ECM-21 Pre-meeting Workshops 24 August 2003

1. Single Crystal and Powder Diffraction Software Workshop

Powder Diffraction: 09:00 to 12:30
Single Crystal: 13:30 to 17:00

Organised by:
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Main theme: 'Crystallographic Software Wizardry in Single Crystal and Powder Diffraction'. Different speakers will show participants some of the advanced features in available crystallographic software; 20 minute live sessions that show 1 to 2 problems on using the power tools in the various crystallographic software packages in handling tricky problems that might not always be appreciated. It is requested that participants will read up on the software prior to the workshop via its webpage at http://www.ccp14.ac.uk/projects/ecm21-durban2003/, to ensure that presenters can go straight into their software demonstrations with very minimal introduction.

Speakers and talks:

Powder Diffraction - Morning

Powder Session 1a: (9:00am to 9:20am) - Phase Identification and Search Match tricks using the ICDD CD-ROM - Brian O'Connor, Head of School of Physical Sciences, Curtin University of Technology, Perth, Western Australia, Australia

Powder Session 1b: (9:20am to 9:40am) - Powder Indexing of large volume cells (including protein data) using Crysfire - Robin Shirley, University of Surrey, Guildford, UK

Powder Session 1c: (9:40am to 10:00am) - "Limits of powder indexing of impure samples using whole profile methods" - McMaille powder indexing software - Armel Le Bail, Laboratoire des Fluorures - CNRS ESA 6010, Universite du Maine, Faculté des Sciences, Le Mans, France

Powder Session 1d: (10:00am to 10:20am) - "Structure Solution using Direct methods" - EXPO Structure Solution Software - demonstrated by Martin Attfield, UMIST Centre for Microporous Materials, Department of Chemistry, UMIST, Manchester, UK

Questions: (10:20am to 10:30am)

(Morning tea/coffee: 10:30am to 11:00am)

Powder Session 2a: (11:00am to 11:20am) - Structure Solution using real space methods and the FOX software - Radovan Cerny - Laboratoire de Cristallographie, l'Universite de Geneve, Switzerland

Powder Session 2b: (11:20am to 11:40am) - Quantitative Phase Analysis (crystalline and amorphous) using MAUD for Java - Mauro Bortolotti and Luca Lutterotti - Department of Materials Engineering, University of Trento, Italy

Powder Session 2c: (11:40am to 12:00am) - Rietveld refinement of complex inorganic materials using Fullprof - Juan Rodriguez-Carvajal - Laboratoire Leon Brillouin (CEA-CNRS) and Service de Physique Statistique, Magnetisme et Supracondutivite Magnetisme et Diffraction Neutronique (CEA/DSM/DRFMC/SPSMS/MDN)

Powder Session 2d: (12:00am to 12:20pm) - Rietveld Structure Refinement of protein powder diffraction data using GSAS -Jon Wright - ESRF, Grenoble, France.

Questions: (12:20pm to 12:30pm)

(Lunch: 12:30pm to 1:30pm)

Single Crystal - Afternoon

Single Crystal 3a: (1:30pm to 1:50pm) - Using CCDs for visually finding tricky cells, supercells and incommensurate cells - "Precession Wallpaper or how to treat hexagonal structures with an incommensurate vector" (Refer: Twin analysis using combined Phi-Chi scans and Using the Nonius KappaCCD for twin analysis) - Rob W. W. Hooft - Bruker Nonius BV, Delft, The Netherlands.

Single Crystal 3b: (1:50pm to 2:10pm) - Advanced absorption correction options using Platon and Euhedral - Martin Lutz, Bijvoet Center for Biomolecular Research, Utrecht University, The Netherlands

Single Crystal 3c: (2:10pm to 2:30pm) - Data processing of Bruker and Nonius CCD data using the WinGX Single Crystal suite, incorporating Sortav - Louis Farrugia - Department of Chemistry, University of Glasgow, Scotland.

Single Crystal 3d: (2:30pm to 2:50pm) - Structure Solution: SnB (Shake-n-Bake) - solving difficult structures - Charles M. Weeks, Hauptman-Woodward Institute, Buffalo, New York, USA

Questions: (2:50pm to 3:00pm)

(Afternoon tea/coffee: 3:00pm to 3:30pm)

Single Crystal 4a: (3:30pm to 3:50pm) - Structure Solution: Dirdif fragment searching to easily solve structures that direct methods won't - Bob Gould, Structural Biochemistry Unit ICMB, University of Edinburgh, Scotland.

Single Crystal 4b: (3:50pm to 4:10pm) - Refinement on weak/problematic small molecule data using Shelxl97 - Alexander Blake, School of Chemistry, University of Nottingham, UK

Single Crystal 4c: (4:10pm to 4:30pm) - Is the local geometry sensible?: Crystals to CCDC Mogul geometry validation - David Watkin, Chemical Crystallography, Oxford University, UK

Single Crystal 4d: (4:30pm to 4:50pm) - Is the structure kosher?: -non-trivial applications of Platon, Addsym and intra/inter-molecular validation - Ton Spek, Bijvoet Center for Biomolecular Research, Utrecht University, The Netherlands

Questions: (4:50pm to 5:00pm)

Cambridge Crystallographic Structural Database

Time: 9:30 to 12:30; 13:30 to 16:00

Organised by:
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The CCDC collates and distributes the Cambridge Structural Database (CSD) which contains comprehensive crystal structure data for small organic and metal-organic compounds. The CSD system consists of the database itself, and accompanying software including:

- ConQuest (for search and retrieval of crystal structures)
- Vista (for numerical analysis)
- Mercury (for crystal structure visualisation)
- IsoStar (knowledge about intermolecular interactions)
- Mogul (knowledge about molecular geometries)

The CCDC now also provides enCIFer for CIF editing and undertakes the development of a range of applications software: GOLD for protein-ligand docking, SuperStar for predicting protein-ligand interactions, Relibase+ for easy searching of protein-ligand complexes and DASH for structure solution from powder diffraction data.

During the workshop we plan to provide attendees with a greater knowledge of the Cambridge Structural Database (CSD) and its associated software. We will provide background information about the CCDC and its activities, including detailed coverage of CSD content, and software which can be used to help make editing CIFs easier: enCIFer. We will present and demonstrate all the products which comprise the CSD System. The DASH program for structure solution from powder diffraction data will also be presented along with a brief overview of the other applications software.

3. Protein Crystallography Workshop

Time: 9:30 to 12:30; 13:30 to 16:00

Organised by:
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Workshop includes:
Data acquisition and processing; Data quality assessment; Molecular replacement and Refinement and structure validation
Speakers include: Harry Powell, Eleanor Dodson, Garib Murshudov, Roberto Steiner.