

DYNAMOL Crystallographic Course 2012 Program

Venue: Department of Chemistry, Lensfield Road, Todd-Hammied meeting room (ground level)

Friday, 26th of October

09:00 Welcome and general Introduction

09:30 The Cambridge Structural Database - The world's storehouse of high quality chemical structural knowledge (Dr John W. Liebeschuetz)

10:15 Practical molecular design with the help of the Cambridge Structural Database (Dr John W. Liebeschuetz)

11:00 Crystallisation Attempts (Participants)

12:30 Lunch

13:30 Crystallisation Techniques (Dr Julian J. Holstein)

14:00 Validation of crystal quality (Dr Julian J. Holstein)

14:15 Microscope practice and crystal mounting (Dr Tanya Ronson, Dr Julian J. Holstein)

15:00 Crystallographic Concepts (Dr Julian J. Holstein)

16:00 Methods of structure solution, from small molecules to macromolecules (Dr Gérard Bricogne)

Saturday, 27th of October

09:00 Introduction to SHELX programs and file formats (Dr Julian J. Holstein)

09:30 ShelXle a graphical-user interface for SHELXL structure refinements (Dr Christian B. Hübschle)

10:30 Simple structures: Hands-on structure refinement (Dr Tanya Ronson, Dr Christian B. Hübschle and Dr Julian J. Holstein)

12:30 Lunch

13:30 Modelling of disorder in SHELXL (Dr Julian J. Holstein)

14:30 Disordered structures: Hands-on structure solution and refinement (Dr Tanya Ronson, Dr Christian B. Hübschle and Dr Julian J. Holstein)

16:30 Crystallographic literature (Dr Julian J. Holstein)