Semester	AUG 2022
Open to semester	7,13,21
Course code	**CH4194/CH6344**
Course title	**Fundamentals of Solution-State NMR Spectroscopy: Principles and Applications (NKN)**
Credits	4 /4
Course Coordinator & participating faculty (if any)	Jeetender Chugh
Nature of Course	Lectures
Pre-requisites	• Basics of vector calculus, matrix algebra, and trigonometry • Basics of quantum chemistry (wave-function, postulates, operators, time-dependent Schrödinger's equation) • Fundamentals of molecular spectroscopy (desirable)
Objectives (goals, type of students for whom useful, outcome etc)	o To define the fundamental concepts in the field of nuclear magnetic resonance (NMR) spectroscopy o To classify, discuss the theoretical origin and explain the background of NMR experiments o To apply and construct the framework developed towards understanding one- and multi-dimensional NMR experiments o To learn to analyze, compare and contrast experiments towards their application in biomolecular systems o To develop a hands-on training model on the basics of data processing and analysis of biomolecular model systems
Course contents (details of topics /sections with no. of lectures for each)	This is an NKN course, students from IISER Bhopal and Trivandrum would also be attending the lectures. This year it will be taught by a faculty from IISER TVM. • Classical picture of NMR o An introductory class on NMR parameters with simple examples: chemical shift, scalar coupling, integration. Deal with the entity called spin, introduce magnetic moment, magnetogyric (gyromagnetic) ratio, energy level splitting for an isolated spin system, the population in the quantum states o Bloch equations o Predicting the spectrum of AX, AX2, AMX, AM2 X 2 systems, Bloch eq. Limitations • Quantum mechanical picture and application to basic modules o Representation of the wave-function in terms of the density

	matrix, deduction of the equilibrium density matrix, representation of the density matrix with a complete set of spin operators o Time evolution of the density matrix - Liouville von Neumann equation, Baker-Campbell-Hausdorff formula, propagator formalism for deducing evolution of density matrix • Application of density matrix formulation to basic modules and 1D NMR o Spin-echo (chemical shift refocusing, scalar coupling evolution, shift evolution, and refocussing of active scalar couplings as in 2D NMR) o Insensitive Nuclei Enhancement by Polarization Transfer (INEPT) - provide examples of 1 H to X nuclei, 13C to 1 5N Spin-state selective coherence transfer o Basic 1D NMR applications o Brief qualitative description of Fourier Transformation (FT) o Basic one-pulse 1D FT NMR - 1 H and 1 3C (without steadystate enhancement) o Refocussed-INEPT (RINEPT) module for 13C 1D NMR o Distortionless Enhancement by Polarization Transfer (DEPT) - 45o, 90o, 135o and its application to distinguish methyl, methylene, and methine groups • Basic NMR instrumentation and data processing o Description of NMR hardware, recent hardware advancements (cryogenic probe and high-field magnets), factors influencing signal to noise, digital quadrature detection o Pulse features - bandwidth, pulse phase modulation and phase cycling, shaped pulses, offset dependence, gradient pulses (application in phase cycling, coherence selection, solvent suppression) o Data processing - phase correction, reasons for phase artifacts, delayed acquisition, aliasing, folding • Introduction to 2D NMR 7 classes o Basic concepts in multidimensional NMR - “indirect” dimension o Homonuclear 2D experiments: COSY (regular, 60o, DQF) o POF of essential modules: constant-time, semi-constant-time modules o Heteronuclear 2D experiments: single-quantum (HSQC), multiple-quantum (HMQC), multiple-bond (HMBC) Other essential concepts: sensitivity enhancement

	(preservation of equivalent pathways), echo-anti echo, time proportional phase incrementation (TPPI),Transverse Relaxation Optimized SpectroscopY (TROSY) with qualitative discussion on relaxation • Protein NMR spectroscopy o Theoretical description of protein chemical shift assignment o Hands-on data processing training using NMRPipe o Hands-on training with data in SPARKY/CARA • Nucleic Acids NMR o Theoretical description of DNA and RNA CS assignment o Hands-on training with data in SPARKY
Evaluation /assessment	End-Sem Examination-40% Mid-Sem Examination-40% Others-20% over four quizzes%
Suggested readings (with full list of authors, publisher, year, edn etc.)	• Protein NMR Spectroscopy: Principles and Practice. Authors: John Cavanagh, Nicholas J. Skelton, Arthur G. Palmer, III, Wayne J. Fairbrother. Hardcover ISBN: 9780121644918. • Fundamentals of Protein NMR Spectroscopy. Authors: Gordon S. Rule, Kevin T. Hitchens. ISBN 978-1-4020-3500-5. • Spin Dynamics. Author: Malcolm H. Levitt. ISBN: 978-0-470-51117-6 • Understanding NMR Spectroscopy. Author: James Keeler. ISBN: 978-0-470-74608-0