CALICUT UNIVERSITY – FOUR-YEAR UNDERGRADUATE PROGRAMME (CU-FYUGP)

B. Sc. CHEMISTRY

Programme	**B. Sc. Chemistry**				
Course Title	**THEORETICAL CHEMISTRY I – BASIC QUANTUM CHEMISTRY**				
Type of Course	**MAJOR**				
Semester	**III**				
Academic Level	**200 – 299**				
Course Details	Credit	Lecture per week	Tutorial per week	Practical per week	Total Hours
	4	4	-	-	60
Pre-requisites	• Early atom models – John Dalton's atomic theory, the discharge tube experiment and discovery of electrons, the plum-pudding model, the gold foil experiment and the invention of the nucleus, the nuclear model of the atom, failures of the nuclear model. • Mathematical prerequisites - basic understanding of differentiation, partial differentiation, integration, technique of separation of variables. Cartesian and spherical polar coordinate systems. • VSEPR theory, postulates and applications				
Course Summary	Properties of bulk matter can be examined from the viewpoint of thermodynamics. But it is essential to know how these properties stem from the behaviour of individual atoms and molecules. The laws of quantum mechanics decide the properties of the micro-world. The course introduces the basic principles of quantum mechanics and explains how quantum mechanics has revolutionised our understanding of atomic structure and chemical bonding.				

Course Outcomes (CO):

CO	CO Statement	Cognitive Level*	Knowledge Category#	Evaluation Tools used

CO1	*recognize* the importance and the impact of quantum revolution in science.	R	F	Assignment
CO2	*identify* the wave functions of hydrogen atom as atomic orbitals.	U	C	Class tests/Viva
CO3	*apply* the concept of atomic orbitals in chemical bonding (the mixing of wave functions of the two combining atoms).	Ap	C	Seminar/ Class tests
CO4	*relate* the concept of hybridization as linear combination of atomic orbitals of the same atom.	An	P	Class tests/Assignment
CO5	*instill* an atomic/molecular level philosophy in the minds of the students.	C	M	Viva
* - Remember (R), Understand (U), Apply (Ap), Analyse (An), Evaluate (E), Create (C) # - Factual Knowledge(F) Conceptual Knowledge (C) Procedural Knowledge (P) Metacognitive Knowledge (M)				

Detailed Syllabus:

Module	**Unit**	**Content**	**Hrs (45 +30)**	**Marks**
I	**The Quantum revolution and its early impact in atomic structure**		**8**	**21**
	1	Experiments which led to the development and generalisation of quantum theory – black body radiation, Planck's quantum hypothesis, photoelectric effect, Einstein's generalisation of quantum theory	3	
	2	Atomic model partly based on quantum theory – Bohr's theory of the atom, calculation of Bohr radius, velocity and energy of an electron.	3	
	3	Atomic spectra of hydrogen and explanation using Bohr's theory; Limitations of Bohr's theory; Louis de Broglie's matter waves – wave-particle duality; Davisson and Germer experiment.	2	
	Sections from References: **Section A**			

II	**Introductory Quantum Chemistry and the Quantum Mechanical Model of the Atom**		**22**	**42**
	4	Heisenberg’s uncertainty principle and the need of quantum mechanics for the micro world; ***Postulates of quantum mechanics*** - *Wave function postulate*, Physical significance of the wave function, The Born interpretation of the wave function and probability density. Well behaved functions, orthonormal functions	2	
	5	*Time-dependent Schrodinger equation postulate* – Deduction of Time independent Schrödinger wave equation for conservative systems. Laplacian and Hamiltonian operators.	2	
	6	*Operator postulate* - linear and Hermitian operators, eigenfunctions and eigenvalues of an operator. *Eigenvalue postulate*. Hermitian operators have real eigenvalues. *Average value or expectation value postulate*	2	
	7	***Applications of time independent Schrödinger wave equation*** *Particle in a one dimensional box with infinite potential energy walls* – derivation of wave functions and energy, normalization of wave function, plots of wave functions and probability densities, average value of position, average value of momentum, calculation of energy levels and absorption band in butadiene using the particle in a box model.	4	
	8	*Particle in a one dimensional box with finite potential energy walls* (derivation not required) – Introduction to tunnelling, Principle of Scanning Tunnelling Microscopy (STM)	1	
	9	*Particles in a three dimensional box* – separation of variables and derivation of wave functions and energy, degeneracy of states in a cubic box.	2	
	10	*Hydrogen atom* - Hamiltonian operator of H-like systems, separation of nuclear and electronic motions - The Born-Oppenheimer approximation, The Schrodinger equation in spherical polar coordinates, separation of variables	3	
	11	Wave functions or atomic orbitals, radial and angular parts of atomic orbitals. Quantum numbers (n, l, m). Radial functions and their plots, Radial distribution functions and	3	

		their plots, Angular functions and their plots (1s, 2s and $2p_z$ only).		
	12	The Stern - Gerlach experiment and the concept of electron spin, spin quantum number, spin orbitals (elementary idea only). Antisymmetric wave functions and Pauli's exclusion principle.	2	
	13	Exact solution of the Schrodinger equation is impossible for multi-electron atoms - Need for approximation methods.	1	
	Sections from References: **Section A**			
III	**Bonding in Diatomic Molecules**		**12**	**21**
	14	Hamiltonian operator of H_2 molecule - Born-Oppenheimer approximation, approximate theories of chemical bonding – *(ways of mixing of wave functions of different atoms)*.	1	
	15	*Valence bond theory of H_2 molecule* - trial wave function, improvements by including delocalisation of electrons, mutual screening and partial ionic character. Potential energy profile of H_2 molecule formation - equilibrium geometry, Comparison of theoretical and experimental energy profiles.	3	
	16	*Molecular orbital theory of* H_2 molecule –linear combination of atomic orbitals (LCAO), bonding and antibonding molecular orbitals, wave function as product of one electron functions, electron distribution in bonding and antibonding molecular orbitals, overlap integral, normalisation of bonding and antibonding molecular orbitals.	3	
	17	MO diagrams of homonuclear diatomic molecules – He_2, Li_2, Be_2, B_2, C_2, N_2, O_2, F_2; Bond order, stability and magnetic properties of these molecules.	2	
	18	MO diagrams of heteronuclear diatomic molecules - CO and NO; Bond order.	2	
	19	Comparison of VB and MO theories.	1	
	Sections from References: **Section B**			
IV	**Bonding in Polyatomic Molecules**		**6**	**14**
	20	Concept of Hybridization: Need of hybridization, Definition *(mixing of wave functions of the same atom)*	1	

	21	LCAO of the central atom – coefficients of atomic orbitals in the linear combination of sp (BeH_2), sp^2 (BH_3) and sp^3 (CH_4) hybridization (derivation not required)	4	
	22	Other examples of hybridization – Geometry of molecules like PCl_5, SF_6 and IF_7.	1	
	Sections from References: **Section B**			
V	**Open Ended Module: Learning through problem solving and plots**		**12**	
	1	• Plots of wave functions of particle in a box using excel or other software • Plots of angular parts of atomic orbitals using any freeware • Problem solving sections • Connections with inorganic chemistry topics		
	Sections from References: **Section A & Section B**			

Books and References:

Section A

1. D. A. McQuarrie, J. D. Simon, Physical Chemistry – A Molecular Approach, Viva, 2001.

2. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.

3. R.K. Prasad, Quantum Chemistry, 3rd Edition, New Age International, 2006.

Section B

1. James E. Huheey, Ellan A. Keiter, Richard L. Keiter, *Inorganic Chemistry – Principles of Structure and Reactivity*, 4th Edn., Harper Collins, 1993.

2. D. A. McQuarrie, J. D. Simon, *Physical Chemistry – A Molecular Approach*, Viva, 2001.

Further reading

1. F.L. Pilar, Elementary Quantum Chemistry 2 ND 2nd Edn., Dover, 1990.

2. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005

3. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books,2003)

Mapping of COs with PSOs and POs:

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO 1	3	-	-	-	2	2	3			1	2		2
CO 2	2	3	-	-	2	2	3				1		2
CO 3	-	-	1	-	2	2	3			1	3		2
CO 4	-	-	2	3	3	3	2				2		2
CO 5	-	1	-	-	3	3	3		2	2	2		3

Correlation Levels:

Level	**Correlation**
-	Nil
1	Slightly / Low
2	Moderate / Medium
3	Substantial / High

Assessment Rubrics:

- Quiz / Assignment/ Quiz/ Discussion / Seminar
- Midterm Exam
- Programming Assignments (20%)
- Final Exam (70%)

Mapping of COs to Assessment Rubrics :

	Internal Exam	Assignment/viva	Practical skill Evaluation	End Semester Examinations
CO 1		✓		✓
CO 2		✓		✓
CO 3	✓			✓
CO 4	✓	✓		✓
CO 5		✓		