## BT 651 Quantum Chemistry of Atoms and Molecules

**Particles and waves:** Energy, Planck's equation, The Photoelectric effect, The Hydrogen atom, waves;

**Wavefunctions:** Schrödinger's equation, The particle in a box, Zero point energy, Degeneracy, Linear combination of wavefunctions, interpreting wavefunctions, normalization and orthogonality;

**Electrons in atoms:** Orbitals and quantum numbers, probability density diagrams, spin, Pauli exclusion principle, Aufbau method and the periodic table, ionization energies, approximate orbitals, total wavefunction of an atom;

**Electrons in molecules:** Homonuclear and heteronuclear diatomic molecules, total wavefunction for molecules, Hückel theory, Valence bond theory, electronic spectroscopy of atoms and molecules, vibrational spectroscopy, rotational spectroscopy, electron spin resonance and nuclear magnetic resonance;

**Formal quantum theory:** Complex numbers, vectors, operators, states, expectation values, measurement, representation, Heisenberg's uncertainty principle, zero point energy;

**Advanced methods of quantum chemistry:** Angular momentum, Zeeman effect, nuclear magnetic resonance, perturbation theory, the simple harmonic oscillator problem

**References**


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| 1. | Philip S C Matthews, *Quantum Chemistry of Atoms and Molecules*, Cambridge University Press, 2010. |
| 2. | Rabi Majumdar, *Quantum Mechanics in Physics and Chemistry with Applications in Biology*, 2nd Edition, PHI Learning, 2015. |
| 3. | Thomas Engel, *Quantum Chemistry and Spectroscopy*, 3rd Edition, Pearson Education, 2013. |
| 4. | Peter Atkins and Ronald Friedman, *Molecular Quantum Mechanics*, 5th Edition, Oxford University Press, 2012. |