School of Chemistry

Aims and Objectives: Session 2023-2024, Semester 1

Module CH3721: Physical Chemistry Laboratory

Duration: 70 hours

Staff: Professor M. Buck*, Professor M. Buehl, Dr D. G. Pinto, Dr R. Schaub, Dr R. M. Smith, Dr T. van Mourik

(*Coordinator)

Aims: To provide experience in a programme dependent selection of empirical and computational physical chemistry techniques, to reinforce and revise practices of basic analytical techniques and to give experience in experiment planning, error analysis and data handling.

Objectives:

1. Computational Chemistry. To introduce students to modern computational techniques that are widely used in chemistry via the "Gaussian" program.

2. Diffraction. To introduce students to the physical process of diffraction using an optical setup with a HeNe laser. To relate optical transforms and diffraction patterns to periodic objects and understand the basics of Fourier transformation. To use the optical diffraction analogy to understand the use of electron and X-ray diffraction, and electron microscopy to determine crystal structures.

3. Surfaces. Introduction to concepts of surface modification, wetting and adhesion. Learning to control surface properties and to pattern surfaces by preparation of organic monolayers. Characterisation of surfaces via contact angle, optical diffraction, and atomic force microscopy.

4. Kinetics. To be able to understand the methods and approaches required to obtain isothermal kinetic data to determine the order of a reaction and to interpret rate data in terms of mechanism, or to measure the kinetics of an enzyme-catalysed reaction and to treat the data in terms of the Michaelis-Menten model.

5. Data handling. To be able to deduce how and where errors arise in experimental work. To be able to use EXCEL spreadsheets to analyze and plot data and to obtain parameters important in physical chemistry.

6. Vacuum systems and gas adsorption. To learn to safely handle simple vacuum systems and gain a knowledge of gas manipulation, sub-atmospheric pressure measurement, vacuum pumps and liquid nitrogen use. To measure and understand adsorption isotherms and be able to calculate surface areas and pore sizes of adsorbents.

7. Fabrication and performance testing of a dye-modified photovoltaic cell.

8. Introduction to Macromolecular Structure in 3 dimensions, via modelling kits and using NMR spectra of macromolecules.