single- and double- sphere Models; primary and secondary kinetic salt effects. Kinetics of surface reactions, heterogeneous catalysis. Electron transfer reactions.

Unit III: Molecular Spectroscopy: (16 Marks) [22 lectures]

Principles: Transition probability, transition moment, selection rules, intensity of spectral lines. Width of spectral lines and its various causes.

Microwave Spectroscopy: Classification of polyatomic molecules according to symmetry types. The non-rigid diatomic rotor. The Stark effect in hetero-nuclear diatomic molecules, determination of dipole moment. Applications of microwave spectroscopy.

Infrared Spectroscopy: Anharmonic oscillator model, Morse potential. Vibration-rotation spectroscopy. P-, Q-, R-branches of the vib-rotor spectrum. Breakdown of the Born-Oppenheimer approximation. Applications of infrared spectroscopy.

Raman Spectroscopy: The 'Raman effect' and its salient experimental features. The classical and quantum explanation of the 'Raman effect'. Interpretation of Raman spectra of diatomic molecules. Applications of Raman spectroscopy.

Semester II

Paper-VI : CHEM(G)-23: Group-B: Practical : 40 Marks
Course Duration: 120 Hours

Physical Chemistry Experiments -30 Marks
Course Duration: 90 Hours

Experiments involving (i) analytical procedures related to kinetics and equilibrium (ii) polarimetry (iii) conductometry (iv) potentiometry (v) pH-metry (vi) colorimetry, (vii) surface phenomena (viii) viscosity, excluding types/experiments performed in previous semester

Examination:

In the examination one experiment or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the records including theory, experimental data, data processing and result are to be submitted within six (6) hours.

Marks Distribution:

Experiment-15, Viva-voce-05, Lab.Records-05, Internal Assessment-05, Total = 30.

Computer Applications in Chemistry (CAC-II): 10-Marks
Course Duration: 30 Hours

To be evaluated internally by continuous assessment

Fortran Programming and application to problems in chemistry

Semester-III

Inorganic Chemistry Special

Paper-VII: CHEM (IS)-31: (85-Marks)

Inorganic Chemistry Special Paper IS-1

Group-A: Theoretical (50-Marks)

Unit I: Group theory and its Applications in Spectroscopy: (18 Marks) [24 Lectures]

The Great Orthogonality Theorem: statement and interpretation, proof of important corollaries; construction of character tables, cyclic groups and construction of their character tables, direct product groups and construction of their character tables, direct product representations. Application of group theoretical methods for (i) selection rules, allowedness/forbiddenness of n-π^* and π-π^* transitions, (ii) splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams, (iii) symmetry aspects of molecular vibrations,justification of Laporte selection rule, vibronic coupling and vibronic polarization of electronically allowed transitions, infrared and Raman activity, selection rules for IR and Raman transition.

Unit II: Advanced Organometallic Chemistry (16 Marks) [22 Lectures]

Stereochemical non rigidity and fluxional behavior of organometallic compounds with typical examples, reactions in fluxional organometallic compounds, catalysis by organometallic compounds Hydrogenation, Wilkinson Catalyst, Tolman Catalytic loop, Syntehses gas-Water gas shift reaction, Hydroformylation (Oxo process), Monsantro Acetic Acid process, Walcker process, Synthetic gasoline – Fischer Tropsch process and mobile process. Polymerization, oligomerization, and metatheses reaction of alkenes and alkynes, Zieggler Natta catalysis, Photodehydrogenation catalyst (Platinum POP)

Unit III: Nuclear Chemistry (16 Marks) [22 Lectures]

Nuclear models: Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism.

Detection and measurement of radiation. Tracer techniques. Study of chemical reactions, isotope exchange reactions, kinetic isotope effect, nuclear activation analyses, charged particle analyses. Principle of nuclear detection, gas detector, ionization chamber, proportional and G. M. detector, dead time of detectors, application of counting statistics in nuclear measurements

Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination,

neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

Paper-VII: CHEM(IS)-31: (Group-B) Practical: 35-Marks
Course Duration 75 Hours

Inorganic Synthesis

Preparation and characterization (by chemical analysis, electronic spectra, conductance and magnetic measurements as applicable) of typical inorganic compounds [at least six (6) compounds derived from at least three (3) different metal ions].

Model Compounds

$[Ni(en)_3]X_2.\ x\ H_2O$ (X = Cl^-, SO_4^{2-}, $S_2O_3^{2-}$)	Mohr's salt
$(Et_4N)_2[NiX_4]$, (X = Cl^-, Br^-)	Ferric alum
	$[Fe(acac)_3]$
$(Et_4N)_2[CuX_4]$, (X = Cl^-, Br^-)	
$[Cu(biguanide)_2]\ SO_4$	
$[Cu(acac)_2]$	Chrome alum
$[Cu(NH_3)_4]\ SO_4.\ H_2O$	$K_3[Cr(C_2O_4)_3].\ 3H_2O\ NO_3.(½)\ H_2O$
	$[Cr(acac)_3]$
	cis- $K_2[Cr(C_2O_4)_2(H_2O)_2]$
	$NH_4[Cr(NH_3)_2\ (NCS)_4].\ xH_2O$
$Et_4N)_2[CoX_4]$, (X = Cl^-, Br^-, I^-)	*(Reineke's salt)*
$Na_3[Co(NO_2)_6]$	
$[Co(NH_3)_6]\ Cl_3$	
$[Co(NH_3)_5\ H_2O]\ Cl_3$	
$[Co(NH_3)_5\ Cl]\ Cl_2$	$(NH_4)_2\ SO_4\ .\ MnSO_4.\ 6H_2O$
$[Co(NH_3)_5\ (N_3)]\ Cl_2$	$(Et_4N)_2[MnX_4]$, (X = Cl^-, Br^-)
$[Co(en)_2(CO_3)]Cl$	$(NH_4)_2[MnF_5]$
$[Co(en)_2(N_3)_2]\ NO_3$	$[Mn(acac)_3]$
$[Co(acac)_3]$ and its nitro derivative	
$[Co(NH_3)_5(SO_3)]_2\ SO_3.2H_2O$	$(NH_4)_2\ [VO(C_2O_4)_2].\ 2H_2O$
$[Co(NH_3)_4(CO_3)]\ NO_3.\ ½\ H_2O$	

Examination : Preparation and purification of one compound and characterization of a (supplied) compound [by estimation of one component or by physicochemical measurement (s) as applicable] in six (6) hours.

Marks Distribution:

Experiment -20, Viva-voce-05, Lab.Records-05, and Internal Assessment-05. Total =35

Semester-III
Inorganic Chemistry Special
Paper-VIII: CHEM (IS)-32: (85-Marks)
Inorganic Chemistry Special Paper IS-2
Group-A: Theoretical (50-Marks)

Unit I: Chemistry of Elements II- Comparative Account: (18 Marks) [24 Lectures]

Design and synthesis, geometric and electronic structures, stereochemistry and bonding, reactivity and reaction pathways of various coordination compounds of transition and non-transition metal ions with halide, pseudohalide, aquo, hydroxo, oxo, carboxylate, amine, amide, polypyridine, azoimine, phosphine, carbonyl, nitrosyl, dioxolene, azophenol, macro-cycle, Schiff base etc. and their mixed mono-, bi- and polynuclear complexes; a closer look at the applications of coordination molecules in different fields of chemistry and related disciplines

Unit II: Inorganic Rings, Cages and Clusters (16 Marks) [22 Lectures]

Introduction, clusters in elemental states, cluster classification, Low nuclearity ($M_3 – M_4$) and high nuclearity cluster ($M_5 – M_{10}$), Metal metal bonding (MO), Carbonyl clusters, skeletal electron (Elm) counting, Wade-Mingos-Luber rule, application of isolobal and isoelectronic analogy, capping rules, carbide, nitride, chalcogenide and halide containing cluster, important examples like Nb, Ta, Mo, W clusters.

Higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevrel compounds, infinite metal chains, cluster-surface analogy, cluster compounds in catalysis.

Unit III: Inorganic Reaction Mechanism (16 Marks) [22 Lectures]

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, inorganic nucleo-philicity scales; like Edward scale, n_{Pt} scale, Gutmann donor number, Drago E & C scale, trans effect, cis effect, reactions without metal-ligand bond breaking, water exchange rates, proton ambiguity, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand.

Paper-VIII: CHEM(IS)-32: (Group-B) Practical: 35-Marks
Course Duration 75 Hours
Inorganic Chemistry Special

Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and or instrumental methods as applicable.

Model Samples

Ores, Minerals, Concentrates:

Dolomite ($CaCO_3$, $MgCO_3$, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys:

Brass (Cu, Zn); Solder / Type metal (Pb, Sb, Sn); Bronze (Cu, Zn, Sn), Aluminium bronze (Cu, Al, Fe, Mn), AlNiCo (Al, Fe, Ni, Co), Cast iron / Steel (Cr, Mn, Ni, P).

At least one ore/ mineral/ concentrate and one alloy should be analyzed during the lab. session.

Examination:

In the examination, two constituents of a real sample (ore/ mineral/ concentrate/ alloy) has to be quantitatively estimated by a candidate and the result of the analysis has to be submitted for evaluation in six (6) hours. All the candidates of a batch may preferably be assigned with the same sample for convenience.

Marks Distribution:
Experiment -20, Viva-voce-05, Lab.Records-05, and Internal Assessment-05. Total =35

Semester-III
Inorganic Chemistry Special
Paper-IX: CHEM (IS)-33: (80-Marks)
Inorganic Chemistry Special Paper IS-3
Group-A: Theoretical (50-Marks)

Unit I: Spectroscopy 1:NMR, ORD/CD (18 Marks) [24 Lectures]

NMR: ^{1}H, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{19}F and ^{31}P-NMR: instrumentation, chemical shift and application; fluxionality, distortion and dynamic equilibria; long-range spin-spin interaction;Identification of compounds like H_3PO_3, H_3PO_2, HPF_2, P_4S_3 etc. Adduct formation reaction: AsF_3 with SO_3. Exchange reaction – exchange in H_2O, factors affecting line width, evaluation of thermodynamic parameter with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Contact shifts. Factors contributing to the magnitude of chemical shift. Applications involving the magnitude of coupling constant – J_{13C-H}, J_{Pt-P}, J_{P-F} etc. NMR spectra of $B_3H_8^-$, $HP_2O_5^{3-}$, $TiF_4.2B$ (B as donor molecule); consequences of nucleii with quadrupole moment in NMR. Double resonance technique. Introduction to pulse and FT NMR, time domain vs. frequency domain, FID, CW vs. FT NMR, rotating frame of reference, relaxation time measurements instrumentation.

EPR: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions. Applications.

Unit II: Spectroscopy 2 EPR, NQR, Mossbauer (16 Marks) [22 Lectures]

CD/ORD: The symmetry origin of the optical activity of molecules, The phenomena of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD): principle, methodology and applications, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application;

NQR: Basic theory, effect of magnetic field in the spectra, relationship between 'q' and molecular structure. Structural information from NQR spectra, Applications.

Mössbauer:Gamma ray emission and absorption by nuclei, Mossbauer effect — conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, Use of Mössbauer spectra in chemical analysis, typical spectra of iron and tin compounds,

Unit III: Spectroscopy 3 I.R., Raman,Mass, PES, ESCA (16 Marks) [22 Lectures]

I.R., Raman: Origin, absorption of radiation by molecular vibrations in polyatomic molecules, effects giving rise to absorption bands, group vibration, limitation of the concept, FTIR, NDIR techniques. Raman Spectrometry: Theory, instrumentation, mechanism of Raman Effect, effect in solids, liquids and gases, Use of symmetry considerations to determine the number of active infra red and Raman lines, differences of IR and Raman spectra, Laser Raman spectra. Application

EI, CI, FD, FAB-Mass, MALDI-TOF; isotropic effect, fragmentation patterns and application in structure elucidation;

Photoelectron spectroscopy: Photo excitation and photo ionization, core level (XPS, ESCA) and valence level (UPS) Photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differention of same element in different environment from XPS, information about the nature of molecular orbital from UPS of simple diatomic molecule e. g. N_2, O_2, CO, HCl etc.

ESCA: Introduction to Electron Spectroscopy for Chemical Analysis (ESCA), Application to the analysis of inorganic samples.

Paper-IX: CHEM(IS)-33: (Group-B) Practical: 30 -Marks
Course Duration 75 Hours

Spectroscopic Studies on Model Compounds: 30 Marks

UV-VIS spectra should be recorded by the students. IR, NMR, MS spectral data of typical compounds (organic and inorganic) may be supplied and the students may be asked to analyze them.

Model Inorganic Compounds

(i).Recording of electronic spectra (of at least 4 different compounds of at least three different metal ions) in water or in ethanol or in suitable solvents, determination of absorption maxima and molar extinction coefficient values and evaluation of crystal field parameters, conductance and magnetic measurements (as applicable) should be carried out by the students. Some model compounds are listed below:

$CuSO_4.5H_2O$, $[Cu(NH_3)_4]SO_4$, $[Cu(en)_2]SO_4$, $(Et_4N)_2[CoX_4]$ (X = Cl^-,Br^-), $[Cu(acac)_2]$; $VOSO_4$, $[VO(acac)_2]$, $(NH_4)_2[VO(C_2O_4)_2].2H_2O$; $CrCl_3.6H_2O$, $K_3[Cr(C_2O_4)_3].3H_2O$, $[Cr(acac)_3]$, $NH_4[Cr(NH_3)_2(NCS)_4]$. xH_2O; $CoCl_2.6H_2O$, $(Et_4N)_2[CoX_4]$ (X = Cl^-,Br^-, I^-), $[Co(NH_3)_6]Cl_3$, $Co(NH_3)_5Cl]Cl_2$, $[Co(NH_3)_5 H_2O]Cl_3$, $[Co(NH_3)_5(N_3)]Cl_2$, $Na_3[Co(NO_2)_6]$,$[Co(acac)_3]$ and its nitro derivative, $[Co(en)_2(CO_3)]Cl$,

$[Co(NH_3)_4(CO_3)]NO_3.(½)H_2O$, $[Co(NH_3)_5(SO_3)]_2SO_3.2H_2O$, $[Co(en)_2(N_3)]NO_3$; $NiSO_4.7H_2O$, $[Ni(NH_3)_6]Cl_2$, $[Ni(en)_3]X_2$. x H_2O (X = Cl^-, SO_4^{2-}, $S_2O_3^{2-}$),

$(Et_4N)_2[NiX_4]$, (X = Cl^-, Br^-), $(NH_4)_2SO_4$. $MnSO_4$. $6H_2O$, $[Mn(acac)_3]$, $(Et_4N)_2[MnX_4]$, (X = Cl^-, Br^-).

(ii). Analysis of supplied UV-VIS, IR, NMR, MS, EPR spectra (as applicable) of model compounds.

Examination:

Recording of electronic spectrum of one compound (organic / inorganic) and analysis of one supplied spectrum (UV-VIS, IR, NMR, MS of one compound, inorganic / organic) in six (6) hours.

Marks Distribution:

Experiment- 15 Viva-voce-05, Lab. Records-05, Internal Assessment-05. Total = 30.

Semester-III
Organic Chemistry Special
Paper-VII: CHEM (\OS)-31: (85-Marks)
Organic Chemistry Special Paper OS-1
Group-A: Theoretical (50-Marks)

Unit I: Spectroscopy: (18 Marks) [24 Lectures]

Mass spectrometry : Basic instrumentation, ion production - E1, C1, FD, FAB and MALDI techniques. Mass spectral fragmentation of typical organic compounds, common functional groups.

Nuclear Magnetic Resonance (NMR) Spectroscopy : Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'- Karplus equation. Classification of molecules. (AB, ABX, AMX, ABC, A_2B_2 etc. types), spin decoupling. FT-NMR. (qualitative idea) and its advantages.

Unit II:Techniques of Chemical Separation (16 Marks) [22 Lectures]

Principles, classification, experimental set up, special features, mechanism of separation procedures, advantages and disadvantages, and applications (analytical and/or industrial) of the following separation techniques.

i. **Chromatography :** Fundamentals, dynamics, plate theory, resolution of mixtures.

   Absorption chromatography-chemical constitution and chromatographic-behaviour, affinity chromatography and chiral chromatography. Partition chromatography-liquid-liquid and reverse phase partition chromatography, paper chromatography, thin layer chromatography (TLC) and ion pair chromatography.

ii. **Gas chromatography (GC) :** Plate theory, gas-solid and gas-liquid chromatography, HPLC. Super critical fluid chromatography, gel permeation chromatography and molecular sieves. Hyphened technique. GC-MS and its applications.

iii. **Electrochromatographic techniques :** Curtain electro-chromatography, reverse osmosis and electro-dialysis and their applications in desalination of water, separation of biomolecules by electrophoresis, capillary electrophoresis.

iv. **Solvent extraction :** Extraction equilibria, partition coefficient and extraction coefficient, extraction by chelation and solvation; solid-phase extraction (SPE), supramolecular extraction with crown ethers, cryptands and rotaxenes.

Unit III:Green Chemistry and Nanoscience (16 Marks) [22 Lectures]

Green Chemistry : Twelve principles of Green Chemistry, Green synthetic methods, catalytic methods, organic synthesis in aqueous media, Ionic liquid, supercritical fluids and microwave. Solvent-free organic reactions.

Nano Science: The nano world (general definition, philosophy), physico-chemical considerations (band structures typical and useful "nano effects"), use of nano particles in organic synthesis.

Paper-VII: CHEM(OS)-31: (Group-B) Practical: 35-Marks
Course Duration 75 Hours

Organic Synthesis

Synthesis of model organic compounds involving typical multi-step reactions, isolation and purification of the intermediate and final products (as applicable) and their characterisation by recrystallisation, chromatographic separation (as applicable), determination of m.p/b.p (as the case may be), and spectral measurements.

Model Experiments/Reactions/Compounds

1. **Beckmann rearrangement :** Benzanilide from benzene.

   Benzene → Benzophenone → Benzophenone oxime → Benzanilide.

2. Synthesis of Heterocyclic compounds :
   i. **Skraup synthesis :** Quinoline from Aniline
   ii. **Fischer indole synthesis :** 2 Phenylindole from phenyl hydrazine.
3. Preparation involving chlorosulphonation
4. Preparation involving Friedel-Crafts reaction
5. Preparation involving diazo-coupling reaction
6. Preparation involving Reimer-Tiemann reaction
7. Coumarin ring synthesis
8. Preparation of indane- 1,3-dione.

At least four experiments to be carried out during lab. session.

Examination : One experiment or a part of it has to be carried out and the product has to be purified by recrystallisation. The yield of the crude product and the m.p. of the recrystallised product are to be noted. Both crude and recrystallised products are to be submitted.

Marks distribution : Experiment 20, viva-voce-05, Lab. record-05, internal assessment-05.

Semester-III
Organic Chemistry Special
Paper-VIII: CHEM (\OS)-32: (85-Marks)
Organic Chemistry Special Paper OS-2
Group-A: Theoretical (50-Marks)

Unit I:Organometallic Chemistry of Transitional Elements (18 Marks) [24 Lectures]

Preparative structural and characteristic aspects. Bonding of hydrocarbon ligands, metallocenes, oxidative insertion, reductive elimination, ligand migration from metal to carbon; organometallics as electrophiles. Davies rules, catalytic nucleophilic addition and substitution, coupling reactions, Heck, Suzuki and Stille reactions, hydrogenetion hydroformylation, carbonylation of methanol, oxidations, alkene polymerisation, Ziegler-Natta reaction, olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, Volhardt co-trimerisation. Fluctional organometallic compounds.

Chemistry and use of organo-derivatives of non-transitional metals- tin, thalium, mercury, lead.

Unit II: Synthetic Methodology II (16 Marks) [22 Lectures]

Organophosphorus compounds-Chemistry of organophosphorus compounds, phosphorus ylids and chiral phosphines.

Organosulphur compounds-Chemistry of organo sulphur compounds, sulphur stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylids, chiral sulphoxide.
Organosilicon compounds - Synthetic uses of silyl ethers, silylenol ethers, TMSCl, TMSI, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acylsilanes; Brook rearrangement, silicon Baeyer Villiger rearrangement.

Unit III: Advanced Pericyclic Reactions (16 Marks) [22 Lectures]

General perturbation molecular orbital theory in cycloadditions :

Reactivity, regioselectivity and periselectivity.

Cheletropic reactions, 1,3-dipolar cycloadditions, cycloaddition involving more than 6 electrons, charged species, three-component and four component cycloadditions.

Ene reactions, group-transfer reactions and eliminations.

Electrocyclic reactions of charged systems (cations and anions)

Sigmatropic rearrangements : [1,j] shifts-[1,5] and [1,7] carbon shifts in neutral systems and [1,4] shifts in charged species : [i,j] shifts- [3,3] shifts, fluctional molecules; [5,5] shifts, [2,3] shifts in ylids.

Paper-VIII: CHEM(OS)-32: (Group-B) Practical: 35-Marks
Course Duration 75 Hours

Qualitative Organic Analysis 2

Identification of single liquid organic compound by physical and chemical tests and preparation of at least one suitable solid derivative after consulting literature.

Functional groups include : amino-(1°,2°,3°), anilido-, nitro-, cyano-, alkcoholic –OH, phenolic –OH, enols, carbonyl (aldehydo-, keto-) carboxylic acids, esters, unsaturation and hydrocarbons.

At least five unknown samples to be performed during lab session.

Examination: Identification of a liquid organic sample under the above headlines, submission of recrystallised derivative and reporting the results in 6(six) hours time.

Marks distribution : Experiment-20, viva-voce-05, Laboratory record-05 internal assessment-05. = Total 35

Semester-III
Organic Chemistry Special
Paper-IX: CHEM (\OS)-33: (85-Marks)
Organic Chemistry Special Paper OS-3
Group-A: Theoretical (50-Marks)

Unit I: Bioorganic Chemistry (18 Marks) [24 Lectures]

The molecules of life

Nucleic acids, purine and pyrimidine bases, nucleosides, and nucleotides. Genetic code of life, replication, transcription and translation of DNA, genetic information transfer and heredity. Types of sugars, deoxy sugars, amino sugars and polysaccharides.

Enzymes :

Catalytic power of enzymes, specificity and regulation. Nomenclature and classification, extraction (large scale production) and purification of enzymes. Immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Mechanism in biological chemistry :

i. Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxy-peptidase-A.

ii. Enzyme catalyzed reactions- Examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergenic processes, proton transfer reactions to and from carbon.

iii. Mechanism of reactions catalyzed by cofactors including coenzyme-A, NAD^+, NADH, FAD and thiamin phosphate.

iv. Chemical synthesis of peptides and proteins. Use of enzymes in organic synthesis.

v. Structural analysis of proteins. Protein folding.

Coenzymes and cofactors : Vitamins, prosthetic groups epoenzymes, structures and biological functions of coenzyme-A, thiamine pyrophosphate, pyrodoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, coenzyme Q, lipoic acid, vitamin -B_{12}.

Unit II: Supramolecular Chemistry (16 Marks) [22 Lectures]

From molecular to supramolecular chemistry : Factors leading to strong binding (non-covalent interactions). New molecular receptors: crown ethers, cryptands, cyclophanes, siderophores, cyclodextrin, and their application in specific recognition processes. Supramolecular reactivity and catalysis, switching devices. Self-assembly of supramolecular aggregates, principles of gene synthesis, catalytic antibodies, molecular channels, transport

processes and carrier design. Supramolecular devices and nanotechnology. Supramolecular photochemistry.

Unit III: Chemistry of Natural Products II (Terpenoids & Carotenoids, Alkaloids, Coumarins and Flavonoids, Steroids, Porphyrins, Prostaglandins) :

(16 Marks) [22 Lectures]

Stereochemistry, reaction and synthesis of terpenoids and carotenoids : zingiberine, santonin, abietic acid, β-carotene.

Stereochemistry, reactions and synthesis of alkaloids; quinine, morphine, camptothecin.

Structure,synthesis and reacations of flavonoids and coumarins.

Reaction and synthesis of steroids **:** cholesterol, bile acid, testosterone, estrone, progesterone.

Structure and synthesis of porphyrins **:** haemoglobin, chlorophyll.

Structure and synthesis of prostaglandins : PGE_2, $PGF_{2\alpha}$.

Paper-IX: CHEM(OS)-33: (Group-B) Practical: 30-Marks
Course Duration 70 Hours

Chromatographic separation techniques and spectroscopic studies of Model compounds

A: Chromatographic separation techniques: Thin layer chromatography, paper chromatography, column chromatography separation of binary mixture of organic compounds and choice of iluents.

B: Recording of electronic spectra of different types of compounds in water, in ethanol or in other suitable solvents, Determination of absorption maxima and molar extinction coefficient values.

Model organic compounds : Aniline, vanillin, p-Nitrophenol, p-Nitroaniline, mesityl oxide, benzoic acid, cinnamic acid, acidic and basic solutions of methyl red, methyl orange and phenolphthalein.

UV-vis spectra of at least 4 different types of compounds are to be recorded during the laboratory session.

Examination: Any one experiment from A or B is to be set during examination.

Marks distribution : Experiment 15, viva-voce-05, lab. record-05, internal assessment 05= 30

Semester-III
Physical Chemistry Special
Paper-VII: CHEM (\PS)-31: (85-Marks)
Physical Chemistry Special Paper PS-1
Group-A: Theoretical (50-Marks)

Unit I: Equilibrium Statistical Mechanics and Non-equilibrium Thermodynamics (18 Marks) [24 Lectures]

(i) *Elements of classical mechanics*: equation of motion in Newton, Lagrange and Hamilton forms. Poisson bracket notation. Limitations of the Maxwell-Boltzmann procedure.

Gibb's procedure: concept of ensembles – micro-canonical, canonical and grand-canonical. Liouville equation and theorem. Classical Statistical Mechanics (CSM): Partition functions and thermodynamic functions. Fluctuations. Calculation of thermodynamic functions using the three different ensembles.

Inadequacy of CSM. Conditions of validity of CSM.

(ii) *Non-equilibrium thermodynamics*: thermodynamic fluctuations around equilibrium. Entropy production, energy flux, thermodynamic force. Phenomenological laws and Onsager 'reciprocity relations'. Applications.

Unit II:Advanced Quantum Mechanics-I (16 Marks) [22 Lectures]

N-dimensional vector space, matrix representation of operators, projection operators, hermitian operators. Heisenberg's uncertainty principle (operator method), Heisenberg's equation of motion, constant of motion. Virial theorem, parity and time-reversal symmetry. Angular momentum operator (in polar coordinates), commutation relation, step-up and step-down operator.

Many-electron Hamiltonian, its commutation with L^2 and L_z operators. Spin operators and Pauli spin matrices. Many electron atom and construction of wave function representing a spectroscopic state.

Unit III Mathematical Methods in Chemistry (16 Marks) [22 Lectures]

Solution of differential equations. Series solutions – Hermite, Legendre. Properties of special functions – gamma, delta functions. Matrices and determinants. Vector calculus. Coordinate transformations. Legendre and Laplace transformations. Fourier analysis.

Semester III
Physical Chemistry Experiments
Paper-VII: CHEM(PS)-31: (Group-B) Practical: 35-Marks
Course Duration: 90 Hours

Experiments involving (i) analytical procedures related to kinetics and equilibrium (ii) polarimetry (iii) conductometry (iv) potentiometry (v) pH-metry (vi) colorimetry, (vii) surface phenomena (viii) viscosity, excluding types/experiments performed in previous semester

Examination:

In the examination one experiment or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the records including theory, experimental data, data processing and result are to be submitted within six (6) hours.

Marks Distribution:

Experiment-20, Viva-voce-05, Lab.Records-05, Internal Assessment-05, Total = 35.

Semester-III
Physical Chemistry Special
Paper-VIII: CHEM (\PS)-32: (85-Marks)
Physical Chemistry Special Paper PS-2
Group-A: Theoretical (50-Marks)

Unit I: Advanced Quantum Mechanics-II (18 Marks) [24 Lectures]

Time-independent Perturbation Theory: Rayleigh-Schrodinger perturbation theory for non-degenerate states. Brillouin-Wigner perturbation theory. Applications – expression for polarizability, energy of the ground state of the helium atom.

Degenerate perturbation theory: Stark effect, lifting of degeneracy in a magnetic field – the $^1P_1$ state of the helium atom.

Unit II: Photochemistry-I (16 Marks) [22 Lectures]

Electronic spectroscopy: Singlet and triplet states. Transition between states, selection rules. The Franck-Condon principle. The vibrational structure of electronic spectra – absorption and emission. The different types of electronic transitions (i) π-π^*, n-π^* (e.g. in HCHO): their characteristic features and effect of the surrounding medium (solvent and H^+) (ii) Charge transfer spectra including MLCT and LMCT.

Fluorescence and phosphorescence spectra – their characteristic features: quantum yield, lifetime, quenching and heavy-atom effect.

Unit III:Polymers (16 Marks) [22 Lectures]

Definition and classification of polymers, including tacticity. Polymerization reactions – initiation, propagation, termination steps; inhibition, chain transfer and co-polymerization. Kinetics and mechanisms of addition and condensation polymerization, including the effect of catalysts.

Crystallinity and glass temperature. Different types of polymers – electrically conducting, fire resistant, medical prosthesis, biodegradable etc. Degradation of polymers – the possible pathways and effect on the environment.

Molar mass of polymers – definitions, and the different experimental techniques of determination. Thermodynamics of polymer solution. Polymer conformations.

Semester III
Physical Chemistry Experiments
Paper-VIII: CHEM(PS)-32: (Group-B) Practical: 35-Marks
Course Duration: 90 Hours

Experiments involving (i) analytical procedures related to kinetics and equilibrium (ii) polarimetry (iii) conductometry (iv) potentiometry (v) pH-metry (vi) colorimetry, (vii) surface phenomena (viii) viscosity, excluding types/experiments performed in previous semester

Examination:

In the examination one experiment or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the records including theory, experimental data, data processing and result are to be submitted within six (6) hours.

Marks Distribution:

Experiment-20, Viva-voce-05, Lab.Records-05, Internal Assessment-05, Total = 35.

Semester-III
Physical Chemistry Special
Paper-IX: CHEM (PS)-33: (80-Marks)
Group-A: Theoretical (50-Marks)

Unit I: Advanced Quantum Mechanics-III (18 Marks) [24 Lectures]

The Variation Method: Molecular systems: Rayleigh-Ritz variation principle and some simple applications. Linear Variation Theory, its characteristic features. Overview of the Born-Oppenheimer approximation. Characteristics of many-electron systems, role of electron spin. The 'independent particle model' (IPM) and its limitations. Huckel, Hartree and Hartree-Fock methods. Electron correlation.

Unit II :Group Theory – I (16 Marks) [22 Lectures]

Groups, sub-groups, classes and characters, classes of symmetry operations, symmetry point groups, matrix representation. Representation of symmetry operator – transformation of basis vector, symmetry transformation of operators, reducible and irreducible representations. The Great Orthogonality Theorem (GOT) and its consequences; construction and application of character tables, representation of cyclic groups. Use of group theory in quantum mechanics: direct product, 'projection operator', 'symmetry adapted linear combination' (SALC). Applications: Huckel theory of pi-electrons - butadiene and benzene as examples.

Unit III : Electrochemistry (16 Marks) [22 Lectures]

The Debye-Huckel theory of ionic activity coefficient, derivation of the 'limiting law', extended forms of the law. The Debye-Huckel-Onsager (DHO) theory of electrolytic conduction. 'Electrophoretic' and 'relaxation' effects. Wien and Debye-Falkenhagen effects. Applications of the DHO theory.

Structure of electrified interfaces, electrical double layers and 'zeta potential'.

Rate equation for electrode processes, kinetic derivation of the Nernst equation. Overvoltage. Butler-Volmer equation, Tafel equation, exchange current density.

Semester III
Physical Chemistry Experiments
Paper-IX: CHEM(PS)-33: (Group-B) Practical: 30-Marks
Computer Application in Chemistry (CAC-III)
Course Duration: 90 Hours

Matrix Manipulation and Diagonalisation of matrices

Solution of Problems Related to Huckel Theory for Conjugated Pi-electron Systems

Examination:

In the examination one problem or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the relevant records of the same are to be submitted within six (6) hours.

Marks Distribution:

Programming-15, Viva-voce-05, Lab.Records-05, Internal Assessment-05, Total = 30.

Semester-IV

Inorganic Chemistry Special
Paper-X: CHEM (IS)-41: (75-Marks)
Inorganic Chemistry Special Paper IS-4
Group-A: Theoretical (50-Marks)

Unit I: Group theory and its Applications in Bonding: (18 Marks) [24 Lectures]

Application of group theoretical methods for (i) construction of SALC's and their use in calculation of π MO's under the Huckel approximations, (ii) calculation of MO's of ABn type and sandwitch type molecules, (iii) study of hybridization. (iv) Conservation of orbital symmetry in pericyclic reactions,

Splitting of orbitals and free ion terms in weak crystal fields, symmetry and multiplicities of energy levels in strong crystal fields, correlation diagrams.

Effect of lowering of symmetry on the orbitals and energy levels, correlation table

Unit II: Advanced Bioinorganic Chemistry (16 Marks) [22 Lectures]

Bioenergetic principle and role of ATP, chemistry of respiration, DNA polymerization, metal ion interaction with nucleoside and nucleotide, metal ion transport and storage proteins, ferritin, transferrin, ceruloplasmin. Metal ion transport across biological membrane, enzymatic and ionophoric transport. Study of metalloprotein and metalloenzyme: catalase, peroxidase, superoxide dismutase, ceruloplasmin, cytochrome oxidases, Ascorbate oxidase, Role of metal ions in different hydrolytic enzymes: Carbonic anhydrase, Carboxypeptidase, Urease, Toxic effects of metals and non metals. Specific examples of Pb, As, Hg, F,

Unit III: Structure and Properties of Solids (16 Marks) [22 Lectures]

Defects in solids, point, line and plane defects. Determination of equilibrium concentration of Schotky and Frenkel defects. Stoichiometric imbalance in crystals and non stoichiometric phases, color center in ionic crystals, band theory, band gap, metals and insulators, semiconductors, hoping semiconductors rectifiers and transistors, Bonding in metals; free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, superconductors; meissner effect, elementary concepts of BCS theory, ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals, cooperative magnetism, Illustrative examples of ionic, covalent and hydrogen bonded solids; perovskite, ilmenite and rutile; spinel and inverse spinel, silicates: pyroxene, amphibole, talc, mica, clay, zeolite, ultramarine;

Semester-IV

Paper-X: CHEM(IS)-41: (Group-B) Practical: 25-Marks
Course Duration 75 Hours
Inorganic Chemistry Special

Advanced Physicochemical Experiments

Model Experiments

(a). Equilibrium studies on inorganic reactions:

1. Determination of composition of complexes formed in solution by spectrophotometric methods:

(a). Mole-ratio method

(b). Slope- ratio method

(c). Job's method of continuous variation

Model systems:

(i). Fe^{III}-sulfosalicylic acid complex

(ii). Fe^{II}- (1, 10- phenanthroline) complex

(iii). Cu^{II}- ethylenediamine complex

(iv). Zn^{II}-alizarin-S complex

2. Determination of stability constants of metal-ligand complexes by spectrophotometric method:

Model systems:

(i). Fe^{III}-sulfosalicylic acid complex

(ii). Fe^{II}-(1, 10-phenanthroline) complex

(ii). Charge transfer complex

3. Determination of stability constants of metal-ligand complexes by pH-metric methods:

Model systems:

(i). Cu^{II}- glycinate complexes

(ii). Cu^{II}-sulfosalicylate

(b). Kinetic studies on inorganic reactions:

4. Kinetic study on consecutive reactions:

Model system:

Determination of the rates of consecutive aquation of the complex, $H[Co^{III}(DMGH)_2Cl_2]$, by conductance method (where, DMGH = dimethylglyoximate monoanion).

5. Kinetics studies on redox reactions:

Model system:

Determination of the rate constants of reduction of the complex, $[Co(NH_3)_5 (N_3)]Cl_2$, by aqueous Fe^{2+} ions by spectrophotometric method.

6. Kinetics studies on linkage isomerism:

Model system:

Kinetic investigation of transformation of the complex, $[Co(NH_3)_5 (ONO)]Cl_2$ to $[Co(NH_3)_5 (NO_2)]Cl_2$ by spectrophotometric method.

7. Kinetics studies on substitution reactions:

Model system:

Kinetic investigation of the substitution reaction $[Co(NH_3)_5 (SO_3)^+] + NO_2^- \rightarrow$ by spectrophotometric method.

8. Kinetics studies on protolysis reaction:

Model system:

Kinetic investigation on protolysis of the complex, $[Co(NH_3)_5 (CO_3)^+]$ ion by spectrophotometric method.

Examination:

In the examination one experiment or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the records - including theory, experimental data, data processing and result are to be submitted within six (6) hours.

Marks Distribution:

Experiment-15, Lab. Records-05, Internal Assessment-05. Total = 25.

Semester-IV

Inorganic Chemistry Special
Paper-XI: CHEM (IS)-42: (75-Marks)
Inorganic Chemistry Special Paper IS-5
Group-A: Theoretical (50-Marks)

Unit I: Synthetic Methodology for Transition and Non-transition Metal Compounds: (18 Marks) [24 Lectures]

Ligand design and ligand synthesis: polypyridine, Schiff base, oxime, macrocycle, tripod, podand, coronand, cryptand, octopus, tailoring and appending of pendant arm, electron reservoir, ligand topology and molecular mechanics, coordination compound design and synthesis: self-assembly, structure-directed synthesis, building block, metalloligand, polymeric ensembles (chain, sheet, network), supramolecular framework, molecular machine, biomodelling, molecular/crystal engineering

Unit II: Magnetochemistry (16 Marks) [22 Lectures]

Different magnetic materials, experimental arrangement for determination of magnetic susceptibility: Gouy method, Faraday methiod, Vibrating sample magnetometer, SQUID, NMR method, anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic systems, Pascal's constants , use of Pascal's constants in structure determination, two sources of paramagnetism, spin and orbital effect, spin orbit coupling, Lande interval rule, energies of J level, Curie equation, Curie law and Curie-Weiss law,

First order and second order Zeeman effect, temperature independent paramagnetism, van Vleck equation and its applications, quenching of orbital contribution, magnetic properties of transition metal complexs in cubic and axially symmetric crystal field, high spin/low spin equilibrium, magnetic behavior of lanthanides and actinides, magnetic exchange interaction and magnetic materials.

Unit III: Complex Equilibria (16 Marks) [22 Lectures]

Different pH-potentiometric, spectrophotometric, voltammetric) tools and methods (slope-ratio, mole-ratio and Job's method of continuous variation) of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes, equilibria in biomolecular systems.

Paper-XI: CHEM(IS)-42: (Group-B) Practical: 25-Marks

Grand Viva-voce

Grand Viva-voce examination shall be conducted jointly by the external and internal Examiners. Short questions on the theoretical principles, experimental methodologies and instrumentations etc. of the different experiments included in the entire practical syllabus of semesters-I, -II, -III and -IV may be asked, Maximum time for viva-voce examination of a candidate shall not normally exceed 20 minutes.

Semester-IV

Inorganic Chemistry Special
Paper-XII: CHEM (IS)-43: (100-Marks)
Inorganic Chemistry Special Paper IS-6
Group-A: Theoretical (50-Marks)

Unit I: Analytical techniques: Isolation, Characterization and Structure Detremination (18 Marks) [24 Lectures]

Classification of chromatographic separation, distribution of analyte between phases, adsorption and partition chromatography, Basics of liquid chromatography, reverse and normal phase, gradient elution, solvent selection, and classes, Ion exchange and Ion chromatography, HPLC: basic concept, different detector system and simple application, GC, GL and GS chromatography: basic principle, different detectors and applications.

Kinetics of solid state reaction by DTA, DSC and TGA methods.

Crystal forms, lattice, primitive cell, crystal system and symmetry, non primitive lattices, crystal classes, space groups, crystals and their properties,

Principle of electron, neutron and X-ray diffraction methods in determining the structure of molecules. Lattice planes, indices, Braggs condition, reciprocal lattice, Braggs law in reciprocal space.

Unit II: Supramolecular Chemsirty (16 Marks) [22 Lectures]

Concept and language, designing of building blocks, molecular valences, supramolecular orbitals, supramolecular arrays: ribbon, ladder, rack, braded, grid; harnessing non-covalent forces to design functional materials

Definition, building block and spacer, molecular valency, supramolecular orbitals, non-covalent forces: pallet of hydrogen bondings, pi-pi and C-H…pi interactions, geometry setter, allosterism, proton and hydride sponges, principle of three C's, lock and key principle, host-guest interaction, self organization and self complementarity, receptors, superstructures in inorganic, metallo-organic, organometallic compounds, supramolecular devices, dendrimers.

Unit III: Chemistry of Elements III (16 Marks) [22 Lectures]

Dinitrogen and dioxygen complexes, Iso- and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures , uses, Bonding in dirhenium complexes.

Mixed valence compounds of Fe, Cu, Pt; Fe-S compounds, cobaloxime related compounds, conformational changes and thermochromism of Ni(II) compounds, Ru(II) and Ru(III) compounds, oxo compounds of Ru and Os, Rh(I) and Ir(I) carbonyl halide and carbonylhydrides.

Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo-blue, W-blue, Pt-blue, W-bronze, Ru-red.

Paper-XII: CHEM(IS)-43: (Group-B) Practical: 50-Marks

Course Duration: 100 Hours

Inorganic Special

Project Work & Seminar-

Project work:

During Semester-IV, each candidate shall carry out some investigative work independently or under the supervision of one or more guides(s), who may be Teacher / Guest Teacher / Member of P.G Board of Studies of the College / University / Scientist of any Recognized Research Institute. The work may be carried out either in the College / University itself or in any Recognized Research Institute, with the approval of the appropriate authority of the College/ University. Duration of the work shall be four weeks (approximately 90-100 hours). The findings of the project work should be submitted in the form of a dissertation for evaluation by a Board of Examiners.

Seminar:

Each candidate shall present his /her project work in a departmental seminar during a period not exceeding 20 minutes. Performance of the candidates in the seminar shall be evaluated jointly by External and Internal Examiners (including the guide).

Marks Distribution:

Project Dissertation-30 Project Seminar 20 Total = 50..

Semester-IV

Organic Chemistry Special
Paper-X: CHEM (OS)-41: (75-Marks)
Organic Chemistry Special Paper OS-4
Group-A: Theoretical (50-Marks)

Unit I: Photo Organic Chemistry and Free Radical Reactions (18 Marks) [24 Lectures]

Photo Organic Chemistry

Basic principles, Jablonsky diagram, exciplex, photochemistry of alkenes-intramolecular reactions of olefinic bond- geometrical isomerism, cyclization reactions, rearrangements of 1,4 and 1,5 dienes. Photochemistry of carbonyl compounds intramolecular reactions of saturated-, cyclic- and acyclic-, α,β-unsaturated- and β,γ-unsaturated carbonyl compounds, cyclohexadienones. Intramolecular cycloaddition reaction-dimerization and oxetane formation. Norrish type I and type II reactions, di-pi-methane rearrangements.

Photochemistry of aromatic compounds : isomerisation, addition and substitution reactions. Miscellaneous photochemical reactions. Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction.

Free Radical Reactions:

a) Methods of generation and detection of free radicals (trapping, ESR, NMR- CIDNP).

b) Reactivity pattern of radicals, substitution and addition reactions, neighbouring group assistance. Reactivity of typical aromatic and aliphatic substractes at a bridge head, the effect of solvent on reactivity, oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes. Radical rearrangement.

c) Radical cations and radical anions, single electron transfer reactions, SRN1 reactions.

Unit II: Advance Spectroscopy (16 Marks) [22 Lectures]

Nuclear Magnetic Resonance (NMR) spectroscopy : Chemical shift values and correlation of protons bonded to carbon atom in aliphatic, olefinic, aromatic compounds, alcohols, aldehydes, phenols, enols, carboxylic acids, amines, amides and mercaptans; chemical exchange: effect of deutaration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique (FT-NMR), nuclear overhauser effect (NOE), ^{19}F and ^{31}P NMR (examples).

Carbon-13 NMR spectroscopy : Chemical shifts(additive shift parameters in alkanes, alkenes, cyclohexane and its derivatives,benzenoid systems) for aliphatic alkenes, alkyne, aromatics, hetero- aromatics and carbonyl carbon atoms, coupling constants. Two dimensional NMR spectroscopy-COSY (1H-1H correlation), NOESY, DEPT, INEPT, APT, HMQC (heteronuclear multi-quantum coherence, 1-bond ^{1}H-^{13}C correlation) HMBC and INADEQAUATE technhiques. Pulse sequences of various 2D NMR spectroscopic techniques.

Unit III: Advanced Stereochemistry **(16 Marks) [22 Lectures]**

A. Stereochemistry of polycyclic system :

a) Conformation and reactivity of fused polycyclic systems- perhydrophenanthrenes, perhydroanthracene, steroids.

b) Dynamic Aspects **:** Cyclisation reactions, Baldwin Rule; elimination, addition and rearrangement reactions.

B. Chiroptic properties:

a) Optical activity **:** Principles, emperical rules and correlations, calculation of optical rotation.

b) Optical rotatory dispersion (ORD) **:** Principles, cotton effects, empirical rules- axial haloketone rule, octane rule, Lowe's rule, Determination of configuration and conformation.

c) Circular dichorism (CD) **:** Principle, applications- determination of configuration, the exeiton chirality method; study of conformational changes, secondary structure of proteins

Semester-IV
Paper-X: CHEM(OS)-41: (Group-B) Practical: 25-Marks
Course Duration 75 Hours
Organic Chemistry Special

Separation, purification and identification of organic compounds in binary mixture (two solids) using chemical tests and TLC

At least 4 samples are to be worked up during the lab session.

Examination:

Any one sample to be worked up during examination. of 6 hrs.

Marks distribution : Experiment 15, lab. records-05, internal assessment 05.

Semester-IV

Organic Chemistry Special

Paper-XI: CHEM (OS)-42: (75-Marks)

Organic Chemistry Special Paper OS-5

Group-A: Theoretical (50-Marks)

Unit I: Advance Organic Synthesis : (18 Marks) [24 Lectures]

Disconnection approach : Synthones and synthetic equivalents, functional group interconversions and order of events in organic synthesis. One group - C-X and two groups C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis. principles of protection of alcohol, amine, carbonyl and carboxyl groups.

One group C–C and two group C–C disconnections (typical examples), use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reactions, 1,3- and 1,5- di-functionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensation, Michael addition and Robinson annealation. Ring synthesis: saturated heterocycles synthesis of 3-, 4-, 5-, and 6-membered rings, aromatic heterocycles in organic synthesis.

Unit II: Oxidation And Reduction of Functional Groups: (16 Marks) [22 Lectures]

Oxidation reactions : Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Woodward and Prevost Reaction, synthetic reactions of epoxides, diastereo-selective epoxidation of homoallylic alcohols, photosensetised oxidation of alkenes, oxidation of ketones to αβ-unsaturated ketones. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium (III) nitrate.

Reduction reactions : Catalytic hydrogenation-the catalyst, selectivity of reduction, reduction of functional groups,stereochemistry and mechanism, homogeneous hydrogenation.

Reduction by dissolving metals-reduction with metal and acid, reduction of carbonyl compounds, Birch Reduction.

Reduction by hydride transfer reagents-aluminium alkoxides, LAH and $NaBH_4$, lithiumhydridoalkoxyaluminates, lithiumaluminiumhydride-aluminiumchloride reagents, di-isobutylaluminiumhydride, sodiumcyanoborodydride, trialkylborohydrides.

Other methods-desulphurisation of thio-acetals, di-imides, low-valent titanium species, trialkyltinhydrides.

Unit III: Dynamic Aspects of Stereochemistry : (16 Marks) [22 Lectures]

Stereoselective and stereospecific synthesis, enantio- and diastereo-selective synthesis; n-facial selectivity, Cieplak model, carbohydrates as chiral pool material.

Diastereoselective reactions **:** Addition to prochiral and chiral carbonyl compounds, reactions of chiral enolates; α-substitution of prochiral ketones (RAMP/SAMP and related methodologies); aldol reactions, addition to C=C bonds, conjugated addition.

Enantioselective reactions : Chiral catalysis sharpless epoxidation and dihydroxylation; asymmetric cyclopropanation; asymmetric hydrogenation, CBS reduction; baker's yeast mediated reduction; enzyme mediated hydrolysis and esterification of meso compounds. Enantioselective synthesis.

Paper-XI: CHEM(OS)-42: (Group-B) Practical: 25-Marks

Grand Viva-voce

Grand Viva-voce examination shall be conducted jointly by the external and internal Examiners. Short questions on the theoretical principles, experimental methodologies and instrumentations etc. of the different experiments included in the entire practical syllabus of semesters-I, -II, -III and -IV may be asked, Maximum time for viva-voce examination of a candidate shall not normally exceed 20 minutes.

Semester-IV

Organic Chemistry Special
Paper-XII: CHEM (OS)-43: (100-Marks)
Organic Chemistry Special Paper OS-6
Group-A: Theoretical (50-Marks)

Unit I: Heterocyclic Chemistry II : (18 Marks) [24 Lectures]

Fused systems **:** nomenclature.

Synthesis and reactions of

(i) Azoles : pyrazole, imidazole, oxazole and thiazole.

(ii) Diazine **:** pyridazine, pyrimidine and pyrazine

(iii) purine, pteridine and folic acid.

ANRORC and Vicarious nucleophilic substitutions in heterocycles.

Unit II: Chemistry of Natural Products III (Biogenesis and Biosynthesis) : (16 Marks) [22 Lectures]

Introduction : Primary and secondary metabolites, biogenetic hypothesis, elucidation of biosynthetic pathways.

Biosynthesis of terpenoids and steroids.

Shikimic acid pathway : Biosynthesis of flavonoids and coumarins.

Biosynthesis of alkaloids.

Biosynthesis of fatty acids and prostaglandins.

Unit III: Medicinal Chemistry : (16 Marks) [22 Lectures]

Different types of drugs. Drug-receptor interactions, mechanisms of drug action. Drug designing and synthesis. Structure-Activity Relationship (SAR) and Quantitative Structure Activity Relationship (QSAR) with special reference to antimalarials, antibiotics, anticholenergics and CNS active drugs. Concepts of LD_{50} and ED_{50}. Antibiotics: penicillins, cephalosporins, tetracyclines, newer generation of antibiotics. Vitamins: vitamin-Bcomplex, vitamin C, vitamin K, Cardiovascular drugs, local anti-ionfective drugs.

Paper-XII: CHEM(OS)-43: (Group-B) Practical: 50-Marks

Course Duration: 100 Hours

Organic Special

Project Work & Seminar-

Project work:

During Semester-IV, each candidate shall carry out some investigative work independently or under the supervision of one or more guides(s), who may be Teacher / Guest Teacher / Member of P.G Board of Studies of the College / University / Scientist of any Recognized Research Institute. The work may be carried out either in the College / University itself or in any Recognized Research Institute, with the approval of the appropriate authority of the College/ University. Duration of the work shall be four weeks (approximately 90-100 hours). The findings of the project work should be submitted in the form of a dissertation for evaluation by a Board of Examiners.

Seminar:

Each candidate shall present his /her project work in a departmental seminar during a period not exceeding 20 minutes. Performance of the candidates in the seminar shall be evaluated jointly by External and Internal Examiners (including the guide).

Marks Distribution:

Project Dissertation-30 Project Seminar 20 Total = 50..

Semester-IV

Physical Chemistry Special
Paper-X: CHEM (PS)-41: (75-Marks)
Physical Chemistry Special Paper PS-4

Unit I: Quantum Statistics: (18 Marks) [24 Lectures]

Symmetry properties of wave functions for many-particle systems.

Bose-Einstein (BE) and Fermi-Dirac (FD) distribution, including their derivation.

Applications of FD statistics: Fermi temperature and Fermi energy, heat capacity of metals.

Applications of BE statistics: Planck equation for blackbody radiation, Bose-Einstein condensation.

Unit II: Molecular Interactions (16 Marks) [22 Lectures]

Molar polarization, Mosotti-Clausius and Debye-Langevin equation – their derivation, uses and limitations. Onsager equation. Ferro-electricity. Intermolecular forces, London dispersion force and Lennard-Jones potential. Hydrogen bonding. Dielectric effects on absorption and emission spectra in solution. Lippert equation.

Unit III: Solid State Chemistry (16 Marks) [22 Lectures]

Crystal structure: Crystal symmetry, unit cell, diffraction of X-rays by crystals, reciprocal lattice, structure factors and systematic absences.

Crystal defects and non-stoichiometry: Schottky and Frenkel defects, colour centres.

Electronic properties: Kronig-Penny model, band theory, electrical and thermal conductivity of metals, semi-conductors and insulators.

Magnetic properties: Classification of materials into dia-, para-, ferro- and antiferro-magnetic types. Magnetic susceptibility and Curie's law.

Semester IV
Physical Chemistry Experiments
Paper-X: CHEM(PS)-41: (Group-B) Practical: 25-Marks
Computer Applications in Chemistry (CAC-IV): 25-Marks
Course Duration: 90 Hours

Matrix Manipulation and Diagonalisation of matrices

Solution of Problems Related to Huckel Theory for Conjugated Pi-electron Systems

Excluding excercises or experiments performed in previous semesters,

Examination:

In the examination one problem or a part of it shall be assigned to a candidate by lottery and the same has to be completed and the relevant records are to be submitted within six (6) hours.

Marks Distribution:

Programming-15, Lab.Records-05, Internal Assessment-05, Total = 25.

Semester-IV

Physical Chemistry Special
Paper-XI: CHEM (PS)-42: (75-Marks)
Physical Chemistry Special Paper PS-5
Group-A: Theoretical (50-Marks)
Paper XI

Unit I: Group Theory-II: (18 Marks) [24 Lectures]

Applications of Group Theory: Hybridization involving *s, p, d*- orbitals, LCAO approximation, LCAO-MO-Π bonding, three-centre bonding.

Crystal field splitting of free ion terms in weak and strong crystal fields (tetrahedral and octahedral) – energy level diagrams, symmetry and multiplicity of energy levels. Correlation diagrams. Selection rules for electronic transitions, vibronic coupling. Laporte selection rules.

Symmetry of normal vibrations, selection rules for vibration and Raman spectra.

Unit II: Photochemistry-II (16 Marks) [22 Lectures]

Interaction of radiation with matter. Spontaneous and stimulated emission, Einstein **A** and **B** coefficients.

Time-dependent Perturbation Theory, variation of constants, Fermi 'golden rule'.

Principle of the LASER. Different types of lasers. Uses of lasers.

The salient features of Raman spectroscopy, 'Resonance Raman' spectroscopy, second harmonic generation, 'Surface Enhanced Raman' spectroscopy.

Unit III: Advanced Molecular Spectroscopy-I (16 Marks) [22 Lectures]

Mass spectrometry: Principles, basic instrumentation. Ion production – EI, CI, FI, FD, FAB and MALDI techniques. Mass-spectral fragments of organic compounds, interpretation of spectra. Applications.

Mossbauer spectroscopy: Principles, basic instrumentation. Spectral parameters and spectral display. Quadrupole and magnetic interactions. Applications.

Photoelectron spectroscopy: Photo-excitation and photo-ionization. Core level and valence level photo-ionization (XPS, ESCA, UPS). Detection of atoms in molecules, chemical shift. Applications.

Paper-XI: CHEM(PS)-42: (Group-B) Practical: 25-Marks

Grand Viva-voce

Grand Viva-voce examination shall be conducted jointly by the external and internal Examiners. Short questions on the theoretical principles, experimental methodologies and instrumentations etc. of the different experiments included in the entire practical syllabus of semesters-I, -II, -III and -IV may be asked, Maximum time for viva-voce examination of a candidate shall not normally exceed 20 minutes.

Semester-IV

Physical Chemistry Special
Paper-XII: CHEM (PS)-43: (100-Marks)
Physical Chemistry Special Paper PS-6
Group-A: Theoretical (50-Marks)

Unit I: Non-equilibrium Statistical Mechanics and Reaction Dynamics
(18 Marks) [24 Lectures]

Brownian Motion: The (i) Einstein and (ii) Langevin approach

Reaction Dynamics:

(i) Chemical reaction, and probe at the elementary level ($HI + Cl \rightarrow HCl + I$)

(ii) Collision of two particles, motion in the centre of mass coordinates, classical scattering, impact parameter, calculation of trajectory.

(iii) Scattering cross-section and intermolecular potential.

Unit II: Advanced Molecular Spectroscopy- II (16 Marks) [22 Lectures]

Principles, basic instrumentation and interpretation of spectra in

(i) NMR (ii) ESR (iii) NQR spectroscopy. Fourier transforms. Two-dimensional NMR spectroscopy.

Unit III: Biophysical Chemistry (16 Marks) [22 Lectures]

The primary, secondary, tertiary and quaternary structures of proteins and enzymes. Function of proteins and enzymes. Nucleic acids: DNA, RNA, helix-coil transition, A, B and Z conformations.

Free energy changes in biological reactions: ATP-ADP inter-conversion. Biopolymer interactions – electrostatic, hydrophobic and dispersion forces. Multiple equilibria involving various types of binding processes. Thermodynamic aspects of biopolymer solutions – osmotic pressure, membrane equilibrium, muscular contraction, energy generation in mitochondrial system. Structures and functions of the cell membrane, ion-transport across biological membranes, muscle contraction and nerve function.

Application of fluorescence spectroscopy in elucidating the structure and function of biomolecules.

Paper-XII: CHEM(PS)-43: (Group-B) Practical: 50-Marks

Course Duration: 100 Hours

Physical Chemistry Special

Project Work & Seminar-

Project work:

During Semester-IV, each candidate shall carry out some investigative work independently or under the supervision of one or more guides(s), who may be Teacher / Guest Teacher / Member of P.G Board of Studies of the College / University / Scientist of any Recognized Research Institute. The work may be carried out either in the College / University itself or in any Recognized Research Institute, with the approval of the appropriate authority of the College/ University. Duration of the work shall be four weeks (approximately 90-100 hours). The findings of the project work should be submitted in the form of a dissertation for evaluation by a Board of Examiners.

Seminar:

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Marks Distribution:

Project Dissertation-30 Project Seminar 20 Total = 50..

Inorganic Chemistry Books

Course ID : CHEM (G): 11, 21, CHEM(IS) 31-33;:41-43

1. Advanced Inorganic Chemistry- F. A. Cotton & G. Wilkinson, John Wiley
2. Inorganic Chemistry- J.E. Huheey, E.A. Keiter & R. L. Keiter, Harper & Row
3. Chemistry of Elements- N. N. Greenwood & A. Earnshaw
4. Concept and Models of Inorganic Chemistry-Douglass, McDaniel & Alexander
5. Coordination Chemistry- S. F. A. Kettle
6. Theoretical Approach to Inorganic Chemistry-A. F. Willams
7. Inorganic Chemistry-D. F. Shriver, P. W. Atkins & C. H. Langford
8. Chemical Applications of Group theory- F. A. Cotton
9. Molecular Symmetry & Group Theory- R. L. Carter
10. Introduction to Ligand Fields- B. N. Figgis
11. Introduction to Ligand Field Theory- C. J. Ballahausen
12. Valence- C. A. Coulson
13. Chemical Crystallography-L. W. Bunn
14. Solid State Chemistry- C. N. R. Rao
15. Ionic Crystal Lattice & Nonstoichiometry-N. N. Greenwood
16. Inorganic Reaction Mechanism- M. L. Tobe
17. Mechanism of Inorganic Reactions- Katakis & Gordon
18. Kinetics and Mechanism of Reactions of Trans. Metal Complexes- R. G. Wilkins
19. Determination and use of Stability Constants- A. E. Martell & R. J. Motekaitis
20. An Introduction to Bioinorganic Chemistry-D. R. Williams
21. Inorganic Chemistry of Biological Processes-M. N. Hughes
22. Bioinorganic Chemistry-E. I. Ochiai
23. Bioinorganic Chemistry- R. W. Hay
24. Elements of Bioinorganic Chemistry- G. N. Mukherjee & A. Das
25. Organometallic Chemistry of Transition Metals-R.H. Cabtree
26. Organometallic Chemistry- R. C. Mehrotra & A. Singh
27. Nuclear and Radio Chemistry-Friedlander, Kennedy & Miller
28. Radioactiviry Applied to Chemistry- A. C. Wahl & N. A. Bonner
29. Magnetochemistry- Selwood
30. Intriduction to Magnetochemistry- Earnshaw
31. Environmental Analysis- S. M. Khopkar
32. Physical Methods in Inorganic Chemistry-R. S. Drago
33. Instrumental Methods in Chemical Analysis- Willard, Meritt and Dean
34. Instrumental Methods in Chemical Analysis- G. W. Ewing
35. Vogel`s Text Book of Quantitative Chemical Analysis
    G. H. Jeffery, J. Bassett, J. Mendham & R. C. Denny
36. Advanced Experiments in Inorganic Chemistry-G. N. Mukherjee (U. N. Dhur)
37. Macro and Semi-micro Qualitative Inorganic Analysis- A. I. Vogel
38. Semi-Micro Qualitative Inorganic Analysis- G. N. Mukherjee (C.U.Press)
39. Quantitative Chemical Analysis- Kolthoff, Sandel, Meehan & Bruckenstein
40. Synthesis and Characterizations if inorganic Compounds-W. L. Jolly

Organic Chemistry Books

Course ID : CHEM (G): 12, 22, CHEM(OS) 31-33;:41-43

1. Organic Chemistry- I. L. Finar, Vols. 1 & 2, ELBS
2. .Adv. Organic Chemistry: Reaction, Mechanism- Jerry March
3. Adv. Organic Chemistry-F. A. Carey & R. J. Sundberg
4. Organic Chemistry (3^{rd}. edn) -Hendrikson, Cram, Hammond
5. Organic Chemistry- Clayden, Greeves, Warren & Wolthers
6. Organic Chemistry- R. T. Morrison & R. N. Boyd
7. Organic Reaction Mechanics- A. Gallego, M. Gomer & M. A. Sierra
8. A Guide Book to Mechanism of Organic Reactions-Peter Sykes
9. Reaction Mechanism in Organic Chemistry- S. M. Mukherjee & S. P. Singh
10. Structure and Mechanism in Organic Chemistry- C. K. Ingold
11. Physical Organic Chemistry-J. Hiine
12. Physical Organic Chemistry-N. S. Isaacs
13. Orbital Symmetry and Organic Reactions-T. L. Gilchrist & R. C. Storr
14. Some Modern Methods in Organic Synthesis-W. Carruthers
15. Principles of Organic Synthesis-Norman, Coxon & Blakie
16. Current Trends in Organic Synthesis-C.Scolastico & F. Nicotra
17. Frontier Orbitals and Organic Chemcal Reactions-I. Fleming
18. Pericyclic Reactions- Gill & Willis
19. Pericyclic Reactions- S. M. Mukherjee
20. Stereochemistry-E. Eliel & S. H. Wilen
21. Stereochemistry- D. Nasipuri
21. Stereochemistry of Organic Compounds- P. Kalsi
22. NMR in Chemistry-A Multinuclear approach—W. Kemp
23. Application of N. M. R. Spectroscopy in Organic ChemistryL- L. M. Jackman M.
24. Interpretation of ^{13}C –NMR Spectra- F. W. Werli & T. W. Wirthlin
25. Mass Spectrometry-Organic Applications-K. Biieman
26. Free Radicals in Organic Chemisrey—Fossey, Lepost & Sorbs
27. Elements of Organic Photochemistry-D. O. Cowan & K. L.Drisco
28. Application of Organotransition Metal in Organic Synthesis-S.G. Davies
29. Comprehensive Heterocyclic Chemistry- A. R. Katritzky, & C. W. Rees (eds)
30. Heterocyclic Chemistry-J. A. Joule &K. Mills
31. Natural Product-A. Pelter
32. Natural Products: Chemistry & Biological Significance-Mann,Davidson,Hobbs,Banthrope,Harbome & Longman
33. An Introduction to Medicinal Chemistry-(3^{rd}.edn) G. L. Patrick
34. Fundamentals of Medicinal Chemistry-G. Thomas
35. Supramolecular Chemistry: Concepts & Perspective- J. M. Lehn
36. Experimental Organic Chemistry: Principles & Practice-L. M. Harwood & C. J. Roodey
37. Experiments and Techniques in organic Chemistry-Pasto, Johnson & Miller
38. Spectrometric Identification of Organic Compounds-(6^{th}. edn)-Silverstein & Webster
39. An Introduction to Experimental Organic Chemistry- Robert, Gilbert, Rodewaid & Wingrove
40. Systematic Qualitative Organic Analysis-H. Middleton
41. Hand Book of Organic Analysis- H. T. Clarke
42. Text Book of Practical Organic Chemistry-A.I. Vogel

Physical Chemistry Books

Course ID : CHEM (G): 13, 23, CHEM(IS) 31-33;:41-43

1. Physical Chemistry: A Molecular Approach-D. A. McQuarrie & J. D. Simon
2. Physical Chemistry- R. S. Berry, S. A. Rice & J. Ross
3. Introduction to Quantum mechanics- L. Pauling & E. B. Wilson
4. Quantum Mechanics J. L. Powel & B. Crasemann
5. Elementary Quantum Chemistry-F. L. Pilar
6. Quantum Chemistry- I. N. Levine
7. Chemical Kinetics-K. J. Laidler
8. Fundamentals of Chemical Kinetics-S. W. Benson
9. Theoretical Chemistry- S. Glasstone
10. The Principles of Chemical Equilibrium-K. Denbigh
11. The Physical Chemistry of Surfaces- N. K. Adams
12. Physical Chemistry of Surfaces- A. W. Adamson
13. Introduction to Molecular Spectroscopy-G. M. Barrow
14. Fundamentals of Molecular Spectroscopy- C.W. Banwell
15. Introduction to Quantum Mechanics- D. J. Griffith
16. Group Theory and Chemistry—D. M. Bishop
17. Thermodynamics and an Introduction to Thermostatistics- H. B. Callen
18. Coulson`s Valence- R. McWeeny
19. Modern Electrochemistry-J.O`M. Bockris & A. K. N. Reddy
20. Principles of Physical Biochemistry- K. E. van Holde, C. Johnson & P. S. Ho
21. Polymer chemistry-P. J. Flory
22. Microwave Spectroscopy-C. H. Townes & A. L. Schawlow
23. Symmetry and Spectroscopy- D. C. Harris & M. d. Bertolucci
24. Solid State Physics- A. J. Dekker
25. Introduction to Solid State Physics- C. Kittel
26. Chemical Kinetics and Dynamics- J. I. Seinfeld, J. S. Francesco & W. L. Hase
27. Text Book of Physical Chemistry- S. Glasstone
28. Statistical Mechanics- D. A. Mcquarrie
29. Statistical Mechanics-B. B. Laud
30. Statistical Mechanics- K. Huang
31. Practical Physical Chemistry- A. M. James & F. F. Prichard
32. Findlay's Practical Physical Chemistry- B. P. Levit
33. Experimental Physical Chemistry- Shoemaker & Garland
34. Introduction to Magnetic Resonance-A. Carrington & A. D. McLachlan
35. NMR, NQR, EPR and Mossbauer Spectro. in Inorganic Chemistry- R. V. Parish
36. Macromolecules:Structure and Function- F. Wold, Prentice-Hall
37. Principles of Biochemistry- A.L. Lehninger
38. Programming with FORTRAN - S. Lepschutz & A. Poe (Schaum Series)
39. Computer Programming in FORTRAN 77- V. Rajaraman
40. Computational Chemistry- A. C. Norris, John Wiley
41. Computational Chemistry- A. Konar
42. Computers in Chemistry – K. V. Raman, TMH
43. Electricity and Magnetism (Vol I) – J.H. Fewkes & J. Yarwood, OUP
44. Atomic Physics (Vol II) – J. Yarwood , OUP
45. Biochemistry – Voet and Voet