School of Chemistry

Aims and Objectives: Session 2023-2024, Semester 2

Module CH3431: Chemistry Workshop

Course Title: Crystallographic Structure Determination

Duration: 16 hours

Lecturer: Dr J. A. McNulty

Aims: X-ray crystallography is a very powerful tool used to determine the structures of compounds in the solid state. The aim of this workshop is to build on the introduction to diffraction given in CH2701 and to develop a theoretical understanding of crystallography, i.e. the structure of periodic solids and their study by X-ray diffraction.

Objectives:

1. Understand periodicity in 3 dimensions and be familiar with unit cells, crystal systems and space groups.

2. Identify symmetry elements in periodic solids.

3. Understand the conditions for diffraction from periodic solids.

4. Understand the reciprocal relationship between the diffraction pattern (structure factors) and the crystal structure (electron density).

5. Understand the origin of systematic absences and how to derive space groups from X-ray diffraction data.

6. Understand the procedures for crystal structure solution from single crystal X-ray diffraction.