Course (Unit) Title	**Quantum Mechanical Approach to Atomic and Molecular Structure and Molecular Spectroscopy**
Course (Unit) Code	CHE202G3
Credit Value	03 (45 hours of lectures and tutorials)
Objective/s	• Outline quantum mechanical principles to understand atomic and molecular structure • Illustrate chemical bonding in molecules using quantum mechanical principles • Define crystal systems and diffraction methods • Understand the basic principles of molecular spectroscopy and their applications
Intended Learning Outcomes	• Explain the atomic and molecular structure of simple molecules using quantum mechanics • Describe the bonding in homo and hetero nuclear diatomic and poly atomic molecules • Analyze structure of crystals and their characterizations • Identify the transitions between rotational, vibrational and electronic states to the spectra of diatomic and polyatomic molecules • Solve realistic problems related to molecular spectroscopy
Contents	**Quantum Mechanics (14 hours)** • The origins of quantum mechanics, derivation of Schrödinger wave equation, quantum mechanical principles, applications of Schrödinger wave equation to a particle moving in one, two and three-dimensional boxes, degeneracy • The Born interpretation of wave function, polar coordinate system, Born-Oppenheimer approximation, solution of time-independent Schrödinger wave equation for the hydrogen atom and hydrogen like ions, radial and angular functions, radial probability and angular probability functions, orbital shapes, radial distribution curves, many electron atoms, electron penetration and orbital energies, calculation of effective nuclear charge **Molecular Structure and Chemical Bonding (9 hours)** • LCAO method, variation principle, introduction to Hartree's self-consistent field approximation method, valence bond and molecular orbital approaches in diatomic (homo nuclear and hetero nuclear) and polyatomic molecules, hybrid orbitals, ionic compounds, calculation of r_+ and r_- from inter nuclear distance, band theory, conductors, semiconductors and insulators

	Crystal Systems and Diffraction Methods (7 hours) • Introduction to crystals, types of crystals, symmetry elements, point groups, space lattice and unit cell, Miller indices, diffraction methods **Molecular spectroscopy (15 hours)** • Molecular properties: Electrical properties (dipole moment, permittivity, polarizability), magnetic properties (magnetic moment, magnetic susceptibility) • Introduction to molecular spectroscopy of diatomic and polyatomic molecules • Rotational spectroscopy: Moment of inertia, rotors and their symmetry, quantization of rotational energy, selection rule, isotope effects, intensity • Vibrational spectroscopy: Harmonic oscillator, quantization of vibrational energy, selection rule, isotope effects, anharmonicity, fundamental and overtone transition, hot bands, vibrational modes. • Ro-vibrational spectroscopy: Selection rules, parallel and perpendicular vibration • Raman spectroscopy: Raman and Rayleigh scattering, Stokes and anti-Stokes scattering, rotational and vibrational Raman spectra • Electronic spectroscopy: Potential energy curve, classification of electronic states, electronic selection rules, Franck-Condon principle, fluorescence, phosphorescence
Teaching and Learning Methods / Activities	Lectures, Tutorials and Assignments
Evaluation	In-course Assessments 30% End of Course Examination 70%
Recommended References	• Atkins, P. and de Paula, *Physical Chemistry*, 10th edition Oxford: Oxford University Press, 2014 • Atkins, P and Paula, J. D., *Physical Chemistry*, 9th Edition, Oxford University Press, 2010 • Ira N. Levine, *Physical Chemistry*, 6th Edition, Mr Graw Hill Education, 2009 • Aruldhas, G., *Molecular Structure and Spectroscopy*, 2nd Edition, PHI Learning Pvt. Ltd., 2011. • Brown, J. M., *Molecular Spectroscopy*, 1st Edition, Oxford University Press, 1998. • Sruve, W. S., *Fundamentals of Molecular Spectroscopy*, Wiley Inter science, 1st Edition, 1989.