NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI

Department of Chemistry

COURSE PLAN			
Course Title	Quantum Chemistry and Group Theory		
Course Code	**CH 605**	**No. of Credits**	**3 (Theory)**
Department	**Chemistry**	**Faculty**	**Dr. S. ANANDAN**
Pre-requisites Course Code	**NIL**		
Lab Course Coordinator(s) (if, applicable)	**-----**		
E-mail	**sanand@nitt.edu**	**Mobile No.**	**+91-9444052074**
Course Type	☑ **Core course** ☐ **Elective course**		

COURSE OVERVIEW

This is a three credit course offered to I year M.Sc. Chemistry students. Three theory classes will be conducted per week. This course provides a thorough understanding of the subject through lectures, tutorials, course work and demonstrations.

COURSE OBJECTIVE

To introduce the basic principles, importance and applications of Quantum Chemistry and Group Theory to the I year M.Sc. Chemistry students.

COURSE OUTCOMES (CO)

Students would become familiar with the

- ✓ The failures of Classical Physics.
- ✓ Quantum mechanical postulates.
- ✓ Schrodinger equation.
- ✓ Quantum mechanical results.
- ✓ Group theory - Symmetry Operations.
- ✓ Application of group theory.

COURSE TEACHING AND LEARNING ACTIVITIES

S.No.	**Week**	**Topic**	**Mode of Delivery**
1	I week of August	A brief introduction about the course and syllabus will be discussed. **Unit-I** The Failures of Classical Physics – Black Body Radiation-photoelectric effect-Bohr's Quantum theory	C&T, PPT
2	II week of August	Wave Particle Duality-Uncertainty Principle. Operator Algebra, Linear and Hermitian operators, Quantum mechanical postulates	C&T, PPT

3	III week of August	Schrodinger equation and its solution to the problem of a particle in one and three dimensional boxes.	C&T, PPT
4	IV week of August	**Unit-II** Schrodinger equation for hydrogen atom and its solution, the origin of electronic quantum members and physical significance	C&T, PPT
5	I week of September	Radial probability density-significance of magnetic quantum number with respect to angular momentum. Hydrogen molecule ion and hydrogen molecule-Pauli's exclusion principle.	C&T, PPT
6	II week of September	Term symbols for electronic state in atoms –LS and JJ coupling. Born Oppenheimer approximation, Mulliken designation of molecular orbitals.	C&T, PPT
7	III week of September	**Unit-III** Quantum mechanical results for a simple harmonic oscillator and rigid rotator, Solution of Schrodinger equation for harmonic oscillator	C&T, PPT
8	IV week of September	Rigid rotor, derivation of Eigen function and Eigen value for hydrogen atom - MO theory of bonding, and MO treatment of H-bonded systems, ethylene, butadiene and benzene.	C&T, PPT
9	I week of October	Approximation methods; Perturbation and variation method, wave functions for many electron atoms – Hartree – Fock SCF method, Slater Orbitals	C&T, PPT
10	II week of October	**Unit-IV** Group Theory-I: Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups	C&T, PPT
11	III week of October	Reducible and Irreducible Representation; Character Tables,	C&T, PPT
12	IV week of October	Orthogonality Theorem–Its Consequences.	C&T, PPT
13	I week of November	**Unit-V** Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization,	C&T, PPT
14	II week of November	classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy, systematic procedure for determining Symmetries of Normal Modes of Vibrations,	C&T, PPT
15	III & IV week of November	Chemical applications of group theory – AB2 and AB3.	C&T, PPT

COURSE ASSESSMENT METHODS				
S.No.	**Mode of Assessment**	**Week/Date**	**Duration**	**% Weightage**
Theory				
1	Group Task (Quiz/working model)/Assignment/Surprise test	II week of August	50 minutes	5
2	Test I	I week of September	60 minutes	20
3	Group Task (Quiz/working model)/Assignment/Surprise test	I week of October	50 minutes	5
4	Test II	IV week of October	60 minutes	20
5	End semester	I week of December	3 hours	50
Total (100)				

ESSENTIAL READINGS : Textbooks, reference books Website addresses, journals, etc

Text Books

1. I. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 1994.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill 1994.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers, 1988.

Reference Books

1. D. A. McQuarrie, 'Quantum Chemistry', University Science Books, 1983.
2. F.A. Cotton, 'Chemical Applications of Group Theory', 2nd Edn., Wiley Eastern Ltd., 1990.
3. R.K. Prasad, Quantum Chemistry, TMH, 1995
4. P.W. Atkins, 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.

COURSE EXIT SURVEY (mention the ways in which the feedback about the course is assessed and indicate the attainment also)

1. Feedback from students during class committee meetings.
2. Anonymous feedback through questionnaire at the end of the semester.

COURSE POLICY (including plagiarism, academic honesty, attendance, etc.)

1. Test I and II will be conducted during assessment period respectively.
2.Retest will be conducted for students who do not appear for the test I & II due to ill health or any other genuine reasons.
3. 75% attendance is compulsory for writing the end semester exam.
4. No formative assessment only Redo if students are absent for final examination.

ADDITIONAL COURSE INFORMATION

The faculty will be available for consultation at times as per the intimation by the faculty. Students can get prior permission either through email: sanand@nitt.edu or mobile no.: +91-9444052074

Faculty-in-charge _____ **CC-Chairperson** _____ **HOD** _____