NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI

DEPARTMENT OF CHEMISTRY

COURSE PLAN – PART I			
Name of the programme and specialization	M.Sc.(Chemistry)		
Course Title	Molecular Spectroscopy		
Course Code	CH 608	No. of Credits	3 (Theory)
Course Code of Pre-requisite subject(s)	Nil		
Session	January 2021	Section (if, applicable)	-
Name of Faculty	Dr. Sarthak Mandal	Department	Chemistry
Official Email	smandal@nitt.edu	Telephone No.	+91 8158805377
Name of Course Coordinator(s) (if, applicable)	Dr. R. Karvembu		
Official E-mail	kar@nitt.edu	Telephone No.	+914312503636
Course Type (please tick appropriately)	☑ Core course	☐ Elective course	

Syllabus (approved in BoS)

Unit I : Rotational Spectroscopy:

Interaction of radiation with matter–Spectroscopic Transitions-Einstein coefficients- transition probability- Born-Oppenheimer approximation- selection rules-intensity and width of spectral lines-Fourier transformation- Principal moments of inertia - Diatomic and polyatomic molecules- selection rules – Diatomic Rigid Rotor – Non Rigid Rotor – Nonlinear poly atomic molecules- Effect of Nulcear spin –Inversion Phenomenon – The Stark Effect

Unit II: Vibrational Spectroscopy

Polyatomic molecules -harmonic and anharmonic oscillators-Morse potential-selection rules–Fermi Resonance-Group Frequencies - normal modes of vibrations of polyatomic molecules-selection rules- Group theoretical approach to spectral activity - Vibration- Rotation spectroscopy-selection rules- FT- IR spectrometer – Instrumentation and sampling

Unit III: Raman Spectroscopy

Fundamentals- quantum mechanical description- Selection rules -rotational Raman - vibrational Raman spectra— Resonance Raman – Surface Enhanced Raman –Non-linear effects – Instrumentation and sampling

Unit IV: Atomic and Electronic spectroscopy

Atoms and molecules-term symbols- Russel – Saunders coupling – Racah Parameters – Zeeman Effect - Frank Condon principle- Vibronic Tranistions- selection rules- parity, symmetry and spin selection rules-polarization of transitions- Instrumentation and sampling - electronic spectra of conjugated systems Fluorescence Spectroscopy – Jablonski Diagram- Kashas rules- Quenching

Unit V: Electron spectroscopy

Photoelectric effect, basic principles of electron spectroscopy, classification - electron energy analysis-photon sources - UV, X-ray, synchrotron, theory, angular dependence-cross section and its determination-valence and core photoemission - Koopmans' theorem

References:

1. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th edn. Tata McGraw Hill, 1996.
2. J. M. Hollas, Modern Spectroscopy, 4 th Edn, John Wiley & Sons, 1992.
3. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn, Oxford University Press, 2005.
4. D. C. Harris and M. D. Bertolucci, Symmetry and Spectroscopy, Dover, 1989.
5. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, Wiley Interscience, 1983.

COURSE OBJECTIVES

To introduce the basic concepts and the applications of various molecular spectroscopic techniques to the M. Sc. students

MAPPING OF COs with POs

Course Outcomes Students will learn about	Programme Outcomes (PO) (Enter Numbers only)
1. Fundamentals of interactions of electromagnetic radiation with matter	
2. Rotational spectra of diatomic and polyatomic molecules	
3. Vibrational IR and Raman spectra of polyatomic molecules	
4. Electronic spectroscopy of atoms and molecules	
5. Fundamentals and applications of photoelectron spectroscopy	

COURSE PLAN – PART II

COURSE OVERVIEW

This course is offered to I year M.Sc.(Chemistry) students. This is 3 credit theory course. Three theory classes will be conducted per week.

COURSE TEACHING AND LEARNING ACTIVITIES (Add more rows)

S.No.	Week/Contact Hours	Topic	Mode of Delivery
1	III week of January	**Unit I** Electromagnetic radiation: its interaction with matter - Einstein coefficients – Transition probability - Born-Oppenheimer approximation	Online Mode (MS Team)

2	IV week of January	Rotational spectra: Diatomic and polyatomic molecules - selection rules, rotational Raman spectra - vibrational spectra of diatomic molecules	Online Mode (MS Team)
3	I week of February	Rotational character of vibration spectra - morse potential of real molecules - selection rules	Online Mode (MS Team)
4	II week of February	**Unit II** Vibrational Spectroscopy: Polyatomic molecules - harmonic and anharmonic oscillators - selection rules	Online Mode (MS Team)
5	III week of February	normal modes of vibrations - selection rules – Fourier transformation in IR spectroscopy	Online Mode (MS Team)
6	IV week of February	**Unit III-** Raman spectroscopy – fundamentals– IR/ Raman instrumentation.	Online Mode (MS Team)
7	I week of March	Resonance Raman – Surface Enhanced Raman –Non-linear effects – Instrumentation and sampling	Online Mode (MS Team)
8	II week of March	**Unit IV** Atomic Electronic spectroscopy: Atoms and molecules - term symbols - Frank Condon principle - vertical transitions -	Online Mode (MS Team)
9	III week of March	selection rules - parity, symmetry and spin selection rules	Online Mode (MS Team)
10	IV Week of March	Polarization of transitions - fluorescence and phosphorescence - Russell Sanders coupling -	Online Mode (MS Team)
11	I week of April	**Unit V** Electron spectroscopy: Photoelectric effect, basic principles	Online Mode (MS Team)
12	II week of April	Photon sources - UV, X-ray, synchrotron, theory, angular dependence - cross section and its determination -	Online Mode (MS Team)
13	III week of April	Koopmans' theorem - Introduction to ESCA - Auger electron spectroscopy - EXAFS.	Online Mode (MS Team)

COURSE ASSESSMENT METHODS (shall range from 4 to 6)

S.No.	Mode of Assessment	Week/Date	Duration	% Weightage
1	Assessment I (Assignment/Quiz)	II week of Feb	30 minutes (Online Mode)	5
2	Assessment II (Class Test 1)	IV week of Feb	60 minutes (Online Mode)	30
3	Assessemnt III (Assignment/Quiz)	II week of March	30 minutes (Online Mode)	5
4	Assessment IV (Class Test 2)	IV week of March	60 minutes (Online Mode)	30
CPA	Compensation Assessment*	III week of April	60 minutes (Online Mode)	30
6	Final Assessment *	IV week of April	2 hrs	30

Theory = Total (100)

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 (including compensation assessment to be specified)

MODE OF CORRESPONDENCE (email/ phone etc)
E-mail: smandal@nitt.edu/ Phone: +91 8158805377

COMPENSATION ASSESSMENT POLICY
For those students who missed Test I and Test II due to genuine reasons, Compensation assessment will be conducted during III week of April 2021

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.
- The above policy against academic dishonesty shall be applicable for all the programmes.

ADDITIONAL INFORMATION, IF ANY

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

FOR APPROVAL

5/2/2021 08/02/2021

Course Faculty: Dr. S. Mandal CC- Chairperson Dr. R. Karvembu HOD: Dr. S. Velmathi