STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI

Course Schedule – November 2023– April 2024

Department : Chemistry

Name/s of the Faculty : Dr. Avila Josephine B

Course Title : INORGANIC CHEMISTRY – II

Course Code : 19CH/MC/IC64

Shift : SHIFT I

Week & No. of hours	Units & Topics	Teaching Methodology	Text & References	Method of Evaluation
Nov 22 – 23, 2023 2 hrs	**Unit 1** **Transition Elements** 1.1 General Properties of Transition Metals 1.2 Ti, V, Cr, Mn Groups, Fe, Co, Ni Groups - A Comparative Study with respect to the Oxidation States, Oxides and Complexes	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 3. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry*. New Delhi: Vikas, 2001 4.Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994. 5. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, Butterworth-Heinemann, 1997	Quiz
Nov 24-30, 2023 5 hrs	1.3 Biological Importance of Transition Metals-Biological Roles of Mo,Fe,Co,Cu,Zn (Metal Containing Proteins and Enzymes and their Biological Roles)	Power point Presentation	1. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry*. New Delhi: Vikas, 2001 2. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 3. Lee J.D. Concise Inorganic Chemistry.	Short answer questions

			London: ELBS, 2008. 4. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994. 5. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, Butterworth-Heinemann, 1997	
Dec 1-7, 2023 5 hrs	**Unit 2** **Chemistry of Coordination Compounds** Introduction – Ligands-Monodentate, Bidentate and Polydentate Ligands, Coordination Sphere, Coordination Number, Chelate Effect	Lecture & Discussion	1. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001 2.Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008.	**III component Assignment Unit 1.3 (10 marks)**
Dec 8-9, 2023 2022 2 hrs	2.1 Nomenclature of Coordination Compounds	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	Worksheet based on nomenclature and isomerism of coordination compounds
Dec 11-15, 2023 5 hrs	2.2 Isomerism – Linkage, Ionization, Hydrate, Coordination, Coordination Position 2.2 Isomerism Geometrical and Optical Isomerism of 4 and 6 – Coordinate Complexes **3.1** Sidgwick's Effective Atomic Number Rule (EAN), 18 Electron Rule,.	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	**III Component MCQ Unit 2 and Unit 3.1 (20 marks)**

Dec 16 – 22, 2023 2022 5 hrs	Valence Bond Theory (VBT), Hybridization, Geometry and Magnetic Properties of Coordination Compounds, Drawbacks of VBT 3.2 Crystal Field Theory - Crystal Field Splitting in Octahedral, Tetrahedral and Square Planar Complexes, Crystal Field Stabilization Energy.	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	**Problem solving** Worksheet
Jan 3 – 6, 2024	3.2 Spectrochemical Series, Low and High Spin Complexes, factors influencing the magnitude of Crystal Field Splitting, Jahn Teller Effect	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	**Problem solving** Worksheet
Jan 8 – 12, 2024	**C.A. Test** **Unit 2, 3.1,3.2, Unit 1(1.1 & 1.2)**			
Jan 13, 2024 1hr	3.3 Applications of Coordination Compounds in Qualitative and Quantitative Analyses Potassium Ferrocyanide Potassium Ferricyanide	Powerpoint Presentation	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 3. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry.* New Delhi: Vikas, 2001	quiz
Jan 18 -20, 2024	3.3 Applications of Coordination Compounds in Qualitative and Quantitative Analyses Alizarin, Ferroin, DMG, Oxine, Cupferron and EDTA	Powerpoint Presentation	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008	quiz

			3. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry.* New Delhi: Vikas, 2001	
Jan 22-29, 2024 5 hrs	4.1 Lanthanides – Lanthanide Series, their Position in the Periodic Table, Properties of Lanthanides, Lanthanide Contraction and its Consequences	Lecture & Discussion	1. Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 3. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry.* New Delhi: Vikas, 2001	Short answer questions Worksheet
Jan 30 – Feb 2, 2024 3 hrs	4.2 Isolation of Lanthanides - Ion Exchange Chromatography 4.3 Actinide – Actinide Series, Position in the Periodic Table, Properties of Actinides.	Lecture & Discussion	1.Lee J.D. Concise Inorganic Chemistry. London: ELBS, 2008. 2. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 3. Cotton, F.A., and G. Wilkinson.*Advanced Inorganic Chemistry.* New Delhi: Wiley Eastern, 2008.	Group Discussion
Feb 3, 2024 1 hr	4.3 Comparison between Lanthanides and Actinides	Lecture & Discussion	1. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 2. Gopalan R, V. Ramalingam. *Concise Coordination*	Group Discussion

			Chemistry. New Delhi: Vikas, 2001 3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994. 4. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, Butterworth-Heinemann, 1997	
Feb 5- 6, 2024 2 hrs	4.4 Extraction of Thorium from Monazite and Uranium from Pitch Blende	Lecture & Discussion	1. Puri. B.R., L.R. Sharma., & C.I. Kalia Principles of Inorganic Chemistry. New Delhi: Milestone, 2008 2. Gopalan R, V. Ramalingam. *Concise Coordination Chemistry*. New Delhi: Vikas, 2001 3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994. 4. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, Butterworth-Heinemann, 1997	Group Discussion
Feb 7 – 14, 2024	4.4 Extraction of Uranium from Pitch Blende 5.1 Metal Carbonyls - Preparation, Properties and Structure of Ni	Lecture &	1. James, E., Huheey & Ellen A.Keiter. Principles of Structure and Reactivity. Pearson, India, 2011. 2. Gopalan R, V.	**III Component test (Unit 4) MCQ Test (20 marks)**

	Carbonyls 5.2 Preparation and Structure of Metal Alkyls and Aryls of Li and Al	Discussion	Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	
Feb 15 – 22, 2024	5.1 Metal Carbonyls - Preparation, Properties and Structure Fe Carbonyls	Lecture & Discussion	1. James, E., Huheey & Ellen A.Keiter. Principles of Structure and Reactivity. Pearson, India, 2011. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	
Feb 23 – 24, 2024 2 hrs	5.2 Preparation and Structure of Metal Alkyls and Aryls of Li			
Feb 26 – Mar 1, 2024 5 hrs	5.2 Preparation and Structure of Metal Alkyls and Aryls Al 5.2 Structure of Metal Alkene Complexes			
Mar 2, 2024 1 hr	**Revision**			
Mar 4 –8, 2024	**C.A. Test** **Unit 4 and Unit 5 (5.1)**			
Mar 9 – 16, 2024 2 hrs	5.2 Preparation and Structure of Metal Alkyls and Aryls of Ti.	Lecture & Discussion	1. James, E., Huheey & Ellen A.Keiter. Principles of Structure and Reactivity. Pearson, India, 2011. 2. Gopalan R, V. Ramalingam.	Short answer test

			Concise Coordination Chemistry. New Delhi: Vikas, 2001	
Mar 18 - 19, 2024 2 hrs	5.3 Ferrocene - Preparation, Properties and Structure	Lecture & Discussion	1. James, E., Huheey & Ellen A.Keiter. Principles of Structure and Reactivity. Pearson, India, 2011. 2. Gopalan R, V. Ramalingam. Concise Coordination Chemistry. New Delhi: Vikas, 2001	quiz
Mar 20-22, 2024 2 hrs	**REVISION FOR END SEMESTER EXAMINATION**			

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI

Course Schedule: November - April 2024

Department : CHEMISTRY

Name/s of the Faculty : Dr. Revathy Rajagopal

Course Title : PHYSICAL CHEMISTRY III

Course Code : 19CH/MC/PC64

Shift : I

Week & No. of hours	Units & Topics	Teaching Methodology	Text & References	Method of Evaluation
Nov 22 – 23, 2023 (Day Order 1 & 2)	**Unit 1 Electrochemistry** I 1.1 Migration of Ions, Conductivity, Ostwald's Dilution Law, Variation of Conductance with Dilution, Types of Conductometric titration, Kohlrausch's Law, Ionic Mobility, Transport Number and Ionic Conductance	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on transport number, ionic conductance, conductivity
Nov 24-30, 2023 (Day Order 1 to 6)	1.2 Transport Number - Determination by Hittorf's and Moving Boundary Methods 1.3 Debye Hŭckel Theory of Strong Electrolytes, Debye-Falkenhagen effect, Wien effect 1.4 Activity Coefficient, Mean Activity Coefficient and Ionic Strength	Lecture/ Power point presentation/ demonstration	Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on Activity coefficient, activity and ionic strength
Dec 1-7, 2023 (Day Order 1 to 6)	**Unit 2 Electrochemistry II** 2.1 Concept of Electrochemical Cell, Galvanic Cell, Reversible and Irreversible Cells, Half Cells, Electrode and Cell Reactions, Nernst Single Electrode Potential, Cell Representation, Terminology and Conventions	Lecture/ Power point presentation/ demonstration	Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on Worksheet on writing cell representatio ns and cell reactions

Dec 8-9, 2023 (Day Order 1, 3)	2.2 Reversible Electrodes, Standard Hydrogen Electrode, Calomel Electrode, and Equation of EMF of Cells- Standard Electrode Potentials, Sign Convention, Electrochemical Series, Significance, Applications. Weston Cadmium Cell, EMF – Measurement Poggendorff's Compensation Method, Redox Potential	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	
Dec 11-15, 2023 (Day Order 2 to 6)	2.3 Applications of EMF Measurements: Application of Gibbs - Helmholtz Equation in the Calculation of ΔG, ΔH, ΔS, Temperature Coefficient of EMF of Galvanic Cells, Equilibrium Constant,	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013.	Numerical on unit 1, 2.1 & 2.2 **III Component (20 Marks)**
Dec 16 – 22, 2023 (Day Order 1 to 6)	2.3 (Contd..) Determination of pH using Glass, Hydrogen and Quinhydrone Electrodes, Potentiometric Titration	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on numerical on Nernst equation
Jan 3 – 6, 2024 (Day Order 1 to 4)	2.4 Types of Reversible Cells, Concentration Cells with and without Transference. Liquid Junction Potential (cell reversible with respective to cations and anions) Derivation - Significance of Salt Bridge	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on numerical on Nernst equation
Jan 8 – 12, 2024	**C.A. Test – I**			

Jan 13, 2024 (Day Order 1)	**Unit 3 Chemical Kinetics** 3.1 The Rate Equation, Order and Molecularity of Reactions with Examples	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006.	Worksheet on evaluating order of reaction
Jan 18 -20, 2024 (Day Order 4 to 6)	**Unit 3 Chemical Kinetics** 3.1 The Rate Equation, Order and Molecularity of Reactions with Examples, Derivation of Rate Constants for Zero, First, Second (Equimolar and Non-Equimolar Reactant Concentrations) and n th Order Reactions, Characteristics of Fractional Order Reactions,			
Jan 22-29, 2024(Day Order 1 to 6)	**Unit 3 Chemical Kinetics** 3.1 The Rate Equation, Order and Molecularity of Reactions with Examples, Derivation of Rate Constants for Zero, First, Second (Equimolar and Non-Equimolar Reactant Concentrations) and n th Order Reactions, Characteristics of Fractional Order Reactions, Half Life Time, Methods of Determination of Order of Reaction	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013.	Assignment on Numerical III Component 10 Marks
Jan 30 – Feb 2, 2024 (Day Order 1 to 4)	3.2 Collisions and Encounters, Effect of Temperature on Reaction Rate, Concept of Activation Energy, Energy Barrier, Effect of Catalyst, Arrhenius Equation, Calculation of Arrhenius Parameters	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	**Group Discussion**

Feb 3, 2024 (Day Order 2)	**3.2** Effect of Catalyst, Arrhenius Equation, Calculation of Arrhenius Parameters	Lecture	Atkins, P.W. Elements of Physical Chemistry	**Group Discussion**
Feb 5- 6, 2024 (Day Order 5 to 6)	**3.2** Effect of Catalyst, Arrhenius Equation, Calculation of Arrhenius Parameters	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	**Group Discussion**
Feb 7 – 14, 2024 (Day Order 1 to 6)	**3.3** Theories of Reaction Rates, Collision Theory of Bimolecular Reactions, Limitations of Collision Theory, Activated Complex Theory of Bimolecular Reactions, Transition State Theory –Thermodynamic Derivation of Rate Constant for TS, Eyring's Equation (No Derivation), Significance of ΔH^*, ΔG^* & ΔS 3.4 Photochemical Rate Law, Kinetics of Hydrogen-Chlorine, Jablonski diagram - Laws of photochemistry- Quantum Efficiency **Unit 4 Catalysis** 4.1 Catalytic Reactions- Characteristics, Homogenous Catalysis- Acid-Base Catalysis, Kinetics of catalysis 4.2 Enzyme Catalysis- Michaelis – Menton Mechanism, Effect of Temperature, pH and subtrate concentration on catalysis	Lecture/ Power point presentation/ demonstration	Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	

Feb 15 – 22, 2024 (Day Order 1 to 6)	**4.3** Heterogenous Catalysis- Kinetics of Surface Reactions, Unimolecular and Bimolecular Surface Reactions, Effect of pH on Catalysed Reactions	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013.	**Numerical in unit 3 & 4 III Component (20 Marks)**
Feb 23 – 24, 2024 (Day Order 1 & 5)	**4.3** Heterogenous Catalysis- Kinetics of Surface Reactions, Unimolecular and Bimolecular Surface Reactions, Effect of pH on Catalysed Reactions	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013.	**Numerical in unit 3 & 4 III Component (20 Marks)**
Feb 26 – Mar 1, 2024 (Day Order 2 to 6)	**Unit 5 Colloids and Surface Chemistry** 5.1 Colloidal systems- classification, reparation and roperties of colloids	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	**Short answer test**
Feb 23 – 24, 2024 (Day Order 1 & 5)	5.2 Adsorption - Physisorption and Chemisorption- Types of Adsorption Isotherms, factors affecting adsorption	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	**Short answer test**

Mar 2, 2024(Day Order 1)	5.2 Adsorption - Physisorption and Chemisorption- Types of Adsorption Isotherms, factors affecting adsorption	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006.	**Short answer test**
Mar 4 –8, 2024	**C.A. Test – II**			
Mar 9 – 16, 2024 (Day 6 & Day Order 1 to 6)	**5.3** Freundlich Adsorption Isotherm - Limitations. Derivation of Langmiur Adsorption Isotherm; BET Adsorption Isotherm - Postulates and Equation. Determination of Surface Area	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Quiz
Mar 18 - 19, 2024 (Day Order 2 to 3)	**5.3**Freundlich Adsorption Isotherm - Limitations. Derivation of Langmiur Adsorption Isotherm; BET Adsorption Isotherm - Postulates and Equation. Determination of Surface Area	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	Worksheet on isotherms
Mar 20-22, 2024 (Day Order 4 to 6)	**5.3**Freundlich Adsorption Isotherm - Limitations. Derivation of Langmiur Adsorption Isotherm; BET Adsorption Isotherm - Postulates and Equation. Determination of Surface	Lecture/ Power point presentation/ demonstration	Atkins, P.W. Elements of Physical Chemistry. Oxford University, 2013. Bajpai.S. Physical Chemistry. New	Worksheet on isotherms

	Area **REVISION**		Delhi: Shobanlal Nagin Chand, 2006. Puri, B.R., Sharma, L.R.& Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co, Jalandar, Delhi, 2018	

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI

Course Schedule: November 2023 - April 2024

Department : Chemistry

Name/s of the Faculty : Dr. Mary Teresita V

Course Title : Spectroscopy

Course Code : 19CH/MC/SP 64

Shift : I

Week & No. of hours	Units & Topics	Teaching Methodology	Text & References	Method of Evaluation
Nov 22 – 23, 2023 (Day Order 1 & 2) 1 Hr	**Unit -1 Introduction** 1.1 Electromagnetic Spectrum	Lecture & Discussion	Banwell, *Fundamentals of Molecular Spectroscopy, 4th Ed, 2010* Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010	Quiz
Nov 24-30, 2023 (Day Order 1 to 6) 5 Hrs	1.2 Microwave Spectroscopy: Rotational Transitions, Theory of Rotational Spectroscopy, Rotation of Homonuclear and Heteronuclear Diatomic Molecules, Selection Rule, Forbidden Transitions, Instrumentation 1.3 Calculation of Moment of Inertia and Reduced Mass	Lecture & Discussion	Banwell, *Fundamentals of Molecular Spectroscopy, 4th Ed, 2010* Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010	Work sheet
Dec 1-7, 2023 (Day Order 1 to 6) 5 Hrs	**Unit -2 Vibrational Transitions: FTIR and Raman Spectroscopy** 2.1 Modes of Vibration, Conditions of Sensitivity to IR 2.2 Characteristic Frequencies of Functional Groups and Aromatic Compounds	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010	Test
Dec 8-9, 2023	2.3 IR Pattern of Simple Organic Compounds	Spectral problem group	Sharma Y.R, *Elementary Organic Spectroscopy:*	Solving Spectral

(Day Order 1, 3) 1 Hr		discussion	*Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	problems as a group
Dec 11-15, 2023 (Day Order 2 to 6) 5 Hrs	2.4 Theory of Raman Spectroscopy, Instrumentation, Comparison with IR, Mutual Exclusion Principle **Unit – 3** **Electronic Transitions: UV Visible Spectroscopy** Theory of Electronic Spectroscopy, Laws of Light Absorption-Beer-Lambert's Law,	Lecture & Discussion	Banwell, *Fundamentals of Molecular Spectroscopy, 4th Ed, 2010* Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test & Quiz
Dec 16 – 22, 2023 (Day Order 1 to 6) 5 Hrs	Definitions of chromophore, auxochrome, bathochromic and hypsochromic shifts. Franck Condon Principle Factors Affecting UV Absorption, Solvents, Parameters of UV Plot	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test
Jan 3 – 6, 2024 (Day Order 1 to 4) 2 Hrs	Woodward - Fieser Rules as Applied to Aliphatic Dienes and α,β Unsaturated Aldehydes and Ketones UV Spectra of Simple Organic Compounds -Toluene and Cresol	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Solving problems

Jan 8 – 12, 2024	**C.A. Test – I** **Unit 1,2 & 3 (No instrumentation)**			
Jan 13, 2024 (Day Order 1)	No Hours for this Day order			
Jan 18 -20, 2024 (Day Order 4 to 6) 3 Hrs	Unit -4 **Nuclear Magnetic Resonance Spectroscopy** 4.2 Theory of NMR Absorption- Magnetic Properties of Nuclei (Magnetic Moment, g Factor) and Theory of Nuclear Resonance. Larmor Precession Frequency, Resonance Condition and Relaxation Processes 4.3 Factors Affecting Chemical Shift Electronegativity, Hybridization	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004 Williams D.H., Fleming I., *Spectroscopic Methods in Organic Chemistry*, Tata McGraw-Hill, 2004.	Test
Jan 22-29, 2024 (Day Order 1 to 6) 5 Hrs	4.2 Shielding and Deshielding, van der Waals Deshielding, H-Bonding, Diamagnetic and Paramagnetic Anisotropy 4.3 Spin-Spin Coupling, (n+1) Rule and its Origin, Pascal's Diagram, Chemical Shift Values 4.4 Factors Influencing Spin Coupling Constants, Vicinal	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic*	

	and Geminal Coupling.		*Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004 Williams D.H., Fleming I., *Spectroscopic Methods in Organic Chemistry*, Tata McGraw-Hill, 2004.	

Jan 30 – Feb 2, 2024 (Day Order 1 to 4) 3 Hrs	4.1 ^{13}C NMR Spectra, Spin Decoupling Techniques – Advantages 4.1 NMR Spectra of Simple Organic Compounds – CH_3Cl, CH_3CH_2OH, $C_6H_5CH_3$, CH_3CHO and CH_3COOH	Lecture & Discussion Spectral Problems Group Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test Solving the problems as a group
Feb 3, 2024 (Day Order 2) 1 Hr	4.1 Instrumentation of Microwave spectroscopy 2.1 Principle, Instrumentation of IR & Raman 3.1 Instrumentation, Block Diagram of Double Beam Spectrophotometer 4.4 Instrumentation and Sample Handling and Standards Employed in NMR 5.2 Instrumentation of Mass spectrometry	Group Assignment	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004 Williams D.H., Fleming I., *Spectroscopic Methods in Organic Chemistry*, Tata McGraw-Hill, 2004.	**Third Component Assignment & Test (30 Marks)**

Feb 5- 6, 2024 (Day Order 5 to 6) 2 Hrs	Unit -5 **Mass Spectrometry** 4.2 Theory and Rules of Fragmentation,	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test
Feb 7 – 14, 2024 (Day Order 1 to 6) 4 Hrs	5.1 Molecular Ion, Base Peak, Nitrogen Rule, Isotope Peaks and Metastable Peaks	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test
Feb 15 – 22, 2024 (Day Order 1 to 6) 5 Hrs	5.2 McLafferty Rearrangement, Retro Diel's Alder Rearrangement	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand	Test

			Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	

Feb 23 – 24, 2024 (Day Order 1 & 5) 3 Hr	5.3 Fragmentation Patterns of Various Functional Groups – Aliphatic & Aromatic hydrocarbons IR & NMR Spectral problems of simple compounds	Lecture & Discussion Group Presentation	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test **Third Component** **(20 Marks)**
Feb 26 – Mar 1, 2024 (Day Order 2 to 6) 4 Hrs	5.3 Fragmentation Patterns of – Aliphatic & Aromatic alcohols , ethers and amines	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Test
Mar 2, 2024 (Day Order 1)	No Hours for this Day order			
Mar 4 –8, 2024	**C.A. Test – II** **Unit 4 & 5 (No instrumentation)**			
Mar 9 – 16, 2024 (Day 6 & Day Order 1 to 6) 5 Hrs	5.3 Fragmentation Pattern – Aliphatic & Aromatic carboxylic acids and	Lecture & Discussion	Sharma Y.R, *Elementary Organic Spectroscopy:*	Test

	its derivatives, halogen containing compounds		*Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	
Mar 18 - 19, 2024 (Day Order 2 to 3) 2 Hrs	Conjoint problems	Group discussion	Sharma Y.R, *Elementary Organic Spectroscopy: Principles and Chemical Applications,* S Chand Publications, 2010 Jag Mohan, *Organic Spectroscopy: Principles and Applications*, Alpha Science International Ltd.,UK, 2004	Solving the problems as a group
Mar 20-22, 2024 (Day Order 4 to 6) 3 Hrs	**END SEMESTER EXAM REVISION**			

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI

Course Schedule: November- April 2024

Department : CHEMISTRY

Name/s of the Faculty :Dr. X*, Dr. Revathy Rajagopal

Course Title : COMPUTERS IN CHEMISTRY

Course Code : 19CH/ME/CC55

Shift : I

Week & No. of hours	Units & Topics	Teaching Methodology	Text & References	Method of Evaluation
Nov 22 – 23, 2023 (Day Order 1 & 2) 3* 2	**Unit 3: Introduction to MathCad** 3.1 Eigen Values and Eigen Vectors of Matrices **Unit 1: Data Processing and Analysis** 1.1. Elements of Computer Architecture - Creating, Editing, Naming, Renaming and Locating Files, Folders, Directory	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005. F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	MCQ test
Nov 24-30, 2023 3* 2	3.1 Differential and Integral Calculus 1.2 Components of Excel - Spreadsheets, Database, Chart & Building Workbooks	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005. F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	Short answer test

Nov 24-30, 2023 (Day Order 1 to 6) 3* 2	3.3 Histograms, Extrapolation and Interpolation in Graphs, Curve Cutting Integration Methods 3.4 Regression Analysis of Experimental Data and its Related Techniques 1.3 Building Formulae, User Made and Statistical Functions, Formatting Cells 1.4 Managing and Organizing Data - Creating Link, Analyzing Data	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Problem test (III Component) 20M
Dec 8-9, 2023 (Day Order 1, 3) 3* 2	3.5 Solutions for Simultaneous Equations by Matrix Methods 1.5 Solving Problems from Physical and Analytical Chemistry (Precision and Accuracy), Standard Deviation using Spectral Data	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	Problem test on excel sheet(III Component) 10M
Dec 11-15, 2023 (Day Order 2 to 6) 3* 2	3.5 Solutions for Simultaneous Equations by Matrix Methods 1.5 Solving Problems from Physical and Analytical Chemistry (Precision and Accuracy), Standard Deviation using Spectral Data	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Assignment III Component(10M)
Dec 16 – 22, 2023 (Day Order 1 to 6)	3.5 Solutions for Simultaneous Equations by Matrix Methods 1.5 Solving Problems from	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Quiz

3* 2	Physical and Analytical Chemistry (Precision and Accuracy), Standard Deviation using Spectral Data			
Jan 3 – 6, 2024 (Day Order 1 to 4)	3.5 Solutions for Simultaneous Equations by Matrix Methods 1.5 Solving Problems from Physical and Analytical Chemistry (Precision and Accuracy), Standard Deviation using Spectral Data	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	Problem test
Jan 8 – 12, 2024	**Unit 1 and Unit 3**			
Jan 13, 2024 (Day Order 1) 3*	3.5 Solutions for Simultaneous Equations by Matrix Methods	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Worksheet
Jan 18 -20, 2024 (Day Order 4 to 6) 3* 2	**Unit 4: CHEM Draw & CHEM 3D Pro 4.1 :** Using CHEM DRAW for Writing Chemical Equations and Representing Schemes of Reaction Mechanisms, Editing, Transporting as Picture to Word Document **Unit 2 Introduction to Graphs2.1** Introduction to Charts - Types, Creating Charts from a Table, Reviewing Graphs	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	Assignment on graphs (III Component) 10M
Jan 22-29, 2024 (Day Order 1 to 6) 3*	**Unit 4: CHEM Draw & CHEM 3D Pro 4.1 :** Using CHEM DRAW for Writing Chemical Equations and Representing Schemes of Reaction Mechanisms, Editing, Transporting as	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	Assignment on graphs

2	Picture to Word Document **Unit 2 Introduction to Graphs2.1** Introduction to Charts - Types, Creating Charts from a Table, Reviewing Graphs			
Jan 30 – Feb 2, 2024 (Day Order 1 to 4)	**Unit 4: CHEM Draw & CHEM 3D Pro 4.1 :** Using CHEM DRAW for Writing Chemical Equations and Representing Schemes of Reaction Mechanisms, Editing, Transporting as Picture to Word Document **Unit 2 Introduction to Graphs2.1** Introduction to Charts - Types, Creating Charts from a Table, Reviewing Graphs	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	**Problem Test**
Feb 3, 2024 (Day Order 2) 3*	**Unit 4: CHEM Draw & CHEM 3D Pro 4.2 :** Using CHEM 3D PRO for Building Molecules and for Measurement of Bond Angles, Bond Energy, Energy Minimization	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005. F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	**MCQ test**
Feb 5- 6, 2024 (Day Order 5 to 6) 3* 2	**Unit 4: CHEM Draw & CHEM 3D Pro 4.3 :** Use of Internet in Chemical Research- XRD, IR, NMR Data **Unit 2 Introduction to Graphs2.2** Solving Problems in Chemistry Plotting Graphs using Theoretical and Experimental Data.	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Short answer test

Feb 7 – 14, 2024 (Day Order 1 to 6) 3* 2	4.2 Internet in Chemical Research- XRD, IR, NMR Data Unit 2 2.3 Trend Line Addition and Determining the Slope and Intercept	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	MCQ test
Feb 15 – 22, 2024 (Day Order 1 to 6) 3* 2	**Unit 4: CHEM Draw & CHEM 3D Pro 4.3 :** Use of Internet in Chemical Research- XRD, IR, NMR Data **Unit 2 Introduction to Graphs2.2** Solving Problems in Chemistry Plotting Graphs using Theoretical and Experimental Data.	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Short answer test
Feb 23 – 24, 2024 (Day Order 1 & 5)	**Unit 4: CHEM Draw & CHEM 3D Pro 4.3 :** Use of Internet in Chemical Research- XRD, IR, NMR Data **Unit 2 Introduction to Graphs2.2** Solving Problems in Chemistry Plotting Graphs using Theoretical and Experimental Data.	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005.	Short answer test
Mar 2, 2024 (Day Order 1)	4.2 Internet in Chemical Research- XRD, IR, NMR Data	Power point presentation and lecture	F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013	MCQ test
Mar 4 –8, 2024	CA II			

Mar 9 – 16, 2024 (Day 6 & Day Order 1 to 6) 3* 2	**Unit 5** **Molecular Mechanics** 5.1Introduction to Cheminformatics in Drug Discovery - 2D Databases and Database searching, Substructure search, property searching, similarity searching 2.4 Using ORIGIN 9.5 for plotting graphs	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005. F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013 Bunin, Barry A. Dordrecht. Chemoinformatics:Theory, Practice, and Products.UK: Springer, 2010.	Worksheet on graphs
	5.2 Representation and manipulation of 2D Molecular Structures, 3D Databases: experimental data sources, Chemical Databases - CHEMDB, KEGG LIGAND, CAS REGISTRY, Chemical searching methods - exact searching, sub structure searching, similarity searching, reaction searching 2.4 Using ORIGIN 9.5 for plotting graphs	Power point presentation and lecture	Ramesh Kumari. *Computers and applications to Chemistry*. New Delhi: Narosa,2005. F. James Holler, Stanley R. Crouch, *Applications of Microsoft Excel in Analytical Chemistry*, UK Cengage Learning : 2013 Bunin, Barry A. Dordrecht. Chemoinformatics:Theory, Practice, and Products.UK: Springer, 2010.	Assignment
Mar 20-22, 2024 (Day Order 4 to 6)	REVISION			