DEPARTMENT OF CHEMISTRY

NATONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI

COURSE PLAN – PART I			
Name of the programme and specialization	**M.Sc. Chemistry**		
Course Title	**Spectroscopy- Applications in Organic and Inorganic Chemistry**		
Course Code	**CH 619**	**No. of Credits**	**3**
Course Code of Pre-requisite subject(s)			
Session	**July 2021**	**Section (if, applicable)**	**-**
Name of Faculty	**Dr. S. Mandal**	**Department**	**CHEMISTRY**
Email	**smandal@nitt.edu**	**Telephone No.**	**8158805377**
Name of Course Coordinator(s) (if, applicable)	**Dr. S. Mandal**		
E-mail	**smandal@nitt.edu**	**Telephone No.**	**8158805377**
Course Type	✓ **Core course**		

Syllabus (approved in BoS)

Nuclear magnetic resonance I: Concept and theory–Larmor frequency - rotating frame and laboratory frame-FT-generation and detection of FID –instrumentation- relaxation phenomena, 1H- NMR- chemical shift - chemical shift anisotropy- spin-spin coupling- mechanism and sign of J coupling- AX, AB, ABC, AMX, AABB, AA′BB′ systems - Karplus relationship- second order effects- chemical shift reagents- double irradiation experiments- 13CNMR –chemical shifts and line intensities- Spin decoupling- Nuclear Overhouser effect

Nuclear magnetic resonance II: Polarization transfer schemes- APT/INEPT/DEPT- dynamic processes by NMR- restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems) - Coalescence temperature- Multi nuclear NMR- 19F, 31P, and 11B spectra- 2-D methods COSY-HETCOR - HSQC - HMQC – TOCSY – INADEQUATE - Interpretation of spectra

Electron paramagnetic resonance: Basic principles-g- value- hyperfine interaction-anisotropy- CW ENDOR and TRIPLE- application to organic radicals and transition metal complexes- zero field splitting - Model system for pulse EPR experiments- Nuclear modulation experiments – ESEEM – HYSCORE- Davies and Mims ENDOR

Mass spectroscopy: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF) – instrumentation- magnetic sector analysis-quadrupole analyser- ion cyclotron resonance (FT)-meta stable ions - study of fragmentation pattern- -bond cleavage- McLafferty rearrangement-retro Alder fragmentation- applications in organic chemistry- isotope distribution analysis.

Mössbauer spectroscopy: Principles – Recoilless emission and absorption--Isomer shift -

Hyperfine- Magnetic Interactions-NQR spectroscopy– Applications of combined spectroscopic techniques in elucidating the structure of organic and inorganic molecules- case studies.

References: 1. D. N. Sathyanarayana, Handbook of Molecular Spectroscopy, From Radio waves to gamma rays, I.K international Publishing house Pvt. Ltd, 2015 2. R. S. Macomber, A Complete Introduction to Modern NMR Spectroscopy, John Wiley & Sons Ltd, 1998.
3. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. A. Vyvyan, Introduction to Spectroscopy, 5thEdn., Brooks Cole , 2010. 4. J. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Wiely-Interscience, 2007. 5. A. Schweigher, G. Jeshcke, Principles of Pulse Electron Paramagnetic Resonance, Oxford University press, 2002. 6. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, John Wiley & Sons, Ltd, 4th and 5thEdn. 2007 & 2013.

COURSE OBJECTIVES

To introduce the basic principles and applications of various spectroscopic techniques such as EPR, NMR, Mass and Mössbauer spectroscopic techniques to the M.Sc. students

COURSE OUTCOMES (CO)

Course Outcomes	**Aligned Programme Outcomes (PO)**
Course Outcomes Students will learn about	
1. Fundamentals of interactions of external magnetic field with magnetic moment of electron or nuclear spin.	
2. Basic principles and applicaitons of EPR spectroscopy	
3. NMR spectra of molecules for structure determination	
4. Mass spectroscopy of molecules	
5. Fundamentals and applications of Mössbauer spectroscopy	

COURSE PLAN – PART II

COURSE OVERVIEW

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

COURSE TEACHING AND LEARNING ACTIVITIES

Sl.No.	**Week**	**Topic**	**Mode of Delivery**

1	I WEEK AUG/2021	**Unit III:** **Electron paramagnetic resonance**: Basic principles-g- value- CW and pulsed EPR, net magnetization, relaxation mechanisms	Online Mode (MS Team)
2	II WEEK AUG/2021	Hyperfine interactions, splitting pattern, g-factor anisotropy, CW ENDOR and TRIPLE-basic principles-Application to organic radicals and transition metal complexes-	Online Mode (MS Team)
3	III WEEK AUG/2021	Zero field splitting -Pulse EPR basics-model system for pulse EPR experiments- Pulse schemes and applications-nuclear modulation experiments - ESEEM – HYSCORE-	Online Mode (MS Team)
4	IV WEEK AUG/2021	**Unit I:** **Nuclear magnetic resonance:** Concept and theory–Larmor frequency - rotating frame and laboratory frame - FT-generation and detection of FID – instrumentation- relaxation phenomena-1H- NMR- chemical shift	Online Mode (MS Team)
5	I WEEK SEPT /2021	-Chemical shift anisotropy- spin-spin coupling- mechanism-sign of J coupling- AX, AB, ABC, AMX, AABB, AA′BB′ systems-	Online Mode (MS Team)
6	II WEEK SEPT/2021	Karplus relationship- second order effects- Chemical shift reagents-double irradiation experiments-13CNMR –chemical shifts and line intensities	Online Mode (MS Team)
7	III WEEK SEPT/2021	**Unit II:** **Nuclear magnetic resonance**: Spin decoupling- Nuclear Overhouser effect–CIDNP-Solomon equations and cross relaxation -Polarization transfer schemes	Online Mode (MS Team)
8	IVWEEK SEPT/2021	APT/INEPT/DEPT- dynamic processes by NMR- restricted rotation (DMF, DMA, biphenyls, annulenes)-Cyclohexane ring inversion, degenerate rearrangements temperature-applications of 19F, 31P, and 11B spectra- other important nuclei -	Online Mode (MS Team)

9	I WEEK OCT/2021	Working of 2-D methods COSY-HETCOR - HSQC - HMQC - interpretation of spectra-structural identification	Online Mode (MS Team)
10	II WEEK OCT/2021	**Unit IV:** **Mass spectroscopy**: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF) –instrumentation	Online Mode (MS Team)
11	III WEEK OCT/2021	Magnetic sector analysis-quadrupole analyzer- ion cyclotron resonance (FT)- determination of molecular formula- meta stable ions - study of fragmentation pattern	Online Mode (MS Team)
12	IV WEEK OCT/2021	Bond cleavage-McLafferty rearrangement- retro Alder fragmentation- applications in organic chemistry- isotope distribution analysis.	Online Mode (MS Team)
13	I WEEK NOV/2021	**Unit V:** **Mössbauer spectroscopy:** Principles and Applications-Hyperfine- Magnetic Interactions-NQR spectroscopy	Online Mode (MS Team)
14	II WEEK NOV/2021	Principles and Applications-Applications of combined spectroscopic techniques	Online Mode (MS Team)
15	III WEEK NOV/2021	Double bond equivalence-case studies and structural identification of organic compounds and inorganic compounds	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)	IV WEEK AUG/2021	30 minutes	5
2	Assessment II (CT – 1)	II WEEK SEPT/2021	1 hour	30
3	Assessment III (Assignment/Quiz)	II WEEK OCT/2021	30 minutes	5
4	Assessment IV (CT – 2)	II WEEK NOV/2021	1 hour	30
CPA	Compensation Assessment*	III WEEK NOV 2021	1 hour	30
5	Final Assessment *	I WEEK DEC 2021	3 hours	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 (preferred mode of correspondence with students, compensation assessment policy to be specified)

MODE OF CORRESPONDENCE (email/phone)

smandal@nitt.edu/8158805377

COMPENSATION ASSESSMENT POLICY

For those students who missed Class Test I and/or Class Test II due to genuine reasons, compensation assessment will be conducted during III week of November 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

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

FOR APPROVAL

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