PROGRAM SCHEDULE

Advanced Methods in X-ray Diffraction Analysis: the XD Programming Package

Buffalo NY, 12-17 May 2003

12th May, Monday

Pre-workshop talk by **Dr. Charles Campana** of Bruker AXS

on *"Solving difficult structures and analyzing twinned and modulated crystals"*

14:00-16:00

Location: Natural Sciences Complex (NSC, Chemistry Building) room 684

Evening

OPENING RECEPTION

At **18:30** a bus* will be available for those who prefer not to walk to the Natural Sciences Complex (abbreviated NSC) where the informal opening reception will take place.

At **21:00** the same bus* will provide transportation from the NSC (at Rensch Loop) back to the motel.

* OPERATED BY "OVER THE FALLS TOURS"

Location of the X-ray Crystallographic Laboratory: Natural Sciences Complex rooms 726-747

13th May, Tuesday

TOPIC: REFINEMENT

Free breakfast served 7.30-8.30 at Bert's (next to NSC lecture halls)

Morning Session 9.00-12.00 Chair: Dr. V. Young

Location: Natural Sciences Complex room 215

Opening ceremony: 8.45-9.00	*Welcoming remarks*	H. Hauptman, Nobel Laureate
Introductory lecture: 9.00-10.00	*X-ray charge density and chemical bonding: the historical background and future prospects*	P. Coppens
coffee break at NSC room 216		
Main lecture: 10.15-11.15	*The multipolar model and least squares refinement*	T. Koritsanszky
Short lectures: 11.15-12.15	*Symmetry restraints and chemical constraints*	P. Mallinson
	The choice of radial functions	P. Macchi

Afternoon Session 13.30-16.30

(tea/coffee will be served 15.00-16.00 in NSC room 216)

Tutorial

Location: Natural Sciences Complex room 218

Presentation by CCR staff

How to access the computer nodes (15 minutes)

Group 1 (beginners)	Group 2 (advanced)
Location: Hochstetter Hall room 139	**Location: Hochstetter Hall room 141**
Teachers: L. Farrugia, P. Mallinson, T. Koritsanszky	**Teachers: P. Macchi, A. Volkov**
getting started with XD (XDINI) *from shelx to XD* *from cif files to XD* *XDLSM input and output files handling*	***description of the new features of XDLSM and XDINI*** *choice of radial functions* *extinction* *improved code performances* *refining difficult parameters* *examples provided by the students*
performing least-squares refinements *worked examples with some datasets* *refining multipole variables* *refining extinction* *refining higher order thermal motion parameters* *wave functions and radial deformation functions* *refining against neutron data*	

Poster Session P10X, 16.30 -17.30, NSC room 218
poster presentations (10 minutes each), experimental techniques

Evening: Informal Dinner at Brewpub

At **18:30** a bus* will provide transportation from the Natural Sciences Complex to the Brewpub (6861 Main Street, Williamsville, NY 14221)

At **21:30** the same bus* will provide transportation from the Brewpub back to the motel

* operated by "OVER THE FALLS TOURS"

14th May, Wednesday

TOPIC:
Fourier methods and analysis of the results

Morning Session 9.00-12.30

Main lecture: *Fourier methods in X-ray charge density;*   P. Mallinson
9.00 - 10.00   *The rho-cif dictionary*

coffee break at NSC room 216

Tutorial 10.15-12.30

Group 1 (beginners)	Group 2 (advanced)
Location: Hochstetter Hall room 139	**Location: Hochstetter Hall room 141**
Teachers: P. Macchi, A. Volkov	**Teachers: P. Mallinson, T. Koritsanszky**
usage of XDFOUR *computing residuals maps with XDFOUR* *computing experimental deformation density maps*	*new features of XDGEOM;* *use of XDFFT and graphical visualization of peaks;* *+ short presentation by L. Farrugia*
usage of XDFFT *Fast Fourier peak search and graphical visualization of peaks* *+ short presentation by L. Farrugia*	*the rho-cif dictionary; producing and retrieving data from an archive file;*
usage of XDGRAPH *graphical visualization of maps (XDGRAPH)*	*XDWTAN, analysis of refinement;* *+ short presentation by L. Farrugia*
usage of XDGEOM *computing geometries (XDGEOM)* *producing cif files*	*learning more from visualization of results through XDGRAPH*
usage of XDWTAN *analysis of refinement* *+ short presentation by L. Farrugia*	***application to user's data***

Afternoon: Tour of Niagara Falls

At 14:00 a bus will meet participants at MOTEL6. Operated by the Niagara Majestic Tours.

15th May, Thursday

TOPIC:
Properties from the electron density

Morning Session 9.00-12.00

Location: Natural Sciences Complex room 218

Main lecture: 9.00-10.00	*Electron density from multipolar model and the derived properties; the electrostatic potential*	P. Macchi

coffee break at NSC room 216

Short lectures: 10.15-12.00	*Theoretical vibrational mode constraint (module XDVIB)*	T. Koritsanszky
	Static deformation densities and their analysis	P. Macchi
	Atomic and molecular partitioning	A. Volkov

Afternoon Session 14.00-18.00
Tutorial 14.00-17.00

(tea/coffee will be served 15.00-16.00 in NSC room 216)

Group 1 (beginners)   **Group 2 (advanced)**

Location: Hochstetter Hall room 139	**Location: Hochstetter Hall room 141**
Teachers: P. Mallinson, T. Koritsanszky, L. Farrugia, P. Macchi	**Teachers: C. Gatti, A. Volkov**
usage of XDPROP: *computing static deformation densities* *reconstructing the total electron density and Laplacian* *reconstructing partial densities (core/valence etc.)* *computing multipole moments (from atomic moments and from Stockholder partitioning)* *extracting d-orbital populations* *computing the electrostatic potential* *usage of XDGRAPH* *graphical visualization of maps (XDGRAPH)*	*use of TOPXD* *searching critical points of the electron density* *integration of the density in the atomic basins (TOPXD)* *producing and visualizing maps* *worked examples also for advanced users*

Poster Session P20X, 17.00 -18.00, NSC room 218
poster presentations (10 minutes each), charge density results and interpretation

16th May, Friday

TOPIC:
Topological Analysis of the charge density

Morning Session 9.00-12.00

Location: Natural Sciences Complex room 218

Main lecture: 9.00-10.00	*The topology of charge density in crystals*	C. Gatti
coffee break at NSC room 216		
Short lectures: 10.15-12.00	*TOPXD: Merging TOPOND and XD*	A. Volkov
	Search of critical points of the density	C. Gatti
	Algorithms for integration, optimization of the performances	A. Volkov
	Interpretation of results	C. Gatti

Afternoon Session 14.00-18.00
Tutorial 14.00-17.00
(tea/coffee will be served 15.00-16.00 in NSC room 216)

Group 1 (beginners) — **Group 2 (advanced)**

Location: Hochstetter Hall room 139 — **Location: Hochstetter Hall room 141**

Teachers: C. Gatti, A. Volkov

Teachers: P. Mallinson, T. Koritsanszky, P. Macchi, L. Farrugia

use of TOPXD
searching critical points of the electron density
integration of the density in the atomic basins (TOPXD)
producing and visualizing maps

topological analysis with XDPROP
analysis of properties along bond paths
visualization of results

new features of XDPROP
computing multipole moments (from atomic moments and from Stockholder partitioning)

extracting d-orbital populations
mathematics on the grid files (+ short presentation)
application to user's data

Poster Session P30X, 17.00 -18.00, NSC room 218
poster presentations (10 minutes each), charge density results and other techniques

17th May, Saturday

Morning session 9.00-12.00
Chair: Prof. A. Pinkerton

Location: Natural Sciences Complex room 218

Main lecture: 9.00-10.00	*Statistical analyses and analyses of geometrical and thermal parameters* *Presentation of a Windows version of XD*	L. Farrugia

coffee break at NSC room 216

Technical discussion: 10.15-10.30	*Choice of a default compiler for the XD package*	A. Volkov
Open presentation: 10.30-11.15	*New results obtained at the meeting*	
Open discussion: 11.15-12.00	*Comments from the participants* *Bug reports* *General questions*	
Closing remarks: 12.00-12.30		P. Coppens