Semester	**7**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 7)**
Paper Code	**C4CH230742T / C4CH230742P**
Credits	**4 (THEORY: 3 PRACTICAL: 1)**
Hours/week	**6 (THEORY: 6 PRACTICAL: 3)**
Category: Core/MDC/SEC/VEC	**CORE**
Theory/Practical/Composite	**COMPOSITE**
Number of Modules	**3**
Syllabus	**Theory:** **Group Theory I (12 lectures)** 1. Groups and their properties: 2. The concept of groups 3. Subgroups, cosets, classes and the related theorems 4. Group multiplication tables and the rearrangement theorem 5. The point group 6. Symmetry elements and symmetry operations (recapitulation) of molecular species 7. Point groups by symmetry operations 8. Molecular point groups 9. Stereographic projection 10. The matrix representations of symmetry operations 11. Theory of group representations 12. Unitary and hermitian matrices 13. Similarity transformation and the invariance of characters 14. Eigen values and matrix equations under such transformations 15. Block diagonalization 16. Direct product of matrices and their characters etc. 17. Matrix representation of point groups 18. Reducible, irreducible and equivalent representations 19. The Great Orthogonality Theorem and its corollaries 20. Character tables 21. The row/column orthogonality of characters 22. Construction of character tables in simple cases (C2v, C3v, C2h etc.) **Photochemistry (12 Lectures)** 1. Preliminaries to molecular orbitals (ethylene, unconjugated and conjugated polyenes, CO, HCHO): possible transitions 2. HOMO and LUMO: spin multiplicities at ground and excited electronic state 3. Born-Oppenheimer approximation and spin-selection rule 4. Electronic transition – allowedness and intensities 5. CT transitions and their intensity 6. Anharmonic potential energy surfaces for electronic states, Frank-Condon principle 7. Applications: e.g. racemization of stilbene on photoexcitation 8. Acid-base properties in first excited electronic state 9. Interpenetrated and isolated structure of excited state:

	consequences 10. Kasha's rule: consequence 11. Decay of excited states by radiative and non-radiative paths: Time scale and selection rule 12. Mirror-image relation between absorption and emission spectrum: 0-0 line 13. Facilitating phosphorescence: l-s coupling 14. Quenching of radiative emission processes 15. Excimer and exciplex formation: outcome in the emission spectrum 16. Quantum yield of radiative processes: Stern-Volmer equation 17. Delayed fluorescence 18. Photostationary state 19. Photosensitized reactions 20. Photochemical equilibrium **Atomic Structure and Atomic Spectra (12 lecture)** 1. Appropriate treatment of Schrödinger equation for Hydrogenic system 2. Solution of radial (complete derivation) 3. Solution of theta and phi part (General expression) 4. Shapes of s, p, d orbitals 5. Hydrogenic wave functions up to n=3 6. Atomic orbitals and their energies 7. Spectroscopic transitions and selection rules. 8. Magnetic moment due to orbital motion of an electron 9. Atoms in an external magnetic field: Zeeman effect 10. Stern-Gerlach experiment: Concept of electronic spin 11. Spin angular momentum: Lande 'g' factor 12. Many-electronic system 13. Spin-orbit coupling, j-j coupling and fine structure 14. Term-Symbol and LS coupling 15. Anomalous Zeeman and Paschen-back effect. **Practical:** Group A •Energy transfer from Lanthanide salts – Binary complexes with antibiotic drug. •Analysis of arsenic content in soil / water in different rural areas using Atomic absorption spectrometer. •Study on Excited state intramolecular protein transfer (ESIPT) proles and their various binary interactions with proteins. Group B •Synthesis of suitable transition metal complexes using the redox non-innocent ligands with azo moiety and isolation the pure product by using different techniques. •Synthesis of suitable transition metal complexes using ligands with imino-quinone functional and isolation the pure product and growing single crystals by using diverse methodologies. •Synthesis and isolation of pure transition metal complexes of

	ligands offering pyridyl/ benzothiazole skeleton. Group C •Synthesis of azido and alkene/alkyne derivatives required for click and metathesis reactions. •Carrying out click reactions between various azido–alkene/alkyne substrates under appropriate catalytic conditions. •Study of intermolecular click reactions for the formation of 1,2,3-triazole derivatives. Group D •Study of clouding behaviour in non-ionic surfactants. •Study of effect of additives on clouding behaviour. •Thermodynamic analysis of clouding behaviour. Group E • Development of a Genetic Algorithm framework including selection, crossover, and mutation operators for atomic coordinates. • Implementation of a Particle Swarm Optimization (PSO) or Artificial Bee Colony method for multidimensional search spaces. •Automation of the Global Optimization codes. Group F •Synthesis of Chemosensor molecules based on PET/ ICT mechanism - i) Isolation and. Purification. •Synthesis of Chemosensor molecules based on PET/ ICT mechanism - ii) Characterization. •Synthesis of Chemosensor molecules based on PET/ ICT mechanism - iii) Photo physical studies. Group G •Synthesis of organic molecules with innocent backbones suitable for supramolecular gelation. •Synthesis of organic molecules with non-innocent backbones for functional gelation and metallogelation. •Purification and characterization of gelator molecules using standard spectroscopic and analytical techniques. Group H •Synthesis and purification of transition metal complexes using macrocylic ligands. •Synthesis and purification of transition metal complexes of ligands containing different heteroatom donor sites, N-heterocylcic carbenes. •Electrochemical characterisation of different metal transition metal complexes to evaluate efficiency in different Proton coupled electron transfer reaction mechanisms.
Course Overview	**Theory:** Composite course that delves into mathematical symmetry, the quantum mechanics of light-matter interactions, and advanced atomic physics, coupled with a diverse, research-oriented laboratory component. • Group Theory I (Module I): Introduces the mathematical framework of symmetry, covering subgroups, classes,

	and point groups. It heavily utilizes matrix algebra to represent symmetry operations, leading to block diagonalization, the Great Orthogonality Theorem, and the construction of Character Tables for point groups like C_{2v}, C_{3v}, and C_{2h}. • Photochemistry (Module II): Investigates the behavior of molecules in electronically excited states. Topics include the Franck-Condon principle, Kasha's rule, and radiative vs. non-radiative decay. It covers advanced kinetic applications such as excimer/exciplex formation, delayed fluorescence, photosensitized reactions, and the calculation of quantum yields using the Stern-Volmer equation. • Atomic Structure and Atomic Spectra (Module III): Provides a rigorous mathematical treatment of the Schrödinger equation for hydrogenic systems, deriving radial and angular wavefunctions. It explores many-electron systems, spin-orbit coupling (LS and $j-j$ coupling), Term Symbols, and the behavior of atoms in magnetic fields (Zeeman and Paschen-Back effects). **Practical:** • Practical Component (Groups A–H): A highly specialized, research-driven laboratory curriculum. Students engage in atomic absorption spectroscopy, synthesis of redox non-innocent transition metal complexes, "click" chemistry (1,2,3-triazoles), surfactant thermodynamics, supramolecular gelation, and the computational implementation of Genetic Algorithms and Particle Swarm Optimization (PSO).
Course Outcomes	**CO1 [Foundations of Group Theory]:** Define the abstract concept of a group, apply group-theoretic constructs (subgroups, cosets, classes, and the rearrangement theorem) to construct group multiplication tables, and assign molecular point groups from symmetry elements and operations using stereographic projections. **CO2 [Matrix Representation Theory]:** Construct matrix representations of symmetry operations, apply similarity transformations to demonstrate the invariance of characters under unitary and Hermitian matrix transformations, and use block diagonalization and direct products to simplify representations. **CO3 [Group Representations & Character Tables]:** Apply the Great Orthogonality Theorem to analyze reducible/irreducible representations and construct character tables for simple point groups like C_{2v}, C_{3v}, and C_{2h}. **CO4 [Photochemical Transitions]:** Evaluate electronic transitions, spin-selection rules, and the Franck-Condon principle to interpret the absorption and emission spectra of molecules. **CO5 [Photophysical Phenomena & Applications]:** Explain Kasha's rule and the mirror-image relation (0-0 line) between

	absorption and emission spectra, and analyze excited-state phenomena including phosphorescence (via spin-orbit coupling), excimer/exciplex formation, delayed fluorescence, photostationary states, and excited-state acid-base behaviour (e.g., stilbene photoracemization), in the context of photosensitized reactions and photochemical equilibria. **CO6 [Excited State Decay Kinetics]:** Analyze the kinetics of radiative and non-radiative decay pathways and calculate quantum yields of emission processes via the Stern-Volmer equation. **CO7 [Hydrogenic Wavefunctions]:** Solve the Schrödinger equation for hydrogenic systems to explicitly derive radial and angular wavefunctions and define the shapes of $s, p,$ and d orbitals. **CO8 [Atomic Transitions & Magnetic Foundations]:** Explain spectroscopic transitions and selection rules for hydrogenic atoms, and relate the magnetic moment arising from orbital motion, electron spin (Stern-Gerlach experiment), and the Landé g-factor to atomic magnetic behaviour. **CO9 [Atomic Spectra & Magnetic Effects]:** Deduce Term Symbols using LS and $j-j$ coupling schemes for many-electron systems, and analyze the spectroscopic splitting of atomic orbitals in external magnetic fields (Zeeman and Paschen-Back effects). **CO10 [Coordination & Macrocyclic Synthesis]:** Synthesize transition metal complexes using redox non-innocent (azo, imino-quinone), pyridyl/benzothiazole, and macrocyclic/N-heterocyclic carbene ligands, isolate pure products via crystallization, and electrochemically characterize their efficiency in proton-coupled electron transfer (PCET) reactions. **CO11 [Click Chemistry]:** Synthesize azido and alkene/alkyne precursors and execute click and metathesis reactions under appropriate catalytic conditions to form 1,2,3-triazole derivatives. **CO12 [Functional Molecule Synthesis & Photophysical Characterization]:** Synthesize, isolate, and characterize chemosensor molecules (via PET/ICT mechanisms) and supramolecular gelators/metallogelators, evaluating their structure and photophysical properties using standard spectroscopic and analytical techniques. **CO13 [Physicochemical & Trace Analysis]:** Investigate lanthanide-antibiotic energy transfer and ESIPT-protein binary interactions, quantify trace arsenic content in environmental (soil/water) samples by atomic absorption spectrometry, and analyze the thermodynamics of clouding behaviour in non-ionic surfactants.

	CO14 [Computational Frameworks]: Develop and implement algorithmic frameworks (Genetic Algorithms, Particle Swarm Optimization) to navigate multidimensional chemical search spaces and optimize atomic coordinates.
Program Outcomes	**PO1: Fundamental Knowledge:** Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2: Laboratory Skills:** Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3: Problem Solving:** Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4: Research Competency:** Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5: Interdisciplinary Applications:** Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6: Communication Skills:** Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7: Ethics and Sustainability:** Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	**Core Curriculum Domain**	**Bloom’s Taxonomy (K-Level)**	**Mapped POs**
CO1	Foundations of Group Theory	**K2** (Understand), **K3** (Apply)	PO1, PO3
CO2	Matrix Representation Theory	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO3	Great Orthogonality & Character Tables	**K4** (Analyze), **K6** (Create)	PO1, PO3
CO4	Electronic Transitions & Franck-Condon	**K4** (Analyze), **K5** (Evaluate)	PO1, PO3
CO5	Photophysical Phenomena & Applications	**K2** (Understand), **K4** (Analyze)	PO1, PO3
CO6	Excited State Decay Kinetics	**K4** (Analyze)	PO1, PO3
CO7	Hydrogenic Wavefunctions	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO8	Atomic Transitions & Magnetic Foundations	**K2** (Understand), **K3** (Apply)	PO1, PO3
CO9	Term Symbols & Zeeman Splitting	**K4** (Analyze), **K5** (Evaluate)	PO1, PO3
CO10	Coordination & Macrocyclic Synthesis	**K3** (Apply), **K5** (Evaluate)	PO2, PO4
CO11	Click Chemistry	**K3** (Apply)	PO2, PO4
CO12	Functional Molecule Synthesis & Characterization	**K3** (Apply), **K6** (Create)	PO2, PO4, PO5
CO13	Physicochemical & Trace Analysis	**K3** (Apply), **K4** (Analyze)	PO2, PO5, PO7

CO14	Genetic Algorithms & PSO Optimization	**K4** (Analyze), **K6** (Create)	PO2, PO4, PO5

Reading/Reference Lists	1. Sears, F.W., Salinger, G.L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition. 2. Metiu, H., Physical Chemistry: Statistical Mechanics, Taylor and Francis 3. Laud, B. B., Statistical Mechanics, New Age 4. Chandler, D., Introduction to Modern Statistical Mechanics 1st Edition, OUP 5. McQuarrie, D. A., Statistical Mechanics, Viva 6. Pathria, R. K., Beale, P. D., statistical Mechanics, Academic Press 7. Cooksy, A., Physical Chemistry: Thermodynamics, Statitical Mechanics and Kinetics, Pearson 8. Levine, I.N., Molecular Spectroscopy, Wiley 9. Huang, K., Introduction to Statistical Physics, Chapman and Hall/CRC 10. Banwell, C.N., McCash E. M., Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill. 11. Barrow, G.M. Molecular Spectroscopy, McGraw-Hill. 12. Hollas, J.M. Modern Spectroscopy, Wiley India. 13. McHale, J. L. Molecular Spectroscopy, Pearson Education. 14. Wayne, C. E. & Wayne, R. P. Photochemistry, OUP. 15. Brown, J. M. Molecular Spectroscopy, OUP. 16. Heimz, P.C., Rajagopalan, R., Principles of Colloid and Surface Chemistry, Marcel Dekker. 17. Ohshima, H., Electrical Phenomenon at Interfaces and Bio-interfaces, Wiley. 18. Ohshima, H., Theory of Colloid and Interfacial Electric Phenomenon, Elsevier. 19. Israelachvili, J.N., Intermolecular and Surface Forces, Academic Press. Practicals: 1. Mukhergee, G.N., University Hand Book Of Undergraduate Chemistry Experiments	
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45	Practical: 40 CA: 38; Attendance:2

Paper Structure for Theory Semester Exam	Answer THREE out of FOUR questions, of 15 marks each.