KTE 211/2 – Group Theory and Spectroscopy

Course Objectives: 1) To introduce the basic concepts of symmetrical elements and point groups.
2) To introduce the principles of molecular spectroscopy and techniques.

Topic	Content	Number of lecture hours	Expected outcome - upon completion of this course, the student should be able to:
1. Group Theory	• Symmetrical elements and operations	3	• Understand the types of symmetrical elements and symmetrical operations in particular with respect to applications of chemical structures. • Differentiate between symmetrical elements and symmetrical operations.
	• Determination of point groups • Basic concept of Group Theory for chemical species	3	• Understand the use of flow-charts for the determination of point groups for wide selection of chemical structures. • Understand the rules and basic concept of class in the context of Group Theory. • Understand the use of matrices in representing the symmetrical operations. • Derive the character for each matrix which represents the symmetrical operation on known base. • Understand the properties of Character Tables and the implications of the members in the Table.

Topic	Content	Number of lecture hours	Expected outcome - upon completion of this course, the student should be able to:
	• The concepts of irreducible representations and reducible representations	3	• Understand the on concept applications of various basis functions. • Identify and derive reducible and irreducible representations. • Understand the reduction process of reducible representation for atomic displacements in chemical species.
	• Application of Group Theory in vibrational spectroscopy and molecular orbitals	3	• Obtain the appropriate orbital for the respective π-bonding in certain molecule. • Derive the symmetry representations of vibrations and determine the Infrared and Raman activity. • Propose the symmetry properties of the mode of molecular vibration. • Determine the type of vibration which can be observed in the Infrared and Raman spectra. • Differentiate among the isomers by using the Group Theory.
2. Spectroscopy	• Basic principles of molecular spectroscopy	1	• Understand the interaction between the electromagnetic wave and mass. • Know the fundamental aspect of electronic transition in atoms and molecules. • Know the basic aspects of rotational and vibrational spectroscopy.
	• Rotational infrared and microwave spectroscopy	2	• Understand the linear, symmetric rotor, spherical rotor and asymmetric rotor molecules. • Explain the spectrum and rotational energy associated with certain molecules. • Know how to determine the moment of inertia for diatomic molecules. • Understand the *isotopic effect* upon moment of inertia.

Topic	Content	Number of lecture hours	Expected outcome - upon completion of this course, the student should be able to:
	• Vibrational spectroscopy	2	• Understand the molecular vibration of diatomic molecules. • Know the principles involved in the infrared/Raman spectra in relation to harmonic and anharmonic oscillation. • Understand the transitions between the stacks of rotational energy levels associated with two different vibrational levels which result in the P, Q and R branches.
	• Electronic spectroscopy for atom and molecule	3	• Understand the atomic structure and quantum number. • Know about the energy associated with the respective atomic and molecular orbitals. • Understand the electronic spectra and the Frank-Condon principle. • Know how to adopt the molecular orbital concept to assume the electronic configuration. • Understand and derive the electronic states arising from configuration.
	• Spectroscopy of UV/FT-IR/FT-NMR	4	• Understand the basic concept associated with the respective techniques of UV/FT-IR/FT-NMR which have well been adopted in the characterisation of chemical compounds.
TOTAL		**24**	