

SEMESTER VII

KU7DSCCHE401: THEORETICAL CHEMISTRY- II

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
VII	DSC	400	KU7DSCCHE401	4	75

Learning Approach (Hours/ Week)			Marks Distribution			Duration of ESE (Hours)
Lecture	Practical/ Internship	Tutorial	CE	ESE	Total	
3	2	0	35	65	100	1.5

Course Description: The course provides fundamental principles and experimental foundations that shaped quantum theory and also quantum vibrational and rotational motion, solving Schrödinger's equation for various systems. The course also covers representations of point groups and the application of the Great Orthogonality Theorem (GOT) to molecular spectroscopy and chemical bonding. Practical sessions utilizing computational chemistry tools will reinforce theoretical concepts through hands-on experiments and visualizations.

Course Prerequisite: Basics of quantum chemistry including operator algebra, eigen values and mathematical skills

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	Enable students to understand the scientific fundamentals governing the behaviour of quantum systems.	U

2	A comprehensive understanding of the fundamental quantum mechanical models, providing insights into the behaviour of particles in confined spaces, harmonic potentials, and rotational motion, respectively	A
3	Learning how to represent scientifically, symmetry operations as matrices and point groups in terms of reducible and irreducible representations	A
4	To analyze representations of point groups and use the Great Orthogonality Theorem to construct character tables and classify symmetry operations.	An
5	Apply skill in challenging computational chemistry problems	A

***Remember (R), Understand (U), Apply (A), Analyse (An), Evaluate (E), Create (C)**

Mapping of Course Outcomes to PSOs

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PSO 7
CO 1	3	1	2	1	1	2	2
CO 2	3	1	2	1	1	2	2
CO 3	3	1	2	1	1	2	2
CO 4	3	1	2	1	1	2	2
CO 5	3	1	2	1	1	2	2

Course Contents for Classroom Transaction:

M O D U L E	U N I T	DESCRIPTION	HOURS
1	QUANTUM MECHANICAL MODELS		10
	1	Quantum Vibrational Motion: –One-dimensional harmonic complete treatment with derivation – Wave functions – Hermite polynomials- Recursion relation–Energy levels –Important features of the problem –comparison with classical results	
	2	Quantum Rotational Motion–Planar rigid rotor (or particle on a ring)– Derivation of the Φ -equation– Energy levels.	
	3	Quantum Rotational Motion–One particle rigid rotator (non-planar rigid rotator or particle on a sphere- complete treatment with derivation of rigid rotor model of diatomic molecule): The wave equation in spherical polar coordinates, separation of variables, the Φ -equation and the Θ -equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics. Space quantization of angular momentum.	
2	ROTATIONAL MOTION AND ONE ELECTRON SYSTEMS (Hydrogen like)		5
	1	One electron quantum system: Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation	

		of variables, the R, Θ and Φ -equations and their solutions (with derivation).	
	2	Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen atom, orbitals, orthonormality of wave functions,	
	3	Radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots.	

	REPRESENTATIONS OF POINT GROUPS		10
3	1	Matrix representation of symmetry operations – Representations of point groups – Matrix representation of point group and its characteristics basis for a representation– Representation based on the character of matrices.	
	2	Representations using vectors –Atomic orbitals positioned on atom in a molecule as basis (H ₂ O and butadiene as examples) – Cartesian coordinates positioned on each atom of molecule as bases (H ₂ O as example)	
	3	Classification of representations: reducible representations and irreducible representations (IR) – construction of IR by reduction (qualitative demonstration only)	

4	GREAT ORTHOGONALITY THEOREM AND ITS APPLICATIONS:	20
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1	Great Orthogonality Theorem: Statement – consequences of GOT, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2v} , C_{3v} , C_{2h} , C_{4v} and C_3 as examples), nomenclature of IR – Mulliken symbols, symmetry species; Reduction formula – Derivation of reduction formula using GOT, reduction of reducible representations, (e.g., Γ_{cart}) using the reduction formula; Relation between group theory and quantum mechanics – Wave functions (orbitals) as bases for IR of point groups.	
2	Applications of GOT to Molecular Spectroscopy: Molecular vibrations – symmetry species of normal modes of vibration, construction of Γ_{cart} – normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments – determination of IR active and Raman active modes of molecules (e.g., H_2O , NH_3 , CH_4 , SF_6) – complementary character of IR and Raman spectra. Spectral transition probabilities – direct product of irreducible representations and its use in identifying vanishing and non-vanishing integrals, transition moment integral and spectral transition probabilities, overlap integrals and conditions for overlap.	
3	Applications of group theory to chemical bonding: Hybridization - Treatment of hybridization in BF_3 , CH_4 and PCl_5 – Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – NH_3 , H_2O and Octahedral examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), construction with projection operator. (NH_3 , H_2O and Octahedral as examples)	
	TEACHER SPECIFIC MODULE: PRACTICALS	30

5	COMPUTATIONAL CHEMISTRY PRACTICALS:		18
	Experiments using modern open source/free computational chemistry packages in computing different parameters of simple molecules (compulsory to do 1 to 5)		
	1	Calculation of the electronic energies (in kcal/mol) of global minimum conformation of simple molecules such as water, ammonia, methane and benzene using HF/STO-3G method.	
	2	Calculation of the resonance energy of benzene using HF/3-21G method.	
	3	Calculation of ionization energy and electron affinity of O ₂ and N ₂ molecules using HF/STO-3G method	
	4	Calculation of IR frequencies of vibrations in water and CO ₂ molecules using HF/3-21G method.	
5	5	Calculation of ring strain energy of cyclopropane using B3LYP/3-21G method.	
General Procedure for above Computational Chemistry Experiments: The software (Avagadro, Firefly/Gamess and Facio) for the above experiments are freely available and can be installed in windows OS. 1. Use Avagadro software to draw/ insert the structure and generate the input file for firefly/Gamess run. 2. Set the firefly/gamess software path in Facio graphics software and run the input file 3. The output file can be analysed using facio.			
OPEN ENDED			12
Directions:			
Use Virtual Labs and Online Tools (e.g., NanoHUB, PhET interactive simulation interface (phet.colorado.edu) of University of Colorado Boulder) for virtual experiments and labs related to quantum mechanics. Use softwares (like Excel, GNUPlot, Mathematica, Geogebra, SciLab) to do the following			

1	Plotting particle in 1D and 3D box, Harmonic oscillator and Rigid rotor wavefunctions	
2	Calculating energies of a particle in 1D and 3D-box, Harmonic oscillator and Rigid rotor	
3	Visualizing probability densities and comparing different scenarios.	
4	Demonstrating GMT based on matrix representations (Use SciLab / Mathematica)	
5	Constructing GMT game with abstract elements using an excel sheet	

Essential Readings:

1. D. A. McQuarrie, "Quantum Chemistry", University Science Books, 1983 (Viva books, 2003).
2. A.K. Chandra, "Introduction to Quantum Chemistry", 4th Edition, Tata McGraw-Hill, 1994.
3. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc., 2009
4. F.A. Cotton, "Chemical applications of Group Theory", 3rd Edition, John Wiley & Sons Inc., 2003
5. Arthur M Lesk, "Introduction to Symmetry & Group theory for Chemists", Kluwer Academic Publishers, 2004
6. Robert L. Carter, 'Molecular Symmetry and Group Theory', Wiley India Edition, 2005

Assessment Rubrics:

Evaluation Type		Marks
End Semester Evaluation (ESE)		65 (50T+15P)
Continuous Evaluation (CCA)		35 (25T+10P)
Theory		25
a)	Test Paper*	10
b)	Assignment	5
c)	Viva-Voce	5
d)	Seminar	5
Practical		10
a)	Skill	4
b)	Record	4
c)	Punctuality	2
Total		100

*Average mark of the best two written tests may be considered for internal mark.