



Accredited with NAAC **A** Grade
12-B Status from UGC

TEERTHANKER MAHAVEER UNIVERSITY
(Established under Govt. of U. P. Act No. 30, 2008)
Delhi Road, Moradabad (U.P.)

PhD PROGRAMME

SYLLABUS FOR DISCIPLINE-SPECIFIC COURSE
CHEMISTRY

Course Code: PDS240127	Advances in Chemistry	L	T	P	C
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Objective:	To familiarize the research scholar with the fundamentals of scientific research.				
Course Outcomes:	On completion of the course, the students will be able to:				
CO 1:	Understand the metal-ligand Equilibria, Substitution reaction & electron transfer reaction in coordination chemistry.				
CO 2:	Understand the addition reaction in C=C and C=O and their stereochemistry involved various organic reactions.				
CO 3:	Understand the Chemical dynamics of chemical compounds.				
CO 4:	Understand in-depth principles of NMR Spectroscopy and interpret the ¹ H NMR spectra of unknown organic compounds.				
CO 5:	Analyze the X-ray diffraction techniques with a description of the procedure for an X-ray structure analysis.				
Course Content:					
Unit 1:	Metal-Ligand Bonding: Molecular orbital theory. Qualitative aspects of metal-ligand sigma bonding in octahedral, tetrahedral, and square planar complexes. Jahn-Teller Effect, Electronic Spectra and of Transition Metal Complexes. Spectroscopic term, terms and microstates for the p ² and d ² configurations, Hund's rules for ground state terms, the correlation of spectroscopic terms into Mulliken symbols, electronic transition selection rules, Orgel diagrams for transition metal complexes (d ¹ -d ⁹ states). Jahn-teller effect and electronic spectra of complexes				
Unit 2:	Reaction Mechanism. Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, and control, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, and isotope effects. Effect of structure on reactivity - resonance and field effects, steric effect.				
Unit 3:	Chemical Dynamics. Methods of determining rate laws, Arrhenius equation, collision theory of reaction rates, steric factor, activated complex theory, ionic reactions, kinetic and thermodynamic control of reactions.				
Unit 4:	Nuclear Magnetic Resonance Spectroscopy: The spinning nucleus, effect of an external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift. Factors influencing chemical shift, anisotropic effect; spin-spin coupling constant, Methods of resolving complex spectra, Applications of PMR in structural elucidation of simple and complex compounds. ¹³ C NMR, Deuterium, fluorine and phosphorus NMR, Structural applications of ¹³ C-NMR.				

Unit 5:	X-ray Diffraction. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of Unit cells from systematic absences in the diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis.
Textbooks:	<ol style="list-style-type: none"> 1. Huheey, J.E. Inorganic Chemistry, Pearson. 2. March, Jerry. Advanced Organic Chemistry: Reactions, Mechanism and Structure, John Wiley. 3. Atkins, P.W. Physical Chemistry, ELBS 4. Kemp, W. Organic Spectroscopy, Macmillan.
Reference Books:	<ol style="list-style-type: none"> 1. Cotton, F.A. and Wilkinson, G. Advanced Inorganic Chemistry, Wiley eastern. 2. Sykes, Peter. A Guide Book to mechanism in Organic Chemistry, Longman. 3. Moore, J.W. and Pearson, R.G. Kinetics and Mechanism, John Wiley and Sons. 4. Barrow, G.M. Introduction to Molecular Spectroscopy, McGraw Hill. 5. Banwell, C.N. Fundamentals of Molecular Spectroscopy, McGraw Hill. <p>*Latest editions of all the suggested books are recommended.</p>
Additional Electronic Reference Material:	<ol style="list-style-type: none"> 1. https://www.youtube.com/watch?v=Rf1luRh6Y5w 2. https://www.youtube.com/watch?v=dfA9t8i38-k 3. https://www.digimat.in/nptel/courses/video/115103104/L01.html 4. https://www.khanacademy.org/science/organicchemistry/spectroscopy-jay/proton-nmr/v/introduction-to-proton-NMR 5. https://www.digimat.in/nptel/courses/video/104108078/L01.html