Quantum Theory of Atoms and Molecules

Dr G.A.D. Ritchie & Dr S. Titmuss **Hilary Term - First Year**

The aim of this course is to introduce the quantum theory required to understand the microscopic properties of elementary particles (electrons etc.), atoms and molecules, to describe some of the important physical and chemical applications of this theory, and to provide an elementary understanding of atomic spectroscopy.

1. Quantisation of energy. Atomic spectra, Bohr theory of H atom, examples of molecular spectra, the photoelectric effect, heat capacities of solids.

2. Wave - particle duality. Wave properties of light: Young's slits, interference and the superposition principle; Particle properties of light: photoelectric effect, blackbody radiation, the Compton effect, radiation pressure, angular momentum of light; Matter waves: electron diffraction, de Broglie relationship, wavepackets, the Heisenberg uncertainty relation.

3. An introduction to quantum mechanics. The time dependent and time independent 1-d Schrödinger equation, the wavefunction and its physical interpretation, normalisation. Particle in free space, wave-particle duality and de Broglie relationship. Boundary conditions; particle-in-a-box, energy levels, wavefunctions, zero point energy, Heisenberg uncertainty principle. Tunnelling. Particle in a box model for electronic transition in polyenes. 2-d Schrödinger equation: particle in a 2-d box, degeneracy, particle on a ring. Extensions to 3 dimensions.

4. The mathematical framework of quantum theory. The postulates of quantum mechanics, operators, eigenfunctions, observables, expectation values, completeness, simultaneous observability and commutation relations.

5. Atomic motion. Quantum mechanical description of the translational, vibrational and rotational behaviour of isolated molecules. Solution of the Schrödinger equation and form of wavefunctions for simple harmonic oscillator and rigid rotor. Heat capacities. Comparison with classical behaviour. Deficiencies of simple models. Particle tunnelling, zero point energy. Introduction to rotational and vibrational spectroscopies.

6. Electronic structure of atoms. Schrödinger equation for 1-electron atoms and form of solutions. Energy levels, orbitals and their representation, quantum numbers and their interpretation, spin-orbit coupling. Many electron atoms, orbitals and the orbital approximation, energy levels, Pauli exclusion principle.

7. Atomic spectra of hydrogen and alkali atoms. Introduction to atomic spectroscopy, absorption and emission spectra. Term symbols for electronic states. Energy levels and selection rules for allowed transitions. Spectra of 1-electron systems and of alkali metals.

8. Electronic structure of molecules. Molecular orbital approximation and the linear combination of atomic orbitals.

Books

P.W. Atkins, *Physical Chemistry* (broad discussion of the basics for the whole chemistry course).
P.A. Cox, *Introduction to Quantum Theory and Atomic Structure* (Oxford Chemistry Primer)
W.G. Richards and P.R. Scott, *Structure and Spectra of Atoms* (good on atomic spectra).
G.A.D. Ritchie and D.S. Sivia, *Foundations of Physics for Chemists* (Oxford Chemistry Primer covering most of the background material on waves and optics in this course.)
N.J.B. Green, *Quantum Mechanics 1: Foundations* (Oxford Chemistry Primer).