

**DEPARTMENT OF CHEMISTRY**  
**NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI**

COURSE PLAN – PART I			
Name of the programme and specialization	M.Sc. Chemistry		
Course Title	CH 605 Quantum Chemistry and Group Theory		
Course Code	CH 605	No. of Credits	3
Course Code of Pre-requisite subject(s)	Nil		
Session	July 2018	Section (if, applicable)	-
Name of Faculty	Dr.L.Cindrella (For Group Theory)	Department	Chemistry
Email	cind@nitt.edu	Telephone No.	3634 (Intercom) 9443765332 (Mobile)
Name of Course Coordinator(s) (if, applicable)	Dr.L.Cindrella		
E-mail	cind@nitt.edu	Telephone No.	3634 (Intercom) 9443765332 (Mobile)
Course Type	<input checked="" type="checkbox"/> Core course <input type="checkbox"/> Elective course		
<b>Syllabus (approved in BoS)</b>			
<p><b>Group theory-I:</b> Elements of group theory, definition, group multiplication tables, conjugate classes, conjugate and normal subgroups, symmetry elements and operations, point groups, assignment of point groups to molecules, Matrix representation of geometric transformation and point group, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, symmetry adapted linear combinations, projection operators. Orthogonality theorem - its consequences.</p> <p><b>Group theory-II:</b> Symmetry aspects of molecular orbital theory, planar <math>\pi</math>-systems, symmetry factoring of Huckel determinants, solving it for energy and MOs for ethylene and 1,4-butadiene, sigma bonding in <math>AX_n</math> molecules, hybridization, tetrahedral, octahedral, square planar, trigonal planar, linear, trigonal bipyramidal systems, hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction, vibrational spectra, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition, IR and Raman activity of fundamentals in <math>CO_2</math>, <math>H_2O</math>, <math>N_2F_2</math>, the rule of mutual exclusion and Fermi resonance.</p> <p><b>References:</b></p> <ol style="list-style-type: none"> <li>1. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers, 1988.</li> <li>2. F. A. Cotton, Chemical Applications of Group Theory, 2<sup>nd</sup> Edn. Wiley Eastern Ltd., 1990.</li> </ol>			

<b>COURSE OBJECTIVES</b>	
To introduce the PG chemistry students to the basic principles of symmetry, postulates of group theory and the chemical applications of group theory.	
<b>COURSE OUTCOMES (CO)</b>	
<b>Course Outcomes</b>	<b>Aligned Programme Outcomes (PO)</b>
Students would become familiar with the	
1. Symmetry and consequence of symmetry of molecules	
2. Group theory concepts	
3. Great orthogonality theorem	
4. Matrix representation of transformation and character table	
5. Chemical applications of group theory in hybridization and spectral response of molecules	

<b>COURSE PLAN – PART II</b>			
<b>COURSE OVERVIEW</b>			
This is a part of the 3 credits course offered to the I year M.Sc. Chemistry students. This component of the course will be conducted as one class per week. Extra classes will be conducted as and when required to work on problems.			
<b>COURSE TEACHING AND LEARNING ACTIVITIES</b>			
<b>S.No.</b>	<b>Week/Contact Hours</b>	<b>Topic</b>	<b>Mode of Delivery</b>
1	I week of Aug	Elements of group theory, definition, group multiplication tables.	C&T, PPT
2	II week of Aug	Conjugate classes, conjugate and normal subgroups, symmetry elements and operations, point groups.	C&T, PPT
3	III week of Aug	Assignment of point groups to molecules, Matrix representation of geometric transformation and point group.	C&T, PPT
4	IV week of Aug	Reducible and irreducible representations, construction of character tables.	C&T, PPT, FC, TPS
5	I week of Sep	Bases for irreducible representation, direct product, symmetry adapted linear combinations.	C&T, PPT

6	II week of Sep	Projection operators, Orthogonality theorem - its consequences.	C&T, PPT
7	III week of Sep	Symmetry aspects of molecular orbital theory, planar $\pi$ -systems, symmetry factoring of Huckel determinants.	C&T, PPT
8	IV week of Sep	Energy and MOs for ethylene and 1,4-butadiene, sigma bonding in $AX_n$ molecules.	C&T, PPT
9	I week of Oct	Hybridization, tetrahedral, octahedral, square planar, trigonal planar, linear, trigonalbipyramidal systems.	C&T, PPT
10	II week of Oct	Hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction.	C&T, PPT, FC, TPS
11	III week of Oct	Vibrational spectra, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition.	C&T, PPT
12	IV week of Oct	IR and Raman activity of fundamentals in $CO_2$ , $H_2O$ , $N_2F_2$ , the rule of mutual exclusion and Fermi resonance.	C&T, PPT

**COURSE ASSESSMENT METHODS (shall range from 4 to 6)**

S.No.	Mode of Assessment	Week/Date	Duration	% Weightage
1	Quiz 1	III week of Sep	30 Minutes	10
2	Test 1	IV week of Oct	1 Hour	15
CPA	Compensation Assessment*	I Week of Nov	1 Hour	10 or 15
6	Final Assessment *		3 Hour	50

**COURSE EXIT SURVEY (mention the ways in which the feedback about the course shall be assessed)**

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

**COURSE POLICY (preferred mode of correspondence with students, compensation assessment policy to be specified)**

**MODE OF CORRESPONDENCE (email/ phone etc): Email / phone**

**COMPENSATION ASSESSMENT POLICY: The % Weightage for the compensation assessment will be as per the missed assessment.**

**ATTENDANCE POLICY (A uniform attendance policy as specified below shall be followed)**

- **At least 75% attendance in each course is mandatory.**
- **A maximum of 10% shall be allowed under On Duty (OD) category.**
- **Students with less than 65% of attendance shall be prevented from writing the final assessment and shall be awarded 'V' grade.**

**ACADEMIC DISHONESTY & PLAGIARISM**

- Possessing a mobile phone, carrying bits of paper, talking to other students, copying from others during an assessment will be treated as punishable dishonesty.
- Zero mark to be awarded for the offenders. For copying from another student, both students get the same penalty of zero mark.
- The departmental disciplinary committee including the course faculty member, PAC chairperson and the HoD, as members shall verify the facts of the malpractice and award the punishment if the student is found guilty. The report shall be submitted to the Academic office.

**ADDITIONAL INFORMATION**

The faculty will be available for consultation at times as per the intimation by the faculty.

**FOR APPROVAL**

Course Faculty *Hindille* 12/7/18 CC-Chairperson *Veeta B. Puri* HOD *GV*