

School of Chemistry

Aims and Objectives: Session 2022-2023

Module CH4717: Fundamentals of Spectroscopy of Molecules and Solids

Duration: 20 hours

Lecturers: Professor S. E. M. Ashbrook* and Dr Renald Schaub

(*Module Convenor)

Aims: The aim of this 4000 level course is to develop a greater understanding and appreciation of the way that electromagnetic radiation interacts with atoms, molecules and solids. Fundamental theory of rotational, vibrational and NMR spectroscopy will be discussed alongside practical aspects of experimental techniques and methods for obtaining structural information from spectra

Objectives:

1. To give a simple description of the nature of electromagnetic radiation and an introduction to the quantum theory.
2. To revise the essential features of the quantum theory of the rotation and vibration of diatomic molecules.
3. To examine the nature and derivation of the Einstein A and B coefficients related to the rates of absorption and emission of radiation by molecules.
4. To consider the nature of selection rules and discuss how they are obtained for vibration-rotation excitations in diatomic molecules.
5. To understand the important interactions that affect solid-state NMR spectra and, in particular, the differences from solution-state NMR spectroscopy.
6. To understand how line narrowing techniques, such as magic-angle spinning (MAS) and decoupling, work and how high-resolution NMR spectra can be obtained.
7. To understand how structural information can be obtained from multinuclear and multidimensional solid-state NMR spectra, and to be familiar with a range of problems and applications where solid-state NMR can be useful