School of Chemistry

Aims and Objectives: Session 2022-2023

Module CH4421: Chemistry Research Skills Laboratory

Lecturers: **Synthesis**: Dr B. A. Chalmers, Dr P. Kilian, Dr J. A. McNulty, Dr I. A. Smellie

Advanced Kinetics: Dr G. Haehner

Advanced Solid State Chemistry: Professor F. D. Morrison

Crystallographic Structure Determination: Dr D. B. Cordes

Advanced Computational Chemistry: Professor M. Bühl, Dr J. B. O. Mitchell, Dr T. van Mourik

Convenor: Dr P. Kilian

Aims: This module develops your independent research and learning skills via integrating advanced practical inorganic, organic and physical chemistry. The module also introduces advanced techniques – single crystal and powder X-ray diffraction, computational quantum chemistry and data analysis using a range of software.

Objectives:

Synthesis:
The major objective is an improvement of problem solving abilities and confidence in independent research work in a chemical laboratory via working on a broadly defined project encompassing organic and inorganic aspects. This will be achieved via:

(1)   use of literature and database searches to gain sufficient knowledge of the specific area of chemistry to allow selection of suitable synthetic strategies and relevant experimental procedures.

(2)   adjusting the identified procedures to available equipment and characterisation techniques.

(3)   performing experimental work with due care and safety.

(4)   recording the results in a laboratory book and communicating of results via written laboratory report in a form of short communication paper.

Advanced Kinetics and Solid State Chemistry:
To be able to plan, organise and research a scientific topic independently.

Students will be allocated problem solving tasks, which will involve:
- Literature/information/background searches as preparation for performing the experiments and the modelling
- Full risk assessment completion as an integral part of the experiment
- Preparation of solutions/materials, setting up experiments and data recording in the laboratory
- Modelling experimental data using software
- Keeping a lab record in a lab book
- Evaluation of the recorded data/data analysis
- Communication of the results in a report

Crystallographic Structure Determination:
The major objective is to give a grounding in the practical aspects of modern single-crystal X-ray diffraction both by carrying out structure solution and refinement of diffraction data and by reporting structural information. This will be achieved via:

(1)   Use of a modern crystallographic GUI and solution and refinement software to fully refine structures, and preparing a final, checked CIF.

(2)   Comparing refined crystallographic data against that of known structures.

(3)   Preparing a report on the structure of crystals using a specified crystallographic format.

Advanced Computational Chemistry:
Going beyond the basics covered in Experiment 1 of the CH3721 lab course, the students will learn about advanced techniques in computational quantum chemistry, including transition state searches, solvation models and corrections for basis set deficiencies. Students will also learn to use quantum chemical program packages in a Linux environment, as they are used on high performance computing platforms.