School of Chemistry

Aims and Objectives: Session 2023-2024, Semester 2

Module CH2701: Physical Chemistry 2

Course Title: Molecular Structure: Spectroscopy and Diffraction

Duration: 14 hours

Lecturer: Professor S. E. M. Ashbrook

Aims: To understand the principles and practical implementation of a range of analytical techniques applied in Physical Chemistry.

To introduce the principles which govern the interaction of radiation (microwaves to X-rays) with atoms and molecules.

To describe the interactions in terms of transitions between different energy levels.

To indicate how such a description can be used to characterise molecules and allow some of their important properties (colour, structure, bond strength, dissociation energies, ionisation energies etc.,) to be determined or explained.

To describe the basic concept of diffraction and explain how it can be used to understand the structure of solids.

Objectives:

1. To understand the nature of electromagnetic radiation, and be able to convert readily between energy, frequency, wavelength and wavenumber.

2. To be able to identify the regions of the spectrum in terms of the different effects they have on atoms and molecules.

3. To appreciate the discrete nature of molecular energy levels and their description in terms of molecular rotations, vibrations and electronic states and, in turn, their links to the structural properties of molecules.

4. To understand the factors determining the position, intensity and linewidth of spectral lines.

5. To appreciate the significant differences between scattering (e.g., Raman) spectroscopies and absorption/emission spectroscopies.

6. To understand the origin of selection rules in absorption, emission and scattering spectroscopies and their relationship to structural and electronic properties of molecules.

7. To understand the basis of molecular electronic spectra, the use of the Born-Oppenheimer approximation and the Frank-Condon principle.

8. To understand the basic concepts of solid-state structure (e.g., lattices and space groups) and of Bragg diffraction.

9. To understand the factors determining the position, intensity and width of reflections in a diffraction pattern and how these can be used to extract information about the solid-state structure.

10. To understand the difference between single crystal and powder X-ray diffraction techniques, the use of synchrotron radiation and the advantages and disadvantages of neutron diffraction, with a focus on practical implementation.