Department of Chemistry

NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI

COURSE PLAN – PART I			
Name of the programme and specialization	**M.Sc.(Chemistry)**		
Course Title	Fundamentals and applications of spectroscopy		
Course Code	**CH 619**	**No. of Credits**	**3 (Theory)**
Course Code of Pre-requisite subject(s)	**Nil**		
Session	**July 2018**		
Name of Faculty	**Dr. A. Sreekanth**	**Department**	**Chemistry**
E-mail	**sreekanth@nitt.edu**	**Telephone No.**	**+91-431-2503642**
Name of Course Coordinator	**Dr. G. Venkatesaprabhu**		
E-mail	**venkates@nitt.edu**	**Telephone No.**	
Course Type	☑ **Core course**	☐ **Elective course**	

Syllabus (approved in BOS)

Nuclear magnetic resonance: Concept and theory–Larmor frequency - rotating frame and laboratory frame-FT-generation and detection of FID –instrumentation- relaxation phenomena, $_{1}H$- 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- $_{13}CNMR$ –chemical shifts and line intensities

Nuclear magnetic resonance: Spin decoupling- Nuclear Overhouser effect–CIDNP-Solomon equations and cross relaxation- 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), organometallic systems. Significance of coalescence temperature- analysis and applications of $_{19}F$, $_{31}P$, and $_{11}B$ spectra- other important nuclei- working of 2-D methods COSY-HETCOR - HSQC - HMQC – TOCSY – INADEQUATE - interpretation of spectra-introduction to solid state NMR- cross polarization – WAHUHA- imaging methods in magnetic resonance.

Electron paramagnetic resonance: Basic principles-hyperfine interaction- zero-field energy levels-McConnal equations –anisotropy- CW ENDOR and TRIPLE-basic principles- application to organic radicals and transition metal complexes- zero field splitting -Pulse EPR basics- model system for pulse EPR experiments- pulse schemes and applications-nuclear modulation experiments – ESEEM – HYSCORE- Davies and Mims ENDOR- distance measurements using ELDOR- NQR fundamentals **Mass**

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

Mössbauer spectroscopy: Principles and applications-Hyperfine- Magnetic Interactions-NQR spectroscopy–Principles and Applications- Applications of combined spectroscopic techniques- double bond equivalence-case studies and structural identification of organic compounds and inorganic compounds

ESSENTIAL READING: Textbooks and Reference books

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.
7. M. Balci, Basic $_{1}$H- and $_{13}$C-NMR Spectroscopy, Elsevier, 2005.
8. J. H. Simpson, Organic Structure Determination using 2D-NMR Spectroscopy, Academic Press, 2008.
9. D. P. E. Dickson, F. J. Berry, Ed. Mossbauer Spectroscopy, Cambridge University Press, 1986.
10. M. H. Levitt, Spin Dynamics- Basics of Nuclear Magnetic Resonance,2ndEdn, John Wiley and sons, 2008.
11. E. Breitmaier, Structure Elucidation by NMR in Organic Chemistry - A Practical Guide, 3rdEdn, John Wiley and Sons, 2002.
12. W. Hendreson, J. S. McIndoe, Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds, John Wiley and Sons, 2005.
13. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds Part A &Part B, 2ndEdn, Wiely, 2009.

COURSE OBJECTIVES

To Introduce the advanced concepts of NMR, EPR and Mass Spectroscopy. Problem solving ablity and interpretation of Spectra.

COURSE OUTCOMES (CO)

Course Outcomes	Aligned Programme Outcomes (PO)
1. To know the importance NMR, EPR, Mass and Mossbauer Spectroscopy.	
2. To understand sampling methods of the analytes to be measured.	
3. To get familarise with the principles,	

operation
and uses of these instruments in industry
4. To conduct demonstration experiments in industry with real samples.

COURSE PLAN – PART II

COURSE OVERVIEW

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

COURSE TEACHING AND LEARNING ACTIVITIES

S.No.	Week	Topic	Mode of Delivery
1	IInd week of July	**Nuclear magnetic resonance:** Concept and theory– Larmor frequency - rotating frame and laboratory frame-FT-generation and detection of FID – instrumentation- relaxation phenomena, $_{1}H$- NMR- chemical shift - chemical shift anisotropy	C&T, PPT
2	Ist week of August	- 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-	C&T, PPT
3	IInd week of August	double irradiation experiments- $_{13}$CNMR –chemical shifts and line intensities	C&T, PPT
	IIIrd week of August	**Nuclear magnetic resonance**: Spin decoupling- Nuclear Overhouser effect–CIDNP-Solomon equations and cross relaxation- polarization transfer schemes- APT/INEPT/DEPT-	
4	IV week of August	dynamic processes by NMR- restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems), organometallic systems. Significance of coalescence temperature-	C&T, PPT
5	I week of September	analysis and applications of $_{19}F$, $_{31}P$, and $_{11}B$ spectra- other important nuclei- working of 2-D methods COSY-HETCOR - HSQC - HMQC – TOCSY – INADEQUATE - interpretation of spectra- introduction to solid state NMR- cross polarization – WAHUHA- imaging methods in magnetic resonance.	C&T, PPT
6	II week of	**Electron paramagnetic resonance**: Basic principles-	C&T, PPT

	September	hyperfine interaction- zero-field energy levels- McConnal equations –anisotropy- CW ENDOR and TRIPLE-basic principles-	
7	III week of September	application to organic radicals and transition metal complexes- zero field splitting -Pulse EPR basics- model system for pulse EPR experiments-	C&T, PPT
8	IV week of September	pulse schemes and applications-nuclear modulation experiments – ESEEM – HYSCORE- Davies and Mims ENDOR- distance measurements using ELDOR- NQR fundamentals	C&T, PPT
9	I week of October	**Mass spectroscopy**: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF) – instrumentation- magnetic sector analysis-	C&T, PPT
10	II week of October	quadrupole analyzer- ion cyclotron resonance (FT)- determination of molecular formula- meta stable ions - study of fragmentation pattern- -bond cleavage-McLafferty rearrangement-	C&T, PPT
11	III week of October	retro Alder fragmentation- applications in organic chemistry- isotope distribution analysis.	C&T, PPT
12	IV week of October	**Mössbauer spectroscopy:** Principles and applications-Hyperfine- Magnetic Interactions-NQR spectroscopy–Principles and Applications- Applications of combined spectroscopic techniques-	C&T, PPT
13	I week of November	double bond equivalence-case studies and structural identification of organic compounds and inorganic compounds	C&T, PPT
14	II week of November	double bond equivalence-case studies and structural identification of organic compounds and inorganic compounds	C&T, PPT

COURSE ASSESSMENT METHODS

S.No.	Mode of Assessment	Week/Date	Duration	% Weightage
Theory				
1	Assignment	I week of Sep	One week	5
2	Test I	12.09.2018	60 minutes	20
3	Seminar	III week of Oct	One week	5
4	Test II	24.10.2018	60 minutes	20
CPA	Compensation Assessment	III week of Nov	60 minutes	20

5	Final Asessment	IV week of Nov	3 hours	50

COURSE EXIT SURVEY

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

COURSE POLICY

MODE OF CORRESPONDENCE (email/ phone etc)

sreekanth@nitt.edu

COMPENSATION ASSESSMENT POLICY

1. This assessment is for those students who missed Test I or Test II due to genuine reasons
2. Compensation assessment will be conducted during the III week of November 2018.

ATTENDANCE POLICY

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

FOR APPROVAL

Course Faculty _____ **CC-Chairperson** _____ **HOD** _____