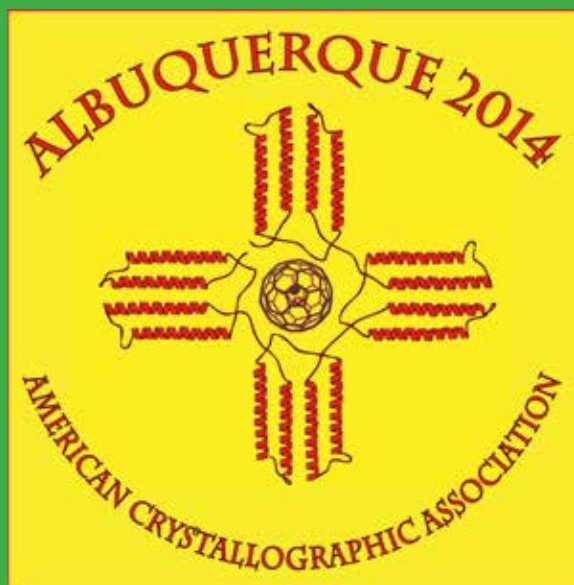


AMERICAN
CRYSTALLOGRAPHIC
ASSOCIATION
ANNUAL MEETING

MAY 24 - 28, 2014
ALBUQUERQUE, NEW MEXICO



Program Book

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION ANNUAL MEETING

MAY 24 - 28, ALBUQUERQUE, NEW MEXICO

Program Chairs: Christine Beavers & Petrus Zwart

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www.AmerCrystalAssn.org

About the ACA

The American Crystallographic Association (ACA) was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction. They will also promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from them.

Membership in the ACA is open to any person who is actively interested in the purposes of the Association and whose application is approved by the ACA Council or its designee. All members are entitled to voting privileges. Student members are very welcome and their contributions to the life and vigor of the association has always been important. The benefits of membership are the same in all categories. These include: voting privileges, RefleXions, the ACA newsletter that is published 4 times per year, complimentary subscription to the Newsletter of the International Union of Crystallography, and Physics Today, a monthly publication of AIP, and reduced rates for the International Tables for X-Ray Crystallography, Structure Reports, Journal of Applied Crystallography, and Acta Crystallographica when purchased for the member's personal use only. The ACA is a member society of the American Institute of Physics (AIP) and an Affiliate Member of the International Union of Crystallography.

The total membership of the ACA is about 1,600. National meetings are held annually. There are 12 Scientific Interest Groups (SIG's) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, Synchrotron Radiation and Young Scientists. Members may join as many of these groups that are of interest them. Each SIG is responsible for organizing sessions at Annual Meetings at least every other year.

The headquarters of the association is located at Hauptman Woodward Medical Research Institute, 700 Ellicott St., Buffalo, NY 14203.

SATURDAY, MAY 24

WK.01 Joint Neutron and X-ray Structure Refinement using Joint Refine in PHENIX

Zoe Fisher, Pavel Afonine, presiding
Cimmarron

This half-day workshop is intended as a somewhat informal and hands-on tutorial. B (is your protein hydrogenous, H/D exchanged or fully deuterated) to the finer nuances of a proper neutron/X-ray refinement. There will also be a focus on careful model building in Coot, taking proper hydrogen bonding and chemistry into account.

08:30 - 09:00

Set up, help participants install PHENIX, distribute practice neutron and X-ray data sets

09:00 - 09:30

Brief introduction on PHENIX Joint Refine, philosophy and approach, what's new and improved over previous versions

09:30 - 10:45

Participants work on PDB preparation, initial refinement parameters, making nuclear and electron density maps for Coot, interpreting maps

10:45 - 11:00 Coffee break

11:00 - 12:30

Continue refinement and model building, finish structure, Q&A.

WK.02 Grazing Incidence SAXS Theory and Data Analysis

Alex Hexemer, Chenhui Zhu, presiding
Dona Ana

Funding for this workshop provided, in part by, Anton Paar, DECTRIS, Rigaku Americas

GISAXS is a unique method for characterizing the nanostructural features of materials, particularly at surfaces and interfaces, which would otherwise be impossible using traditional transmission-based scattering techniques [1]. It is a surface-sensitive tool for probing simultaneously the sample morphology both in-plane and out-of-plane, and is being increasingly utilized to measure the size, shape and spatial organization of nanoscale objects located on top of surfaces or embedded in mono- or multi-layered thin-film materials. Individual GISAXS images serve as static snapshots of nanoscale structure, while successive images provide a means to monitor and probe dynamical processes, including self-assembly or other reorganization events, which occur at nanometer length scales.

Invited Speakers:

Elaine Chan, Advanced Light Source, Lawrence Berkeley National Laboratory

Walter Van Herck, Jülich Centre for Neutron Science JCNS, Germany

Alex Hexemer, Advanced Light Source, Lawrence Berkeley National Laboratory

Zhang Jiang, Advanced Photon Source, Argonne National Laboratory

Joseph Strzalka, Advanced Photon Source, Argonne National Laboratory

Kevin Yager, National Synchrotron Light Source / Center for Functional Nanomaterials, Brookhaven National Laboratory

Morning session 8:00am-12:00pm

Introduction: What can we learn from GISAXS data?

Theory Essentials: GISAXS theory.

Sample preparation, experimental geometries and current GISAXS capabilities at synchrotron beamlines.

Hand-on data reduction and processing using Nika.

Afternoon session 1:00pm-5:00pm

Hand-on GISAXS pattern simulation using BornAgain [v], and HipGISAXS.

Brief introduction of parallel computing for GISAXS simulation.

Open help, Q&A

WK.03 Reciprocal Space Visualization - MAX3D

Jim Britten, presiding
Cimmareon

The workshop will open with a discussion of reciprocal space and a description of how the all of the information on an area detector frame (not just Bragg spots) maps into RS. We will look at examples of “single crystal” diffraction showing crystal quality, protein diffraction, twinning, incommensurate scattering, diffuse scattering, quasicrystal diffraction. We will briefly discuss the origins of various scattering features. We will discuss how scanning strategies can be viewed and optimized to observe targeted diffraction features.

M1:00 - 2:00 Overview Of Max3d Applications and Features

2:00 - 3:00 Step by Step Analyses of Tutorial Data. Participants Should Follow Along on Their Own Computers

3:00 - 3:30 Break / Discussion

3:30 - 4:30 Visualization Optimization and Analyses of Data Provided by Participants

Saturday Evening Activities

First Time Attendee and Student Meeting Orientation

5:30-6:30pm Aztec

The focus of this informal session is to orient ‘young scientists’ and first time attendees to the structure of the ACA Meeting and how to make the most of their experience.

Opening Reception Exhibit Show

7:30pm NE Exhibit Hall

Must have meeting name badge for entry

SUNDAY, MAY 25

Registration Desk.....	7:30am	East Lobby
Speaker Ready Room.....	7:30am	Tijeras
Council Meeting Room.....	7:30am	La Cienega
Exhibit Show.....	10:00am	NE Exhibit Hall
Reception for Undergraduate Students.....	12:00pm-01:30pm	San Miguel
Industrial SIG Meeting.....	12:00pm	Dona Ana

P001 Patterson Award Presentation and Lecture

Martha Teeter, presiding

Brazos

08:00-08:45am P001.01

Synchrotron Radiation Macromolecular Crystallography: Instrumentation, Methods and Applications. John Helliwell

1.1.2 Instrumentation & Methods for Structure Solution of Nano-sized Materials

John Helliwell & Pavol Juhas, presiding
Galisteo

09:00-09:30am **1.1.2.01**
Nanopowder Crystallite Sizes and Shapes as Viewed from XRD and TEM: Examples of EMT Zeolite, Ti- and Mn-oxide Nanoparticles. Daniel Chateigner, Philippe Boullay, Luca Luttrero, Svetlana Mintova.

09:30-10:00am **1.1.2.02**
Preferred Orientation, PDF and Debye Equation. Reinhard Neder.

10:30-11:00am **1.1.2.03**
Developments in Nanostructure Solution from PDF Data. Simon Billinge.

11:00-11:30 **1.1.2.04**
Quantitative Atomic Structure Studies of Nanomaterial Phenomena. Katharine Page.

11:30-12:00am **1.1.2.05**
Stroboscopic Probes of Transient Response to Time Dependent Stresses in Soft Condensed Matter. Daniel Olds, Rex Hjelm.

1.1.4 Frontier of Structure-selective Characterization in Complex Soft Matter Materials

Wei Chen & Yun Liu, presiding
Cimmarron

08:55-09:00am
Introductory Remarks. Wei Chen & Yun Liu.

09:00-09:30am **1.1.4.01**
The Lack of Pore Defects in Vesicles of Binary Lipid Mixtures Above TM. Paul Butler, Andrea Woodka, Lionel Porcar.

09:30-10:00am **1.1.4.02**
Development of *in-situ* Resonant Soft X-ray Scattering for Soft Materials. Cheng Wang, Alexander Hexemer, Anthony Young, Howard Padmore.

10:00-10:15am **1.1.4.03**
Probing the Structures and Dynamics of Polymer Materials Through Selective Deuteration. Kunlun Hong.

10:15-10:30am **Coffee Break**

10:30-11:00am **1.1.4.04**
Anomalous Small Angle X-Ray Scattering on Soft-Hard Hybrid Materials. Byeongdu Lee.

11:00-11:15am **1.1.4.05**
Dynamical Crossover in Soft Colloids below the Overlap Concentration. Wei-Ren Chen.

11:15-11:45am **1.1.4.06**
Characterization of Block Copolymer Lithography Patterns Using Resonant X-ray Scattering. Joseph Kline, Daniel Sunday.

Canadian Division Meeting	12:00pm.....	Cimarron
Demonstration and Q&A on the New wwPDB		
Deposition and Annotation System	5:00pm	Mesilla
Poster Session S (sponsored by Bruker)	5:30pm - 7:30pm	NE Exhibit Hall
Rayonix-YSSIG Mixer (ticket required).....	8:00pm.....	Hotel Andaluz

11:45-12:00pm **1.1.4.07**

Thermo- and Light-Sensitive Hydrophilic Block Copolymer in Water Investigated by SANS. Lilin He.

TR.01 100 Years of Crystallography

Edward Snell, presiding

Brazos

09:00-09:30am **T001.01**

Fun with Crystals, Light and Symmetry - IYCr Outreach Activities. Cora Lind-Kovacs, Martha Teeter.

09:30-10:00am **T001.02**

A Brief History of Women in Crystallography. Martha Teeter.

10:00-10:30am **Coffee Break**

10:30-11:15am **T001.03**

Protein Crystallization Over 200 Years: From Art to Science. Alexander McPherson.

11:15-12:00am **T001.04**

Databases in Crystallography: Past, Present, and Future. Helen Berman, Colin Groom, James Kaduk.

12:00-01:30pm **Lunch Break**

01:30-02:15pm **T001.05**

Changing Practice in Crystallographic Phase Evaluation for Biological Macromolecules. Wayne Hendrickson.

02:15-03:00pm **T001.06**

The Dawn of the Age of Uncertainty. James Holton.

03:00-03:30pm **Coffee Break**

03:30-04:15pm **T001.07**

Synchrotron Radiation in Structural Biology: Past, Present, and Future. Robert Sweet.

04:15-05:00pm **T001.08**

Powder Diffraction: 98 Years as Plan B? Brian Toby.

Poster Preview Session

Bill Duax, presiding

Aztec

9:00-9:10am **T-46**

Automated Protein Crystal Optimisation with TTP Labtech's Dragonfly. Soheila Vaezeslami, Gary Cochrane.

9:10-9:20am **S-17**

Improved Twin Processing with CrysAlisPro. Lee Daniels, Fraser White, Daniel Baker, Zoltan Gal, Oliver Presly, Mathias Meyer.

9:20-9:30am **M-02**

A Set of Tools for Micro-crystallography: Highlights of Rigaku Minstrel DT/HT UV Advances. Pius Padayatti, Max Petersen, Benjamin Liedblad.

9:30-9:40am **M-24**

SAD Phasing of RNA with X-rays at the Iron Absorption Edge. Blaine Mooers, Tzanko Doukov.

9:40-9:50am **S-27**

Structural and Functional Analysis of Lysosomal Phospholipase A2 a Close Homolog of Lecithin-cholesterol Acyltransferase. Alisa Glukhova, James Shayman, John Tesmer.

9:50-10:00am **S-39**

Two Paralogs of FabH in *V.cholerae*: Structures and Kinetics Suggest a Mechanism for Adapta-

SUNDAY, MAY 25

tion in the Initiation of Fatty Acid Synthesis. Jing Hou, Heping Zheng, Matthew Zimmerman, Maksymilian Chruszcz, Mahendra Chordia, Wladek Minor.

10:00-10:30am Coffee Break

10:30-10:40am S-09

Crystal Structure of the Nipah Virus Phosphoprotein Tetramerization Domain. Jessica Bruhn, Katherine Barnett, Jaclyn Bibby, Jens Thomas, Ronan Keegan, Daniel Rigden, Zachary Bornholdt, Erica Ollmann Saphire.

10:40-10:50am M-14

Holistic Integration of Crystallography into an Undergraduate Course on Scientific Communication. Louise N. Dawe.

10:50-11:00am T-06

The Search for New Polymeric CuI/CuII Cyanide Complexes. Peter Corfield, Michael A. Chernichaw, Emma M. Cleary, Julie H. Thoubboron, Joseph F. Michalski.

11:00-11:10am M-22

Phosphates in Z-DNA Dodecamer are Flexible but their P-SAD Signal is Sufficient for Structure Solution. Zhipu Luo, Mirosława Dauter, Zbigniew Dauter.

11:10-11:20am T-11

Accurate Alignment Corrects Errors in Ribosome Structural Analysis and Reveals Essential Function of S9. William Duax, Sam Chen, Connor Huck, Nick Sass.

1.2.1 Industrial Research from Young Scientists

George Lountos & Peter Wood, presiding
Dona Ana

01:30-02:00pm 1.2.1.01

An Experimental and Computational Investigation of Physical Form Diversity of Olanzapine. Rajni M. Bhardwaj, Alastair J. Florence, Sarah L. Price, Susan M. Reutzel-Edens.

02:00-02:30pm 1.2.1.02

The Polymorphism of Dehydro-Aripiprazole. Jacob Trotta, Tarek Zeidan, Renato Chiarella, Mark Oliveira, Magali Hickey, Öm Almarsson, Julius Remenar.

02:30-03:00pm 1.2.1.03

p-aminobenzoic acid (PABA): Solvent Selection and Crystallising the β Polymorph. Ghazala Sadiq, Roger Davey, Rachel Sullivan.

03:00-03:30pm Coffee Break

03:30-04:00pm 1.2.1.04

Discovery of Novel Allosteric Inhibitors of HCV NS3/4a Enzyme via Structure-based Drug Design. Puja Pathuri, Susanne Saalau-Bethell, Andrew Woodhead, Nicola Wilsher, Maria Carr, Gianni Chessari, Joseph Coyle, Lynsey Fazal, Brent Graham, Chris Hamlett, Steven Hiscock, Harren Jhoti, Jon Lewis, Vanessa Martins, Alessia Millemaggi, Chris Murray, David Norton, Mike Reader, Caroline Richardson, Pamela Williams.

Undergraduate Reception

Sponsored by the Society of Physics Students

San Miguel

12:00 - 01:30pm

All undergraduates and their mentors, as well as others who might be interested, are invited to join us for a reception highlighting undergraduate research. Undergraduates presenting posters at the meeting are encouraged to also present them here in this special undergraduate-focused session. In addition to poster presentations, Dr. Cora Lind-Kovacs will be giving a short talk with introductory remarks by ACA President Martha Teeter. Refreshments will be provided; pre-registration is mandatory.



04:00-04:30pm **1.2.1.05**
Contribution of Multifunctional Enzymes to Biomass Hydrolysis. Christopher Bianchetti, Taichi Takasuka, Kai Deng, Hannah Udell, Sam Deutsch, Trent Northern, Brian Fox.

04:30-05:00pm **1.2.1.06**
Crystallography as a Guide for Understanding and Engineering Enzymes in the Chemoenzymatic Synthesis of CMP-sialic Acid. Melissa Matthews, Nhung Huynh, Yanhong Li, Hai Yu, Xi Chen, Andrew Fisher.

1.2.3 Disorder & Inhomogeneity in Complex Materials Probed by PDF

Ram Seshadri, presiding
Galisteo

01:30-02:00pm **1.2.3.01**
Representational Analysis of Extended Disorder in Crystals from Total Scattering Data. James Neilson.

02:00-02:30pm **1.2.3.02**
Exploring the Potential Energy Surface of Hydrated-Amorphous Magnesium Carbonate: The Computational Chemistry and Total Scattering Iterative Methodology. Claire White.

02:30-03:00pm **1.2.3.03**
Emphasis in a Lead-free Compound: Local Symmetry-Breaking in the High Temperature Regime of SnTe. Kevin Knox, Emil Bozin, Christos Malliakas, Mercouri Kanatzidis, Simon Billinge.

03:00-03:30pm **Coffee Break**

03:30-03:45pm **1.2.3.04**
Size-dependent Non-space Filling Atomic Packing in Metallic Nanoparticles. Vicky Doan-Nguyen, Simon Kimber, Diego Pontoni, Benjamin Diroll, Danielle Reifsnnyder, Marcel Miglierini, Xiaohao Yang, Christopher Murray, Simon Billinge.

03:45-04:00pm **1.2.3.05**
Using Dynamic Pair Distribution Function Analysis to Probe the Local Structure of the Superconductor, β FeSe. Allyson Fry, William A. Phelan, James R. Nielson, Tyrel M. McQueen.

04:00-04:30pm **1.2.3.06**
Crystallization of Inorganic Melts Probed by *in-situ* PDF. Daniel Shoemaker.

04:30-05:00pm **1.2.3.07**
Local Structural Effects on the Magnetism of Doped BaxMn8O16 Hollandite Oxides. Efrain Rodriguez, Amber Larson, Pouya Moetakef.

1.2.4 General Interest I

Graciela Diaz de Delgado, presiding
Aztec

01:30-01:35pm Opening Remarks

01:55-02:15pm **1.2.4.02**
Structure of the *Trypanosoma cruzi* Protein Tyrosine Phosphatase TcPTP1, a Potential Therapeutic Target for Chagas' Disease. George Lountos, Joseph Tropea, David Waugh.

02:15-02:35pm **1.2.4.03**
The Story of the Missing Bond or How Good Data and High Quality Electron Density Maps may Mislead You. Sergei Pletnev, Nadya Pletneva, Konstantin Lukyanov, Ekaterina Souslova, Arkady Fradkov, Dmitry Chudakov, Tatyana Chepurnykh, Ilia Yampolsky, Alexander Wlodawer, Zbigniew Dauter, Vladimir Pletnev.

02:35-02:55pm **1.2.4.04**
Selenium-derivatized Nucleic Acids for Structure Determination of the First Protein-Nucleic Acid Complex via MAD and/or SAD Phasing: Se-atom Probe Provides Novel Insights into Enzyme Catalysis. Zhen Huang, Rob Abdur, Oksana Gerlits, Jianhua Gan, Jiansheng Jiang, Jozef Salon, Andrey Kovalevsky, Alexander Chumanevich, Irene Weber, Zhen Huang.

SUNDAY, MAY 25

02:55-03:30pm Coffee Break

03:30-03:50pm **1.2.4.05**

How Do You Know Where Your Refined Model is Wrong? Lynn Ten Eyck, Martin Perez.

03:50-04:10pm **1.2.4.06**

Stabilization of Nitro-Aromatics. Jeffrey Deschamps, Damon Parrish.

04:10-04:30pm **1.2.4.07**

Inhibition of Metallo- β -lactamases by Bisthiazolidines. Javier M. Gonzalez, Mariano Gonzalez, Magda Kosmopoulou, Cecilia Saiz, Valerie Castillo, Graciela Mahler, Robert Bonomo, James Spencer, Alejandro Vila.

04:30-04:50pm **1.2.4.08**

A Century of Small Molecule Crystal Structures. Suzanna Ward, Colin R. Groom, Gregory M. Ferrence.

1.3.1 Career Odysseys

Yulia Sevryugina, presiding

Cimmarron

5:00pm - 6:30pm

This session will present a panel of speakers from varied career paths who will discuss how they came to be in their position, what factors played into their decision, and what their career entails and requires. The panelists will first discuss their own experiences and will then answer questions from the audience.

Panelists:

Dr. Kevin W. Bieg, Senior IP Counsel Sandia National Laboratories

Dr. Ilia A. Guzei

Director of Crystallography, University of Wisconsin, Madison

Dr. Joseph Orgel, Professor, Illinois Institute of Technology

Dr. Jim Pflugrath, Research Scientist, Rigaku Americas

Dr. Claudia J. Rawn

Associate Professor, University of Tennessee at Knoxville

Rayonix-Young Scientists SIG Mixer

High energy fun, great food and some of the most exciting venues make the Young Scientists Mixer a great place to connect with scientists ranging in experience and disciplines. The Mixer is one of the meeting's most popular events and is FREE to registered Students & Postdocs (**ticket required**) and \$28 for all others. The mixer will be held at Ibiza Bar, the rooftop bar within the Andaluz Hotel. The hotel is located within walking distance of the convention center. The Mixer is on Sunday, May 25, beginning at 8:00pm. This event is sponsored in part, by Rayonix.

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Registration Desk	7:30am.....	East Lobby
Speaker Ready Room	7:30am.....	Tijeras
Council Meeting Room.....	7:30am.....	La Cienega
Exhibit Show	10:00am	NE Exhibit Hall
Joint SIG Meeting: Neutron/Materials/Powder	12:00pm	Cimarron
Fiber Diffraction SIG Meeting.....	12:00pm	Dona Ana
Aglient Luncheon Seminar	12:00pm - 1:30pm.....	Ruidoso
Young Scientist SIG Meeting/Travel Funding Winners.....	5:00pm.....	Brazos
Light Source (formerly Synchrotron) SIG Meeting.....	5:00pm.....	Dona Ana
USNCCr Meeting.....	5:00pm.....	La Cienega
Poster Session M.....	5:30pm-7:30pm.....	NE Exhibit Hall

P002 Wood Writing Award Presentation and Lecture

Martha Teeter, presiding
Brazos

08:00-08:45am P002.02
The World of Crystallography on Postage Stamps.
Daniel Rabinovich

2.1.1 Scattering and Energy Storage Materials

Peter Chupas & Lilin He, presiding
Brazos

09:00-09:30am 2.1.1.01
Electrochemical Energy Storage: New Approaches to Decouple Mesoscale Phenomena. Karena Chapman, Kamila Wiaderek, Olaf Borkiewicz, Peter Chupas.

09:30-09:50am 2.1.1.02
Establishing an Atomistic Picture of Gas Sorption With and Without Crystallography: Tools for Advanced Separations. Paul Forster, Keith Lawler, Zeric Hulvey.

10:10-10:40am Coffee Break

10:40-11:00am 2.1.1.04
Dispersion Morphology of Nafion in the Fabrication of Fuel Cell Membrane Electrode Assemblies: Relationships to Electrolytic Fuel Cell Durability and Performance. Rex Hjelm, Cynthia Welch, Andrea Libouriau, Bruce Orlor, Yu-Seung Kim.

11:00-11:20am 2.1.1.05
SANS Investigations of Shale Specimens Retrieved from Different Depth. Jitendra Baha-

dur Lnu, Yuri Melnichenko, Maria Mastalerz, Agnieszka Furmann.

11:20-11:40am 2.1.1.06
in situ Synchrotron-Based X-ray Scattering Studies of Nanoporous Metal-organic Frameworks. Gregory Halder, Karena Chapman, George Shimizu, Simon Iremonger, Tom Woo, Tom Daff.

11:40-12:00pm 2.1.1.07
The Importance of the Experimental Design for *in situ* X-ray Scattering Studies on Battery Materials. Olaf Borkiewicz, Olaf Borkiewicz, Karena Chapman, Fiona Stobridge, Peter Chupas, Clare Grey.

2.1.2 Neutrons in Biology: Structural Enzymology

Zoe Fisher, Paul Langan, presiding
Galisteo

09:00-09:30am 2.1.2.01
Joint X-ray/neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir - Insights for Drug Design. Irene Weber, Mary Jo Waltman, Marat Mustyakimov, Matthew Blakeley, David Keen, Arun Ghosh, Paul Langan, Andrey Kovalevsky.

09:30-10:00am 2.1.2.02
Unraveling the Catalytic Mechanism of DHFR using Neutron and Ultrahigh-resolution X-ray Diffraction. Qun Wan, Brad Bennett, Mark Wilson, Andrey Kovalesky, Paul Langan, Chris Dealwis.

10:00-10:30am Coffee Break

MONDAY, MAY 26

10:30-10:55am **2.1.2.03**

10:55-11:20am **2.1.2.04**

Details of cGMP Binding to the Regulatory Domain of PKG I β Revealed by Joined X-ray/neutron Crystallography. Oksana Gerlits, Gilbert Huang, Matthew Blakeley, Choel Kim, Andrey Kovalevsky.

11:20-12:00am **2.1.2.05**

Is Xylose Isomerase Non-Michaelis? A Combined Quantum Chemical & Neutron Crystallography Study. Matt Challacombe, Nicolas Bock, Andrey Kovalevsky.

2.1.3 Blackboard Sessions: Data Processing with the Pros

Edward Collins, Andrew Torelli, presiding
Aztec

09:00-09:30am **2.1.3.01**

Data Collection and Processing Begins at Home. James Pflugrath.

09:30-10:00am **2.1.3.02**

Data Collection, Reduction and Semi-automatic Structure Solution with HKL-3000. Wlodek Minor, Marcin Cymborowski, Zbyszek Otwinowski, Dominika Borek, Chruszcz Maksymilian.

10:00-10:30am **Coffee Break**

10:30-11:00am **2.1.3.03**

iMosflm and its Tools for Data Analysis. Harry Powell.

11:00-11:30am **2.1.3.04**

XDS Package And Related Tools for X-Ray Data Processing. Keitaro Yamashita.

11:30-12:00pm **2.1.3.05**

Data Processing with the PROTEUM Software Suite. Michael Ruf, Matthew M. Benning.

2.1.4 Wavelengths and Particles as Tools in Structural Analyses

Vivian Stojanoff, Bi-Cheng Wang, presiding
Dona Ana

09:00-09:30am **2.1.4.01**

An Overview of Ultra Short Wavelengths in Macromolecular Crystallography. John Helliwell.

09:30-10:00am **2.1.4.02**

New Capabilities and Challenges for Protein Crystallography Using Neutrons. Dean Myles.

10:00-10:20am **Coffee Break**

10:20-10:45am **2.1.4.03**

Crystallography at Ultra-short wavelength, why not? Vivian Stojanoff, Jean Jakoncic, Veijo Honkimaki, Marco DiMichiel.

10:45-11:10am **2.1.4.04**

Using X-rays to Describe Electronic Fluxes in REDOX Enzymes. Enrique Rudino-Pinera, Enrique Rudino-Pinera, Eugenio De la Mora, Hugo Serrano-Posada, Nizaa Jimenez-Arroyo, Cesar S. Cardona-Felix, Claudia Rodriguez-Almazan.

11:10-11:40am **2.1.4.05**

Expanding the Crystallographer's Toolbox: A SER-CAT Pilot Project Exploring New Applications of Wavelength (Energy)-Dependent Diffraction Data. Bi-Cheng Wang, Palani Kandavelu, Lirong Chen, John Rose, Dayong Zhou, Hua Zhang, Zheng-Qing (Albert) Fu, Unmesh Chinte, James Fait, John Chrzas.

11:40-12:10pm **2.1.4.06**

Native Structural Analyses from Anomalous Diffraction at Low X-ray Energy. Wayne Hendrickson, Qun Liu.

2.1.5 Discovering Emergent Phenomena and Magnetism With Neutron and X-ray Powder Diffraction

Branton Campbell, Anna Llobet Cimmarron

09:00-09:30am **2.1.5.01**
Low Dimensional Magnetism and Topological Magnetic Frustration in Copper Based Delafos-site oxides. Ovidiu Garlea.

09:30-10:00am **2.1.5.02**
Structural Signatures of Stripe-Order Melting and Symmetry-Broken States in the Pseudogap Phases of Nickelates and Cuprates, and Related Materials. Emil Bozin.

10:00-10:30am **Coffee Break**

10:30-10:50am **2.1.5.03**
Discovery of Tripolaron Formation in TbBaMn₂O_{5.75}. Graham King, David Avila-Brande, Esteban Urones-Garrote, Anna Llobet, Susana Garcia-Martin.

10:50-11:10am **2.1.5.04**
Magnetic Critical Phenomena in Parent Superconductor Fe(1+x)Te. Efrain Rodriguez, Chris Stock, Mark Green, Jose Rodriguez.

11:10-11:30am **2.1.5.05**
Structural, Magnetic, and Field Induced Phase Transitions in (Tb/Dy)RuAsO. Michael McGuire, Ovidiu Garlea, Andrew May, Brian Sales.

11:30-12:00pm **2.1.5.06**
Phase Competition Between Structurally Orthorhombic and Tetragonal SDW Phases in the Ba(1-x)NaxFe₂As₂ (0.24 ≤ x ≤ 0.28) Superconductors. Jared Allred, Daniel Bugaris, Omar Chmaissem, Stephan Rosenkranz, Sevda Avci, Pascal Manuel, Dmitri Khalyavin, Aziz Daoud-Aladine, Duck Young Chung, Helmut Claus, Mercouri Kanatzidis, Ray Osborn.

2.2.1 Engaging Undergraduate Students with X-ray Crystallography: Curriculum Development, Undergraduate Research, Equipment Acquisition, and Strategies for Faculty Success

Roger Rowlett, Kraig Wheeler, presiding
Brazos

Funding for this session provided, in part, by Art Robbins Instruments, Crystallographic Resources, Inc.

01:30-02:00pm **2.2.1.01**
Engaging University of Manchester Chemistry Undergraduate Students in Protein Crystallography. John Helliwell.

02:00-02:20pm **2.2.1.02**
Integration of a Benchtop Single-Crystal X-Ray Diffractometer into an Active Undergraduate Research Program in Synthetic Inorganic and Organometallic Chemistry. John Lee.

02:20-02:40pm **2.2.1.03**
Experiences with Teaching Undergraduates Protein Crystallography in a Synchrotron Environment; Case Study at Lund University and the MAX IV Laboratory. Marjolein Thunnissen, Derek Logan, Thomas Ursby.

02:40-03:00pm **2.2.1.04**
Exposing Undergraduates to Protein Crystallography Research. Rachel Powers.

03:00-03:30pm **Coffee Break**

03:30-04:00pm **2.2.1.05**
One Weird Trick Makes Lysozyme Ideal for Training in Macromolecular Crystallography. James Pflugrath, Vijaya Madakasira.

04:00-04:20pm **2.2.1.06**
Benchtop Diffractometers: Implementation of an X-ray Crystallography Consortium of Undergraduate Institutions Based at St. Catherine University. Daron Janzen.

04:20-04:40pm **2.2.1.07**
X-ray Crystallography in the Chemistry Curriculum at the United States Naval Academy.

MONDAY, MAY 26

Wayne Pearson, Jamie Schlessman.

04:40-05:00pm **2.2.1.08**
Involving Undergraduates in Macromolecular Crystallization and X-ray Crystallography Experiments. Leoarnd Thomas, Paul Sims.

2.2.3 Supermolecular Assemblies

Gerald Audette
Galisteo

Funding for this session provided, in part, by Art Robbins Instruments, Fisher Scientific, Rigaku Americas Corporation, and VWR International Co.

01:30-01:35pm
Welcome and thanks to sponsors.

01:35-02:00pm **2.2.3.01**
The Crystal Structure of a Nematode-infecting Virus. Yusong Guo, Corey Hryc, David Wang, Wah Chiu, Weiwei Zhong, Yizhi Tao.

02:00-02:30pm **2.2.3.02**
RNA Polymerase Recycling during Transcription: Solution Structure of RapA and its Binding Site on RNA Polymerase. Smita Kakar, Xianyang Fang, Lucyna Lubkowska, Yan Ning Zhou, Gary Shaw, Ding Jin, Mikhail Kashlev, Yun-Xing Wang, Xinhua Ji.

02:30-03:00pm **2.2.3.03**
Structural Studies of the U6 snRNP. Eric Montemayor, Allison Didychuk, John Hardin, Yasushi Kondo, Elizabeth Curran, Hong Hong Liao, Kristie Andrews, Christine Treba, Kiyoshi Nagai, Samuel Butcher, David Brow.

2.2.4 Producing and Transporting Energy: Thermoelectrics, Superconductors, Photovoltaics, and Magnets

Michael Mcguire, presiding
Cimmarron

01:30-02:00pm **2.2.4.01**
Crystal Chemistry of Ba₈M₁₆P₃₀ (M= Cu/Zn) Clathrates: Phase Transformations Induced by

Electron Doping. Kirill Kovnir.

02:00-02:20pm **2.2.4.02**
Synthesis and Structural Analysis of a New Heterometallic Supramolecular Compound. Patrice Tsobnang Kenfack.

02:20-02:40pm **2.2.4.03**
Neutron Single-Crystal Structural Study of Stephanite, Ag₅SbS₄, Silver Ion Motion. Bryan Chakoumakos, Huibo Cao, Antonio dos Santos.

02:40-03:30pm **Coffee Break.**

03:30-04:00pm **2.2.4.04**
New High-Anisotropy Materials for Permanent Magnetism: Limitations, Goals, and Successes. Vladimir Antropov.

04:00-04:20pm **2.2.4.05**
Magnetic Orders of the Intermetallic Binary Compounds R₅Pb₃ (R=Nd or Tb). Huibo Cao, Jiaqiang Yan.

2.2.5 Automation: from Crystal to Solved Structure

Aina Cohen, presiding
Dona Ana

01:30-02:00pm **2.2.5.01**
Nano-scale to Micro-scale: Detection and Optimization of Submicron Crystals. Joe Luft, Jennifer Wolfley, Elenaor Cook Franks, Angela Lauricella, Raymond Nagel, Stephen Potter.

02:00-02:30pm **2.2.5.02**
Automated Crystal Harvesting with the RodBot. David Sargent, Hsi-Wen Tung, Roel Pieters, Bradley Nelson.

02:30-03:00pm **2.2.5.03**
Efficient Data Collection using Multiple Crystals in High Density Grids. Elizabeth Baxter, Aina Cohen, Jinhu Song, Laura Aguila, Christopher Barnes, Chris Bonagura, Winnie Bremmer, Axel Brunger, Guillermo Calero, Brian Kobilka, Andrew Kruse, Artem Lyubimov, Karl-Magnus Larsson, Scott McPhillips, Erik

Norgren, Yingsu Tsai, Bill Weis, S. Michael Soltis.

03:00-03:30pm Coffee Break

03:30-04:00pm 2.2.5.04

Recent Progress of Robot Based Systems for Crystallography on Beamlines and in the Laboratories. Jean-Luc Ferrer, Xavier Vernede, Yoann Sallaz-Damaz, Christophe Berzin, Michel Pirocchi, Franck Borel, Nathalie Larive.

04:00-04:30pm 2.2.5.05

Automated Merging of Multiple Partial Datasets. Kay Perry.

04:30-05:00pm 2.2.5.06

New Developments for Processing Microcrystal X-RAY Diffraction Data. Graeme Winter, Richard Gildea, David Waterman, Gwyndaf Evans.

2.2.6 Bio SAS Data Analysis withtith US-SOMO

Emre Brooks, Javier Perez, Mattia Rocco, presiding Aztec

01:30-03:00pm Intro and HPLC-SAX Tools

03:00-03:30pm Coffee Break

03:30-05:00pm DMD and Advanced Usage

2014 Margaret C. Etter Student Lecturer Awards

Each Scientific Interest Group (SIG) has the opportunity to select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIG. Students who are selected receive a monetary award of \$250 and a certificate to be presented at the beginning of their lecture.

Congratulations to this year's winners:

BioMac	Yusong Guo, Rice Univ.....	2.2.3.01
Fiber Diffraction	R. S. Madhurapantula, Illinois Inst. of Technology	3.2.1.02
Industrial	Jacob Trotta, Alkermes, Inc.....	1.2.1.02
Light Source.....	Igor Petrik, Univ. of Illinois at Urbana-Champaign	3.1.2.04
Materials Science	William Kerlin, Univ. of Nevada Las Vegas	3.2.2.04
Neutron Scattering.....	Patricia Langan, Los Alamos National Lab	4.1.3.06
Powder Diffraction	Vicky Doan-Nguyen, Univ. of Pennsylvania	1.2.3.04
Small Angle Scattering	Jesse Hopkins, Cornell Univ.....	3.2.5.07
Small Molecule.....	Jordan Cox, Univ. of Buffalo	4.2.5.06
Young Scientist.....	Crysania Linderman, Univ. of Buffalo	3.1.1.05

TUESDAY, MAY 27

Registration Desk.....	7:30am	East Lobby
Speaker Ready Room.....	7:30am	Tijeras
Council Meeting Room.....	7:30am	La Cienega
Small Angle Scattering SIG Meeting	12:00pm	Galisteo
BioMac SIG Meeting.....	12:00pm.....	Dona Ana
Sm Molecules & Service Cr Joint SIG Meeting.....	12:00pm.....	Brazos
Membership Business Meeting.....	5:00pm	Aztec
Poster Session T	5:30pm.....	NE Exhibit Hall

P003 Margaret C. Etter Early Career Award Presentation and Lecture

Martha Teeter, presiding
Brazos

08:00-08:45am P003.01
Exploring the Structures of Clostridial Protein Toxins. Borden Lacy, Stacey Rutherford, Desiree Benefield, Melanie Ohi, Benjamin Spiller.

3.1.1 Etter Early Career Symposium

Yulia Sevryugina, presiding
Brazos

09:00-09:15am 3.1.1.01
Saccharin as a Potential Lead Compound for Anti-Cancer Targeting of Carbonic Anhydrase IX. Brian Mahon, Alex Hendon, Robert McKenna.

09:15-09:30am 3.1.1.02
Structural Studies of NKX2.1 Homeodomain. Lagnajeet Pradhan, Hyun-Joo Nam.

09:30-09:45am 3.1.1.03
Crystal Structure of *Staphylococcus aureus* Type I Signal Peptidase - a Novel Drug Target for Antibiotic-resistant Gram-positive Bacterial Infection. Yi Tian Ting, Paul Young, Edward Baker.

09:45-10:00am 3.1.1.04
Insights into the Structural Plasticity of the Variable Domain of the Receptor for Advanced Glycation Endproducts. Jaime Jensen, Venkata Indurthi, Estelle Leclerc, Stefan Vetter, Christopher Colbert.

10:00-10:30am Coffee Break

10:30-10:45am 3.1.1.05
Consequences of Heavy-atom Ligand Substitution in Cu(I) Emitters. Crysania Linderman, Corey O'Brien, Jordan Cox, Jarrett Coppin, Dinesh (Dan) Patel, Jason Benedict.

10:45-11:00am 3.1.1.06
The Structural Properties of Iron (III), Nickel(II), Copper(II) and Zinc(II) Complexes Containing 12-membered Pyridine- and Pyridol-based Tetra-aza Macrocycles. Kimberly Lincoln, Samantha Brewer, Travis Hayden, Michael Offutt, Ryker Saunders, Kayla Green.

11:00-11:15am 3.1.1.07
The Effect of Template Switching on the Stereochemical Selectivity of Photoactivated [2+2] Cycloaddition Reactions. Eric Reinheimer, Devin Ericson, Zachary Zurfluh-Cunningham, Ryan Groeneman, Leonard MacGillivray.

11:15-11:30am 3.1.1.08
Direct Observation of the Short-lived Excited State Structure of a Dimeric silver(I)-copper(I) Complex via Time-resolved X-ray Laue Diffraction. Katarzyna Jarzemska, Radoslaw Kaminski, Bertrand Fournier, Elzbieta Trzop, Jesse Sokolow, Yang Chen, Robert Henning, Philip Coppens.

11:30-11:45am 3.1.1.09
Thermofluor as a Rapid Method to Determine and Optimize Conditions for Protein Folding. Amadeo Biter, Jean Lin, Kevin Phillips.

11:45-12:00pm 3.1.1.10
Novel Dimer Interface in a Single Domain Response Regulator from a Red Light Sensing Network. Anna W. Baker, Kittikhun Wangkanont, Katrina Forest.

3.1.2 Combined Techniques in One Beamline

Christine Beavers, Petrus Zwart, presiding
Aztec

09:00-09:30am 3.1.2.01

Combining X-ray Spectroscopy and Diffraction to Study the Catalytic Cycle of Photosystem II using Synchrotron and XFEL Sources. Jan Kern, Roberto Alonso-Mori, Rosalie Tran, Johan Hattne, Aaron Brewster, Nathaniel Echols, Sergey Koroidov, Carina Gloeckner, Mohamed Ibrahim, Julia Hellmich, Hartawan Laksmo, Raymond Sierra, Gaungye Han, Sheraz Gul, Johannes Messinger, Athina Zouni, Nicholas Sauter, Vittal Yachandra, Uwe Bergmann, Junko Yano.

09:30-10:00am 3.1.2.02

Tracking Reduction of the bis-Fe(IV) Heme Intermediate in MauG-MADH Crystals using Single Crystal Spectroscopy. Erik Yurl, Babak Andi, Lyndal Jensen, Victor Davidson, Carrie Wilmot.

10:00-10:30am Coffee Break

10:30-11:00am 3.1.2.03

Active Site Redox Assignments in Metalloproteins using Diffraction Spectroscopy. Darren Sherrell, Aina Cohen, Jay Nix, Thomas Spatzal, Oliver Einsle, Ingrid Pickering, Graham George.

11:00-11:30am 3.1.2.04

Correlated Crystallographic and Spectroscopic Investigations of Oxygen Reduction by Engineered Oxygen Reductases. Igor Petrik, Babak Andi, Robert Henning, Allen Orville, Yi Lu.

11:30-12:00am 3.1.2.05

Structural Characterization of the Kynurenine Enzyme Trio and Reaction Cycle Intermediates Reveal Novel Metabolic Connections. Lu Huo, Ian Davis, Aimin Liu.

3.1.3 Solution Structure and Dynamics of Biomolecules

Thomas Weiss, presiding
Galisteo

09:00-09:05am

Welcome & thanks to sponsors

09:05-09:40am 3.1.3.01

Structural Dynamics and Functional Asymmetry Within ATPase Activator Ring Drives σ 54-RNAP Interaction and ATP Binding and Hydrolysis. B. Tracy Nixon, Tatyana Sysoeva, Saikat Chowdhury, Liang Guo.

09:40-10:00am 3.1.3.02

Small-Angle Scattering and Atomistic Modeling of Dilute and Concentrated Monoclonal Antibody Solutions. Nicholas J. Clark, Susan Krueger, Max Watson, Maribel Espinosa, Sekhar Kanapuram, Bruce Kerwin, Arnold McAuley, Joseph Curtis.

10:00-10:30am Coffee Break

10:30-11:10am 3.1.3.03

Structure and Dynamics of Adapter Proteins at the Interface of Cell Membrane and Actin Cytoskeleton. Zimei Bu, Jahan Ali Khajeh, Bela Farago, David Callaway.

11:10-11:35am 3.1.3.04

The Box C/D Structure Reveals the Mechanism of rRNA Methylation: a Study Combining SANS, SAXS and NMR. Frank Gabel, Audrone Lapinaite, Bernd Simon, Lars Skjaerven, Magdalena Rakwalska-Bange, Teresa Carlomagno.

11:35-12:00pm 3.1.3.05

Bio-SANS, A Neutron Toolbox for Biomacromolecules Study. Shuo Qian, Sai Venkatesh Pingali, Volker Urban.

TUESDAY, MAY 27

3.1.4 Exciting Biology from Challenging Systems: Developers

Simon Morton, Gerd Rosenbaum, presiding
Dona Ana

09:00-09:30am 3.1.4.01

Serial Crystallography. Seth Fraden, Sol Gruner, Achini Ophthalage, Michael Heymann, Jennifer Wierman.

09:30-10:00am 3.1.4.02

Bringing Back Room Temperature Crystallography: New Techniques and Methods. Jennifer Wierman, Jonathan Alden, Paul McEuen, Sol Gruner.

10:00-10:30am Coffee Break

10:30-11:00am 3.1.4.03

Serial Crystallography with Sparse Data: collective Orienting and Indexing. Kartik Ayyer, Hugh T. Philipp, Mark W. Tate, Veit Elser, Sol M. Gruner.

11:00-11:30am 3.1.4.04

A Global View of Diffraction Geometry Refinement. David Waterman, Graeme Winter, James Parkhurst, Aaron Brewster, Luis Fuentes-Montero, Johan Hattne, Nicholas Sauter, Gwyndaf Evans.

11:30-12:00pm 3.1.4.05

Cctbx.xfel: New Software to Enable Serial Crystallography. Nicholas Sauter, Johan Hattne, Aaron Brewster, Jan Kern, Junko Yano, Vittal Yachandra.

3.1.5 Earth/Environmental Sciences

Olaf Borkiewicz, Claudia Rawn, presiding
Cimarron

09:00-09:30am 3.1.5.01

Local Structure of Ppal: Implication for Diagenetic environments. Hsiu-Wen Wang, Katharine Page, Reinhard Neder, Michael Cheshire, David Bish.

09:30-10:00am 3.1.5.02

Phase Determination in a Special Argillaceous Rock Formation by μ -XRD. Margit Fabian, Janos Osan, Szabina Torok, Rolf Simon.

10:00-10:30am Coffee Break

10:30-11:00am 3.1.5.03

Beamline 12.2.2: High Pressure Diffraction for the Geosciences at the Advanced Light Source. Christine Beavers, Jason Knight, Bora Kalkan, Junyuan Yan, Alastair MacDowell, Quentin Williams.

11:00-11:30am 3.1.5.04

Synthesis and Crystal Chemistry of $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$ (Mayenite) Doped with Fe. Claudia Rawn, Sabina Ude, Ashfia Huq.

3.2.1 Flesh & Blood: Intact and *in-situ* Connective Tissue Diffraction Studies of Animals Plants and Insect Bodies

Olga Antipova, Joseph Orgel, presiding
Cimarron

01:30-01:45pm 3.2.1.01

Molecular Structure and Organization of the Collagens Whilst in their Tissues as Shown by X-ray Diffraction. Joseph Orgel, Olga Antipova.

01:45-02:05pm 3.2.1.02

Determination of Structural Changes from Non-enzymatic Glycation of Type I Collagen using X-ray Diffraction and their Effect on its Digestion by MMP-I. Rama Sashank Madhura-pantula, Olga Antipova, Joseph Orgel.

02:05-02:25pm 3.2.1.03

in situ Characterization of Cu Dense Inclusion Bodies in Neuronal Stem Cells. Brendan Sullivan, Gregory Robison, Olga Antipova, Yulia Pushkar.

02:25-02:55pm 3.2.1.04

X-ray Diffraction Reveals Structural Aspects of Collagen Fibers in Cardiac Tissues. Olga Antipova, Joseph Orgel.

03:00-03:30pm Coffee Break**03:30-04:00pm 3.2.1.05**

Neutron and X-ray Fiber Diffraction Experiments and Computational Modeling of Pretreatment of Biomass. Paul Langan, Paul Langan, Loukas Petridis, Hugh O'Neill, Sai Venkatesh Pingali, Daisuke Sawada, Roland Schultz, Benjamin Lindner, Volker Urban, Barbara Evans, Art Ragauskas, Jeremy Smith, Brian Davison.

04:00-04:10pm 3.2.1.06

Scanning X-ray Microdiffraction Studies of the Molecular Architecture of *Arabidopsis stem*. Jiliang Liu, Hideyo Inouye, Lee Makowski.

1.1.1. Pathological Fibers: Prions Amyloids & Friends

Olga Antipova & Joseph Orgel, presiding
Cimmarron

04:10-04:20pm 1.1.1.01

Recent Progress in X-ray Diffraction Based Studies of Amyloid, Prion and Fibril based Brain Diseases. Joseph Orgel.

04:20-04:40pm 1.1.1.02

Structural and Pharmacological Studies of Anticonvulsant Carboxamides and Acetylureas. Tatiana Timofeeva, Arkadius Krivoshein, Bhupinder Sandhu, Junhao Huang, Yongli Chen.

04:40-05:00pm 1.1.1.03

Structural Studies of the Prion Protein Bound to the POM Family of Anti-prion Antibodies. Mridula Swayampakula, Pravas Baral, Michael James.

3.2.2 Structural Studies of Radioelements

Paul M. Forster, Alice Smith, presiding
Dona Ana

01:30-02:00pm 3.2.2.01

Supramolecular Chemistry with Hexavalent Uranium. Christopher Cahill.

02:00-02:30pm 3.2.2.02

The Crystal Chemistry of Technetium Oxides and Halides. Efrain Rodriguez, Frederic Poineau, Kenneth Czerwinski, Alfred Sattelberger, Anthony Cheetham, Anna Llobet.

02:30-03:00pm 3.2.2.03

Crystallochemical Trends in a New Family of PuMIn₅ (M = Co, Rh, Ir) Compounds. Paul Tobash, Brian Scott, Jeremy Mitchell, Eric Bauer.

03:00-03:30pm Coffee Break**03:30-04:00pm 3.2.2.04**

Preparation and Structural Analysis of Low Valent Technetium Metal-metal Bonded Species via Solvothermal Reduction of Pertechnetate Salts. William Kerlin, Paul Forster, Alfred Sattelberger, Kenneth Czerwinski.

04:00-04:30pm 3.2.2.05

Structural Topologies of Uranyl Peroxide Cage Clusters. Jie Qiu, Peter Burns.

04:30-05:00pm 3.2.2.06

in situ High Temperature Synthesis and Characterization of Uranium Carbide. Helmut Matt Reiche, Sven C. Vogel.

3.2.3 Computational, Chemical & Biological Crystallography: Complimentary Methods Bridging the Divide

Louise Dawe, Jason Mercer, presiding
Brazos

01:30-02:00pm 3.2.3.01

Predicted Crystallization and Dynamic Structural Models: Recent Experiences from Several Challenging Proteins. Gerald Audette.

02:00-02:30pm 3.2.3.02

Advantages of Refinement using MMFF Force Field for Ligand Geometry. Gregory Warren, Oliver Smart, Brian Kelley, Gerard Bricogne.

TUESDAY, MAY 27

02:30-03:00pm **3.2.3.03**
Comparing Chemistry to Outcome: The Development of a Chemical Similarity Metric, Clustering and Visualization to Macromolecular Crystallography. Edward Snell, Andrew E. Bruno, Amanda M. Ruby, Joseph R. Luft, Thomas D. Grant, Jayaraman Seetharaman, John F. Hunt, Gaetano T. Montelione.

03:00-03:30pm **Coffee Break**

03:30-04:00pm **3.2.3.04**
Jeux Sans Frontieres - Games in Reciprocal Space. Jim Britten, Weiguang Guan, Victoria Jarvis, Hilary Jenkins.

04:00-04:20pm **3.2.3.05**
Shutterless Data Collection Using the Photon-100 Detector: A User's Perspective. Victor Young.

04:20-04:40pm **3.2.3.06**
Extension of Pair-based Structural Homology to Incommensurate Structures. Herbert J. Bernstein, Lawrence C. Andrews.

04:40-05:00pm **3.2.3.07**
RigakuIntegrate : A New Single Crystal Integration Program. Mark Pressprich.

3.2.5 Chemistry and Biology with Novel Scattering Techniques

Jacob Urquidi, presiding
Galisteo

01:30-02:00pm **3.2.5.01**
Enabling Challenging Biological Systems with XFEL Crystallography. Axel Brunger.

02:00-02:30pm **3.2.5.02**
2.9 Å Resolution Protein Structure Obtained Using Whole Cells as the Crystal Production and Delivery Vehicle. Michael Sawaya, Duilio Cascio, Mari Gingery, Jose Rodriguez, Lukasz Goldschmidt, Marc Messerschmidt, Sebastien Boutet, Jason Koglin, Garth Williams, Bruce Doak, Aaron Brewster, Karol Nass, Johan Hattne, Sabine Botha, Robert Shoeman, Daniel

DePonte, Brian Federici, Nicholas Sauter, Ilme Schlichting, David Eisenberg.

02:30-03:00pm **3.2.5.03**
Fluctuation Scattering as a Tool in Energy, Materials, Chemical and Biological Sciences. Peter Zwart, Erik Malmerberg.

03:00-03:30pm **Coffee Break**

03:30-03:50pm **3.2.5.04**
Current Challenges in Accurate Integration of Diffraction Data from X-ray Free Electron Lasers: Refining the Crystal Model. Aaron Brewster, Johan Hattne, Nicholas Sauter.

03:50-04:10pm **3.2.5.05**
HipGISAXS: a High-performance Parallel Computing Code for Simulating Grazing-incidence X-ray Scattering Data. Chenhui Zhu, Slim Chourou, Abhinav Sarie, Xiaoye Li, Elaine Chan, Alexander Hexemer.

04:10-04:35pm **3.2.5.06**
Microemulsions as a New Platform for Studying Membrane Proteins by SAS. Volker Urban, Douglas Hayes, Ran Ye, Sai Venkatesh Pingali, Hugh O'Neill, Rachel Dunlap.

04:35-05:00pm **3.2.5.07**
CryoSAXS as a Method for Measuring Low Resolution Macromolecular Structure. Jesse Hopkins, Andrea Katz, Stephen Meisburger, Matthew Warkentin, Richard Gillilan, Lois Pollack, Robert Thorne.

ACA Members' Business Meeting

5:00pm

Aztec

All are welcome

Toward a better understanding of Functional and Smart Materials. Olivier Gourdon.

4.1.3 Neutrons in Biology: New Instruments & Structures

Zoe Fisher, Andrey Kovalevsky, presiding
Cimarron

09:00-09:20am 4.1.3.01

IMAGINE, a Tunable Quasi-Laue Single crystal Diffractometer for Neutron Protein Crystallography. Flora Meilleur, Andrii Kovalevskyi, Parthapratim Munshi, Tibor Koritsanszky, Robert Blessing, Bryan Chakoumakos, Lee Robertson, Alexandru Stoica, Lowell Crow, Dean Myles.

09:20-09:40am 4.1.3.02

First Results from the Macromolecular Neutron Diffractometer (MaNDi). Leighton Coates.

09:40-10:00am 4.1.3.03

Conceptual Design for a Macromolecular Diffractometer at the ESS. Esko Oksanen, Britt Hansen, Phillip Bentley, Iain Sutton, Richard Hall-Wilton, Peter Willendrup, Ken Andersen.

10:00-10:30am Coffee Break

10:30-11:00am 4.1.3.04

Deciphering How Protonation State Supports Catalysis in Bacterial KDN9P Phosphatase. Karen Allen, Tyrel Bryan, Javier M. Gonzalez, John P. Bacik, Nicholas J. DeNunzio, Clifford J. Unkefer, Tobias E. Schrade, Andreas Ostermann, Debra Dunaway-Mariano, S. Zoe Fisher.

11:00-11:20am 4.1.3.05

Joint Neutron/X-ray Structure of the *E. coli* ABC Transport Receptor Phosphate Binding Protein as a Model of Ion-dipole Interactions. Katherine Sippel, John Bacik, Zoe Fisher, Florante Quiocho.

11:20-11:40am 4.1.3.06

Joint X-ray/neutron Structure of Reversibly Photo-switchable Thermostable Green Protein variant. Patricia Langan, Andrey Kovalevsky,

Leighton Coates, Devin Close, Csaba Kiss, Geoff Waldo, Andrew Bradbury.

11:40-12:00am 4.1.3.07

Neutron Crystallographic Structure of the Inorganic Pyrophosphatase from *Thermococcus thioreducens* at 2.2Å: Insights to a Structure-based Catalytic Mechanism. Joseph D. Ng, Michelle L. Morris, Leighton Coates, Tobias Schrader, Matthew P. Blakeley.

4.1.4 New Algorithms in SAXS/WAXS

Lee Makowski, presiding
Aztec

09:00-09:20am 4.1.4.01

HIPGISAXS: High Performance Computing Code for GISAXS. Alexander Hexemer, Slim Chourou, Abhinav Sarje, Xiaoye Li.

09:20-09:40am 4.1.4.02

SASCALC -- A Fast and Accurate Small-angle Scattering Calculator for Atomistic Ensembles. Joseph Curtis, Hailiang Zhang.

09:40-10:00am 4.1.4.03

WAXS, MD, Fluctuations and Function. Lee Makowski, Hao Zhou, Yu Jing Wang.

10:00-10:30am Coffee Break

10:30-10:50am 4.1.4.04

The SASTBX: New Tools for the Analyses of Biomolecular Small Angle Scattering Data. Petrus Zwart, Haiguang Liu.

10:50-11:10am 4.1.4.06

Progress in Parsimonious Spatial Modeling of Biological SAS Experimental Data. Emre Brookes.

11:10-11:25am 4.1.4.07

Three-dimensional Structure Determination of Large RNAs using Small-angle X-ray Scattering. Yuba Bhandari, Jinbu Wang, Xianyang Fang, Ping Yu, Yun-Xing Wang.

11:25-11:40am **4.1.4.08**

Crystal Structures and Target-Decoy SAXS Rigid Body Modeling of the Bifunctional Flavoenzyme Proline Utilization A. John Tanner.

11:40-11:55am **4.1.4.09**

Improvement and Evaluation of Uncertainty Estimation for Radius of Gyration Derived from Small-Angle X-ray Scattering Experiments. Cody Alsaker, Mark van der Woerd, F. Jay Breidt.

4.1.5 Cool Structures

Shao-Liang Zheng, presiding
Brazos

09:00-09:20am **4.1.5.01**

Symmetry-Guided Synthesis of Highly Porous Materials for Clean Energy Applications. Muwei Zhang, Hong-Cai Zhou.

09:20-09:40am **4.1.5.02**

Utilization of Synchrotron Radiation to Determine the Structures of Weakly- Diffracting Fullerene Crystals. Kamran Ghiassi, Susanne Chen, Armin De Meijere, Marilyn Olmstead, Alan Balch.

09:40-10:00am **4.1.5.03**

Finally! The Structural Secrets of a HD-GYP Phosphodiesterase Revealed. Dom Bellini, Delphine Caly, Yvonne McCarthy, Mario Bumann, Maxwell Dow, Robert Ryan, Shi-Qi An, Martin Walsh.

10:00-10:30am **Coffee Break**

10:30-10:50am **4.1.5.04**

Deceptive Orthorhombic Centered Lattices. Ilia Guzei.

10:50-11:10am **4.1.5.05**

Metal Complexes with BINOL-based Bis(pyridine) Ligands: From Self-sorting to Templating, from Subtle Effects to Unexpected Assemblies. Filip Topic, Maximilian Bogner, Christoph Gütz, Rainer Hovorka, Christoph Klein, Caroline Stobe, Niklas Struch, Gregor Schnakenburg, Arne Lützen, Kari Rissanen.

11:10-11:30am **4.1.5.06**

On a Remarkably Short Bi-Li Bond: Uniting Two Sides of the Periodic Table. Christopher Durr, Malcolm Chisholm, Vagulejan Balasanthiran.

11:30-11:45am **4.1.5.07**

π -Cation Porphyrin Derivatives. W. Robert Scheidt, Beisong Cheng, K. Venugopal Reddy, Kristin Buentello, Allen Oliver.

11:45-12:00am **4.1.5.08**

Cyclopropylammonium Flurbiprofen: 1:1 Salt 1:1:1 Salt Cocrystal and Related Salt/Salt Cocrystal Pairs. Carl H. Schwalbe, Miren Ramirez, Graham J. Tizzard, Peter N. Horton, Barbara R. Conway, Peter Timmins.

4.2.1 General Interest II

Graciela Diaz de Delgado, presiding
Galisteo

01:30-01:35pm **Opening Remarks**

01:35-01:55pm **4.2.1.01**

Advances in Data Quality in Area Detector Diffraction Experiments. Mathias Meyer.

01:55-02:15pm **4.2.1.02**

The Bruker APEX3 Suite - A New Generation of Single Crystal Software. Charles Campana, Joerg Kaercher, Bruce Noll, Michael Ruf.

02:15-02:35pm **4.2.1.03**

Explicit and Implicit Data Merging in Crystallographic Least Squares. Alan David Rae.

02:35-02:55pm **4.2.1.04**

Investigating Data Collection Strategies for High-Speed CCD Detector. Zheng-Qing Fu, John Chrzas, James Fait, Zhongmin Jin, Rod Salazar, John Gonczy, Unmesh Chinte, Palani Kandavelu, John Rose, Bi-Cheng Wang.

03:00-03:30pm **Coffee Break**

03:30-03:50pm **4.2.1.05**

XL Nano-sized Octahedral Coordination Cage

WEDNESDAY, MAY 28

Chunhua Hu, Shangchao Du, Tang-Qing Yu, Huaqiao Tan, Wuping Liao.

03:50-04:10pm **4.2.1.06**

Investigation of Porphyrin-based MOFs as Porous Hosts for Generating Singlet Oxygen. John MacDonald, Francisco Rosales Espinoza, Jiawei Lu, Grace Holliday, Andrew Smith.

04:10-04:30pm **4.2.1.07**

Solid State Behavior of the Muscle Relaxant Thiocolchicoside and Structural Characterization of its Dihydrate Using Powder and Single Crystal Methods. Graciela Diaz de Delgado, Robert Toro, Chun-Hsing Chen, Jines Contreras, Jose Miguel Delgado.

04:30-04:50pm **4.2.1.08**

When the Unseen Hydrogens are the Most Interesting Atoms in the Structure. Larry R. Falvello, Silvia C. Capelli, Elena Forcén-Vázquez, Garry J. McIntyre, Fernando Palacio, Milagros Tomás.

04:50-05:00pm **Closing Remarks**

4.2.2 Exciting Structures

John Rose, Daouda Traore, presiding
Aztec

01:30-01:35pm **Opening Remarks**

01:35-01:55pm **4.2.2.01**

Crystallization of Erg11p - The Cytochrome P450 Target of Azole Antifungal Drug. Franziska Huschmann, Thomas M. Tomasiak, Mikhail V. Keniya, Joseph D. O'Connell III, Sylvia R. Luckner, Kurt Krause, Richard D. Cannon, Janet Finer-Moore, Robert M. Stroud, Joel D. A. Tyndall, Brian C. Monk.

01:55-02:15pm **4.2.2.02**

Crystallographic and Enzyme Kinetics Studies Support Phosphate Transfer in by Metal-free cAMP-dependent Protein Kinase Catalytic Subunit. Amit Das, O. Gerlits, M.M. Keshwani, S.S. Taylor, M.J. Waltman, W.T. Heller, P. Langan, A. Kovalevsky.

02:15-02:35pm **4.2.2.03**

The Crystal Structure of the C-terminal Domain of the Ebola Virus Nucleoprotein (NP). Paulina Dziubanska, Urszula Derewenda, Jeff Ellena, Krystal Haley, Daniel Engel, Zygmunt Derewenda.

02:35-02:55pm **4.2.2.04**

Structural Basis of Cytosolic DNA Recognition by the PYHIN family Innate Immune Receptors AIM2 and IFI16. Tengchuan Jin, Jiansheng Jiang, Mo Huang, Andrew Perry, Patrick Smith, Tsan Xiao.

02:55-03:30pm **Coffee Break**

03:30-03:50pm **4.2.2.05**

Structural Analysis of Ara h 8, an Allergen from Peanuts. Lesa Offermann, Barry Hurlburt, Jane McBride, Makenzie Perdue, Karolina Majorek, Soheila Maleki, Maksymilian Chruszcz.

03:50-04:10pm **4.2.2.06**

Breaking the Crystal Twinning of the Flexible UvsY protein: An Experimental Low Resolution Structure and the Twinned High Resolution structure. Stefan Gajewski, Stephen White.

04:10-04:30pm **4.2.2.07**

Structural & Functional Studies of a Novel RNA-binding Sm-like Archaeal Protein. Peter Randolph, Kanishk Jain, H. Thien Nguyen, Cameron Mura.

04:30-04:50pm **4.2.2.08**

The role of BamA in the Biogenesis of beta-barrel Membrane Proteins in Gram-negative Bacteria. Nicholas Noinaj, Adam Kuszak, Curtis Balusek, Petra Lukacik, Hoshing Chang, Nicole Easley, Trevor Lithgow, JC Gumbart, Susan Buchanan.

04:50-05:00pm **Closing Remarks**

4.2.3 Opportunities with New Sources

Soichi Wakatsuki, presiding
Brazos

01:30-01:40pm Introduction

01:40-02:00pm 4.2.3.01

MX at MAX IV. Marjolein Thunnissen, Roberto Appio, Johan Unge, Derek Logan, Thomas Ursby.

02:05-02:20pm 4.2.3.02

Final Design of Biomedical Beamlines for Micro-crystallography and Highly Automated Crystallography at NSLS-II: Status and Opportunities at FMX and AMX. Dieter Schneider, Robert Sweet, Lonny E. Berman, Dileep Bhogadi, Oleg Chubar, Lin Yang, Sean McSweeney, Martin Fuchs.

02:20-02:40pm 4.2.3.03

Structural Biology at LCLS: Current Capabilities and Future Plans. Sebastien Boutet.

02:40-03:00pm 4.2.3

Visualizing Ultrafast Structural Changes in Photosynthetic Reaction Centres. Richard Neutze.

02:55-03:30pm Coffee Break

03:30-03:50pm 4.2.3.04

Progress Toward Virus Structural Studies using the Linac Coherent Light Source (LCLS). Brenda G. Hogue, Haiguang Liu, Stephan Kassemeyer, Robert Lawrence, Sebina Botha, Dingjie Wang, Daniel James, Ho-Hsien Lee, Tsafirir Mor, Petra Fromme, Raimund Fromme, Uwe Weierstall, John C. Spence, Ilme Schlichting.

03:50-04:10pm 4.2.3.05

Fixed Target Approaches for Sample Delivery in X-ray Laser Diffraction Studies. Geoffrey Feld, Henry Benner, Michael Heymann, Mark Hunter, Tommaso Pardini, Ching-Ju Tsai, Sabastian Boutet, Matthew Coleman, James Evans, Seth Fraden, Stefan Hau-Riege, Tanya Kuhl, Brent Segelke, Matthias Frank.

04:10-04:30pm 4.2.3.06

Time-resolved Crystallography Without Crystals. Dilano Saldin, Kanupriya Pande, Peter Schwander, Marius Schmidt.

04:30-04:50pm 4.2.3.07

Determination of Damage-free Crystal Structure of X-ray Sensitive Proteins using SACLA. Masaki Yamamoto, Kunio Hirata, Kyoko Shinzawa-Itoh, Naomine Yano, Shuhei Take-mura, Koji Kato, Tomitake Tsukihara, Eiki Yamashita, Go Ueno, Hironori Murakami, Takashi Ogura, Hiroshi Sugimoto, Jian-Ren Shen, Shinya Yoshikawa, Hideo Ago.

04:30-04:50pm 4.2.3.08

Serial Femtosecond Crystallography in Lipidic Cubic Phase. Vadim Cherezov.

4.2.4 SAXS with Biomolecular Mixtures

Emre Brookes, Srinivas Chakravarthy,
Javier Perez, presiding
Cimmarron

01:30-02:00pm 4.2.4.01

Modeling Against Small Angle Scattering Data from Polydisperse Samples. Alexey Kikhney, Maxim Petoukhov, Giancarlo Tria, Dmitri Svergun.

02:00-02:20pm 4.2.4.02

Solution Scattering Developments at the Australian Synchrotron SAXS/WAXS Beamline. Nigel Kirby, Stephen Mudie, Adrian Hawley, Nathan Cowieson, Haydyn Mertens, Vesna Samardzic-Boban, Robert Hynson, Lawrence Lee, Anthony Duff, Peta Faulkner, Rachel Kilmister.

02:20-02:40pm 4.2.4.03

EDNA and ISPyB Facilitate Efficient Online Size Exclusion Chromatography Experiments at the ESRF BioSAXS Beamline BM29. Adam Round.

02:40-03:00pm 4.2.4.04

Gaining Functional Insight from SAXS: How

WEDNESDAY, MAY 28

In-line SEC and MALS/DLS can Provide Complementary Structural Information and Quality Assessment in Polydisperse Systems. Alvin S. Acerbo, Michael J Cook, Bill A Miller, Scott E Smith, Irina A Kriksunov, Dolettha M E Szebenyi, Richard E Gillilan.

03:00-03:30pm Coffee Break

03:30-04:00pm **4.2.4.05**

New Developments in the UltraScan Solution MODeler (US-SOMO) HPLC-SAXS Data Analysis Module. Patrice Vachette, Javier Perez, Mattia Rocco, Emre Brookes.

04:00-04:20pm **4.2.4.06**

Analysis of Oligomeric and Allosteric States of GTPase Regulatory Enzymes by Size Exclusion Chromatography Small Angle X-ray Scattering. David Lambright, Andrew Malaby, Sagar Kathuria, Osman Bilsel, Robert Mathews, Thomas Irving, Srinivas Chakravarthy.

04:20-04:40pm **4.2.4.07**

Architecture and Functional Sites of the Inner Nuclear Envelope from NMR, AUC and SAXS data. Sophie Zinn-Justin, Isaline Herrada, Benjamin Bourgeois, Bernard Gilquin, Francois Lallemand, Howard J Worman, Javier Perez.

04:40-05:00pm **4.2.4.08**

Allosteric Regulation of the Catalytic Activity of the Human Phosphatase PTPN4 by its PDZ Domain. Nicolas Wolff, Pierre Maisonneuve, Celia Caillet-Saguy, Bertrand Raynal, Bernard Gilquin, Alain Chaffotte, Javier Perez, Sophie Zinn-Justin, Muriel Delepierre, Henri Buc, Florence Cordier.

4.2.5 Advances in X-ray and Neutron Scattering Techniques under Non-ambient Conditions

Christine Beavers, Gregory Halder, presiding
Dona Ana

01:35-02:05pm **4.2.5.01**

Advances in Neutron High Pressure Research at the Spallation Neutron Source. Antonio M. dos Santos, Jamie J. Molaison, Christopher A. Tulk.

02:05-02:25pm **4.2.5.02**

Behavior of Scandium Tungstate Type Materials under Non-ambient Conditions. Cora Lind-Kovacs, Lindsay Young, Jennifer Gadiant.

02:25-02:55pm **4.2.5.03**

The Response of Negative Thermal Expansion Materials to Pressure. Angus Wilkinson, Leighanne Gallington, Cody Morelock.

02:55-03:30pm Coffee Break

03:30-04:00pm **4.2.5.04**

The use of X-ray Diffraction for Real-Time and *in situ* Monitoring of Solid-State Transformations: Mechanochemical Reactions and Photo-Mechanical Effect. Tomislav Friscic, Oleksandr Bushuyev, Ivan Halasz, Christopher Barrett.

04:00-04:20pm **4.2.5.05**

From Nonporous to Porous: Exploiting High Pressures to Generate Porosity in the Nonporous Molecular Framework Zn(CN)₂. Saul Lapidus, Gregory J Halder, Peter J Chupas, Karena W Chapman.

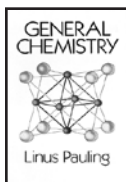
04:20-04:40pm **4.2.5.06**

Photochromism in a New Light: Temperature-Dependent *in situ* Photocrystallographic Study of a Diarylethene. Jordan Cox, Ian Walton, Dinesh Patel, Mengyang Xu, Andrea Markelz, Jason Benedict.

THURSDAY, MAY 29

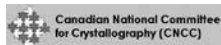
Planning Session for
2015 Meeting

8:30am Dona Ana



Pauling Poster Prize, Canadian and IUCr Poster Prize

The Pauling Poster Prize established by the ACA and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each annual meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of \$250, a complimentary banquet ticket, and a copy of a Linus Pauling book. An additional Pauling Prize sponsored by the Canadian Div. of the ACA and the Canadian National Committee of the IUCr, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory.



IUCr Poster Prize

The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.



Journal of Chemical Crystallography Poster Prize

The best graduate or undergraduate poster presentation in the area of chemical crystallography or small molecule structure determination and analysis is sponsored by Springer's Journal of Chemical Crystallography www.springer.com. The winner will receive their personal choice of books from Springer's extensive portfolio of titles.



Journal on Structural Dynamics Poster Prize

The prize of \$250 is given for excellence in research on structural determination and dynamics of sys-



tems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies and is open to students (graduate and undergraduate) and post-docs.

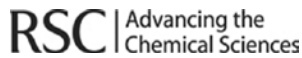
RCSB Protein Data Bank Poster Prize

This prize recognizes a student poster presentation involving macromolecular crystallography. The award will be 2 educational books that will be mailed to the winner after the meeting. An announcement will appear on the RCSB PDB website and newsletter.



CrystEngComm Poster Prize

CrystEngComm (published by the Royal Society of Chemistry) is very pleased to sponsor a prize to be awarded to the best graduate or undergraduate poster presentation in the area of crystal engineering/supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted on the CrystEngComm website (www.rsc.org/Publishing/Journals/CE/about.asp) shortly after the conclusion of the meeting.



Oxford Cryosystems Low Temperature Poster Prize

This prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.



Taylor & Francis Biomolecular Crystallography Poster Prize

This prize is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The winner will receive Bernhard Rupp's book Biomolecular Crystallography donated by the Taylor & Francis Group and will be announced at the banquet on Wednesday.



POSTER HANGING INSTRUCTIONS

Posters beginning with S should be assembled before 11:00am on Sunday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with M should be assembled before 11:00am on Monday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with T should be assembled before 11:00am on Tuesday and be removed at the conclusion of the poster session at 7:30pm.

Please be present at your poster from 5:30 - 7:30pm on the day to which you are assigned and remove your poster at the end of the session.

Sunday Posters



Poster
session
sponsored
by
Bruker

S-01

Applications of Smart Sensitivity Control with Agilent's New Range of S2 CCD Detectors. Tadeusz Skarzynski, Daniel Baker, Fraser White, Zoltan Gal, Mathias Meyer, Przemyslaw Stec.

S-02

Bonding in Group 1 Citrate Salts. James Kaduk, Alagappa Rammohan.

S-03

CCP4: Are you Getting your Updates. Charles Ballard, Eugene Krissinel, Ronan Keegan, Andrey Lebedev, David Waterman, Marcin Wojdyr, Ville Uski.

S-04

Characterization of Mutant Methionine Adenosyltransferases from *Sulfolobus solfataricus*. Eileen Brady, Fengbin Wang, Jonathan Clinger, George Phillips.

S-05

Coping with BIG DATA Image Formats: Integration of CBF NeXus and HDF5 A Progress Report. Herbert J. Bernstein, Jonathan M. Sloan, Graeme Winter, Tobias S. Richter.

S-06

Crystal Structure and Functional Characterization of an Hfq Homolog from *Aquifex aeolicus*. Kimberly Stanek, Jennifer Patterson, Peter Randolph, Cameron Mura.

S-07

Crystal Structure of Phosphoenolpyruvate Carboxylase from *Methylobacterium extorquens*. Ricardo Marti-Arbona, Javier M Gonzalez, Cliff Unkefer.

S-08

Crystal Structure of SgcC a Two-Component FAD-Dependent HpaB-family Monooxygenase from *Streptomyces globisporus*: Substrate Specificity and Carrier-Protein Recognition. Hongnan Cao, Weijun Xu, Jeremy R. Lohman, Craig Bingman, Huiming Ge, Tingting Huang, Ben Shen, George N. Phillips Jr.

S-09

Crystal Structure of the Nipah Virus Phosphoprotein Tetramerization Domain. Jessica Bruhn, Katherine Barnett, Jaclyn Bibby, Jens Thomas, Ronan Keegan, Daniel Rigden, Zachary Bornholdt, Erica Ollmann Saphire.

S-10

De Novo Phasing at SSGCID - Iodide Phasing Revisited. Jan Abendroth, Don Lorimer, Thomas Edwards.

S-11

Disorder in Protein Crystals of 3K9I Revealed by Diffuse X-ray Scattering Data and a Simple Markov Model for Molecular Displacements.

James Clarage, Anam Ahmed, Mary Faltaous, Lukas Cara.

S-12

Enhancing Protein Crystallization Through Synthetic GFP Symmetrization. David Leibly, Mark Arbing, Geoffrey Waldo, Thomas Terwilliger, Todd Yeates.

S-13

Fragment Screening of the Shikimate Pathway in Multi-drug Resistant Gram Negative Bacteria. L. Wayne Schultz, Kristin Sutton, Jennifer Breen, Thomas Russo, Timothy Umland.

S-14

High Impact Crystallography? - A Statistical Analysis of Crystal Structures Reported in the CSD (1997-2012). Amy Sarjeant.

S-15

How to use "Random" Microseeding Before you get your First Crystals. Patrick Shaw Stewart.

S-16

Human Hints: Powerful Tools for Nucleotide Monophosphate Drug Activation. Kimberly Maize, Carston Wagner, Barry Finzel.

S-17

Improved Twin Processing with CrysAlisPro. Lee Daniels, Fraser White, Daniel Baker, Zoltan Gal, Oliver Presly, Mathias Meyer.

S-18

Investigation of Molecular Mechanism of Rhodopsin Activation by Small Angle Neutron Scattering. Utsab Shrestha, Suchithranga Perera, Kurt VanDelinder, Udeep Chawla, Andrey Struts, Shuo Qian, Michael Brown, Xiang-Qiang Chu.

S-19

IUCr Participation in the CODATA / VAMAS Working Group on Nanomaterials. John Helliwell, Daniel Chateigner, Reinhard Neder.

S-20

Micromanufacturing Processes For Beamline Improvements. Diane Bryant, Simon Morton, Peter Zwart, Marc Allaire, Jason Knight, Kurt Krueger, John Pepper, Azer Dauz, Jeff Dickert, Anthony Rozales, Kevin Royal, Banumathi Sankaran, Nathan Smith, John Taylor, Yun Zhou, Corie Ralston.

S-21

Mitotic Kinesin Structure Displays Elusive Near Rigor State of the Motor Domain. Kritica Arora, Parker Anderson, Ana Asenjo, Lama Talje, Monika Joshi, Hernando Sosa, Benjamin Kwok, John Allingham.

S-22

Nanostructured ZnO Thin Films From Colloidal Nanoparticles Deposited by Evaporation. Jose Alberto Alvarado, Hector Juarez, Mauricio Pacio.

S-23

Probing Hierarchical Nanomorphologies in High-performance Organic Solar Cells through Resonant Soft X-ray Scattering. Wei Chen.

S-24

Quasi-racemic Crystallization of Backbone Modified Proteins: Not Quite Centrosymmetric. Dale Kreidler, David Mortenson, Katrina Forest, Samuel Gellman.

S-25

Selective Observation of Slow Dynamics of Proteins in Complex Buffer Solutions. Yun Liu.

S-26

Structural and Functional Analyses of Secretory Proteins and Small Molecule Compounds from *Onchocerca volvulus* as Basis for Rational Drug Design. Amr Moustafa, Markus Perbandt, Christian Betzel.

S-27

Structural and Functional Analysis of Lysosomal Phospholipase A2 a Close Homolog of Lecithin-cholesterol Acyltransferase. Alisa Glukhova, James Shayman, John Tesmer.

Posters-S

- S-28**
Structural Basis for Cofactor Selectivity of a Zinc-containing Alcohol Dehydrogenase from *Streptococcus pneumoniae*. Donghyuk Shin, Sangho Lee.
- S-29**
Structural Characterization and the Design of Isoform Specific Inhibitors of Human Carbonic Anhydrase II and IX. Melissa Pinard, Fabrizio Carta, Jean-Yves Winum, Mayank Aggarwal, Claudiu Supuran, Robert McKenna.
- S-30**
Structural Characterization of 1-deoxy-D-xylulose-5-phosphate Reductoisomerase from *Vibrio vulnificus*. Nikita Ussin, Makenzie Perdue, Lesa Offerman, Maksymilian Chruszcz.
- S-31**
Structural Characterization of the Fungal Effector Protein Avr4. Nicholas Hurlburt, Amanda Kohler, Stephen Bolus, Ioannis Stergiopoulos, Andrew Fisher.
- S-32**
Structural Studies of OleA B C & D: Progress Toward Understanding the Olefin Biosynthetic Pathway. Matthew Jensen, James Christenson, Lawrence Wackett, Carrie Wilmot.
- S-33**
Structural Studies of PqqC Mutants Provide Clues to the Enzymatic Mechanism of this Cofactorless Oxidase. Robert Evans III, Valerie Klema, Florence Bonnot, Judith Klinman, Carrie Wilmot.
- S-34**
Structure of Rv3902c from *Mycobacterium tuberculosis*. Bharat Reddy, Derek Moates, Heung-Bok Kim, Todd Green, Chang-Yub Kim, Thomas Terwilliger, Lawrence DeLucas.
- S-35**
Targeted Taking the Crystals out of X-Ray Crystallography Data From Inorganic Crystalline to Study Thermodynamic Data of Phase in the SiO₂-K₂O-P₂O₅ System. Shahrbanoo Salehi, Dan Bostrum.
- S-36**
The Berkeley Center for Structural Biology Beamlines: Enabling High-Throughput Structure Solution Through Technical Upgrades. Kevin Royal, Marc Allaire, Diane Bryant, Azer Dautz, Jeff Dickert, Simon Morton, Anthony Rozales, Banumathi Sankaran, Nathan Smith, John Taylor, Peter Zwart, Corie Ralston.
- S-37**
The New wwPDB Deposition and Annotation System. Jasmine Young, Zukang Feng, Swanand Gore, Cathy Lawson, Tom Oldfield, Martha Quesada, Sanchayita Sen, Sameer Velankar, John Westbrook, Huanwang Yang.
- S-38**
The Structural Characterization of (147-Tris(2-nitrobenzenesulfonyl)-147-triazaheptane). Travis Hayden, Kimberly Lincoln, Kayla Green.
- S-39**
Two Paralogs of FabH in *V. cholerae*: Structures and Kinetics Suggest a Mechanism for Adaptation in the Initiation of Fatty Acid Synthesis. Jing Hou, Heping Zheng, Matthew Zimmerman, Maksymilian Chruszcz, Mahendra Chordia, Wladek Minor.
- S-40**
X-ray Single Crystal Analysis of n-Type Metallocene Dopants for OTFTs and Other Applications. Evgheni Jucov, Siyuan Zhang, Benjamin Naab, Zhenan Bao, Stephen Barlow, Seth Marder, Tatiana Timofeeva.
- S-41**
X-Ray Structural Study of Chalcogenopyriliium Cyanine-Like Dyes with Rigid Substituents for Signal Processing Applications. Bhupinder Sandhu, Marina Fonari, Tatiana Timofeeva, Yulia Getmanenko, Seth Marder.

Monday Posters

M-01

A Homologue Rescue Approach Increases the Structural Coverage of Tuberculosis Drug Targets. Don Lorimer, Loren Baugh, Garry Buchko, Robin Stacy, Lance Stewart, Thomas Edwards, Wesley Van Vorhis, Peter Myler.

M-02

A Set of Tools for Micro-crystallography: Highlights of Rigaku Minstrel DT/HT UV Advances. Pius Padayatti, Max Petersen, Benjamin Liedblad.

M-03

Anisotropy and Competition of Magnetic and Ferroelectric Phases in Mn_{1-x}CoxWO₄. Jose Luis Garcia-Munoz.

M-04

Bringing Instrumentation to the Undergraduate Laboratory. Bruce C. Noll, Scott D. Phillips, Michael Ruf.

M-05

Correlating Morphology and Hydrogen Adsorption Capacity of Disordered Carbons. Lilin He.

M-06

Crystal Structure of Human EAT2. Mohammed Taha, Hyun-Joo Nam.

M-07

Crystal Structure of [Na₄X][Ag₄₄(SC₆H₄CO₂)₃₀] Nanoparticles. Kristin Kirschbaum, Terry Bigioni, Brian Conn, Anil Desiredy, Wendell Griffith, Jingshu Guo, Bradley Monahan.

M-08

Crystal Structures Determined by Undergraduates in Biochemistry Provide New Insights into a Classic Enzyme. Katherine Kantardjieff, Eric Reinheimer, Clyde Smith, Larry Grant, Dominica Ranieri, Chandra Srinivasan, Christopher Meyer.

M-09

Crystallization and Preliminary Diffraction of a Periplasmic Zn-binding Protein. Erik Yukl.

M-10

Crystallographic studies of a *Yersinia pestis* Outer Membrane Transporter. Stephen Mayclin, Jennifer McCarthy, Nicholas Noinaj, Susan Buchanan.

M-11

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Heterometallic PdII-NiII Complexes. Double C-H Bond Activation and Formation of a Rectangular Tetradibenzotetraaza[14]Annulene. Hamid Khaledi, Marilyn Olmstead, Hapipah Mohd Ali.

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Modern Macromolecular Crystallography - Fun for Kids of All Ages. Pamela Focia, Wayne Anderson, Ludmilla Shuvalova, Allison Penn, Nicole Tanna, Andrew Trandal, Noelle Wands, James Winsor, Tamar Cooney.

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Monoclinic and Rhombohedral Crystals of Inorganic Pyrophosphatase from *T. thioresidens*. Michelle Morris, Anuj Singhal, Joseph D. Ng, Marc Pusey.

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SAD Phasing of RNA with X-rays at the Iron Absorption Edge. Blaine Mooers, Tzanko Doukov.

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SCrALS: Utilizing a High Flux Radiation Source for the Elucidation of Structures from Diffractionally-Challenged Microcrystals. Jeanette Krause, Allen Oliver.

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Searching for the Functional Hydrogen Atom: Joint X-ray/neutron Crystallographic Studies of a Family 11 Xylanase. Andrey Kovalevsky, Qun Wan, Scott Hamilton-Brehm, Kevin Weiss, Zoe Fisher, Marat Mustyakimov, Leighton Coates, Paul Langan.

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Sensor Domain of hHstidine Kinase KinB of *Pseudomonas* - a Helix-swapped Dimer. Kemin Tan, Gekleng Chhor, Andrew Binkowski, Robert Jdrzejczak, Magdalena Makowska-Grzyaska, Andrzej Joachimiak.

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Structural Studies on *Trypanosoma brucei* Flap Endonuclease Wild Type (TbFEN). Faizah AlMalki, Sarah Oates, Svetlana Sedelnikova, Jon Sayers, Peter Artymiuk.

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Structure and Function of Two Putative Virulence Factors from *Francisella tularensis*. Geoffrey Feld, Brent Segelke, Sahar El-Etr, Timothy Carpenter, Sahar El-Etr, Michelle Corzett, Nicholas Fischer, Mark Hunter, Matthias Frank, Amy Rasley.

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Structure and Mechanism of Levoglucosan Kinase: Molecular Insights into the Bioconversion of Levoglucosan. John Bacik, Brian Broom-Peltz, Laura Jarboe, Brian Mark,

Ryszard Michalczyk, Zoe Fisher, Clifford Unkefer.

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Structure of Potential Charge Transfer Polymorph Materials and a Pseudo-Polymorph with Trimeric Perfluoro-o-Phenylene Mercury and Tetrathiafulvalene. Raul Castaneda, Sergiu Draguta, Andrey Yakovenko, Morina Fonari, Tatiana Timofeeva.

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The Bis-iron (IV) Catalytic Intermediate of MauG: an Enzyme Involved in Methylamine Dehydrogenase Maturation. Chao Li, Erik Yukl, Victor Davidson, Carrie Wilmot.

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The Effects of Nano- and Meso-Structural Changes on the Long-Term Cycling Stability in Conversion-Type Electrodes. Kamila Właderek, Tiffany Kinnibrugh, Olaf Borkiewicz, Peter Chupas, Karena Chapman.

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Using a 2-day Mini-Camp to Initiate Faculty and Student Engagement in Protein Crystallography at Predominantly Undergraduate Institutions. Roger Rowlett.

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Why do X-ray Crystallographic Methods Work? Alan Pinkerton.

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X-ray and Fluorescent Studies of Potential Electro-luminescent MOFs. Carlos Ordonez, Qiang Wei, Tatiana Timofeeva.

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X-ray Correlated Single-crystal Electronic Absorption and Raman Spectroscopy at NSLS Beamline X26-C: A Polarized Approach.

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Yes Solvent Molecules Do Matter: Solvatomorphism and Polymorphism of cis- 22-tetrakis(mo nothiosuccinimidato)dimolybdenum(II). Brian Dolinar, Ilia Guzei, John Berry.

Tuesday Posters

- T-01**
Integration of Data Acquisition and Data Analysis for SAXS Experiments at Diamond Light Source. Jun Aishima, Irakli Sikharulidze, Conor Lehane, Tobias Richter, Karl Levik, Matthew Gerring, James Douth, Mark Tully, Katsuaki Inoue, Nick Terrill, Paul Gibbons, Alun Ashton.
- T-02**
Creating a Fluorescence Probe for X-ray Beam Characterization. Randy Alkire, Ralu Divan, C. Suzanne Miller.
- T-03**
Elucidation of Two Closely Related Polymorphs by Single Crystal X-ray Analysis. Alicia Ng, John DiMarco, Rosana Schlanm, Chenkou Wei, Qi Gao, Rat Scaringe.
- T-04**
Understanding the Biological Activity of L-Citrulline a Non-Essential Amino Acid Through Structural Studies. Alessio Caruso, Francesco Caruso, Miriam Rossi.
- T-05**
Ultra-high Resolution Protein Crystallography: Neutron Structure of Crambin at 1.1 Å. Julian Chen, Bryant Leif Hanson, Zoe Fisher, Paul Langan, Andrey Kovalevsky.
- T-06**
The Search for New Polymeric CuI/CuII Cyanide Complexes. Peter Corfield, Michael A. Chernichaw, Emma M. Cleary, Julie H. Thouboron and Joseph F. Michalski.
- T-07**
One Minute SAXS Data at Home - Your Personal SAXS Beamline. Angela Criswell, Mark Del Campo, Katsunari Sasaki.
- T-08**
Built Like A MOF - but a Purely Organic Cage. Lee Daniels, Gang Zhang, Oliver Presly, Fraser White, Iris Oppel, Michael Mastalerz.
- T-09**
Fish Antifreeze Protein Stabilized by a Network of ~400 Interior Waters. Peter Davies, John Allingham, Robert Campbell, Feng-Hsu Lin, Tianjun Sun.
- T-10**
Late-stage Crystal Failures and the Protein Crystal Harvesting Bottleneck. Marc Deller, Robert Viola, Jace Walsh, Marc Elsliger, Bernhard Rupp, Ian Wilson.
- T-11**
Accurate Alignment Corrects Errors in Ribosome Structural Analysis and Reveals Essential Function of S9. William Duax, Sam Chen, Connor Huck, Nick Sass.
- T-12**
DIALS - A Toolbox for Diffraction Data Analysis. Gwyndaf Evans, Graeme Winter, David Waterman, James Parkhurst, Luis Fuentes-Montero, Richard Gildea, Aaron Brewster, Johan Hattne, Nicholas Sauter.
- T-13**
Fragment-Based Discovery of Small Molecule Antagonists of Hyaluronan Binding to CD44. Barry Finzel, Li-Kai Liu.
- T-15**
In situ Manipulation and Patterning of Microcrystals Using Surface Acoustic Waves. Jarrod French, Feng Guo, Tony Huang.
- T-16**
Diterpene Glycosides from the Leaves of Stevia Rebaudiana. Frank R. Fronczek, Mohamed A. Ibrahim, Douglas Rodenburg, Kamilla Alves, James D. McChesney, Chongming Wu, Brian J. Nettles, Sylesh K. Venkataraman, Frank Jaksch.
- T-17**
Towards Establishing Advanced Micro-Beam Capability for Macromolecular Crystallography at the CLS. Pawel Grochulski, Mirek Cygler, Michel Fodje, James Gorin, Shaun Labiuk,

Kathryn Janzen.

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IYCr2014: Experience with 3D Printing of Molecular Models. Marvin Hackert, Lars Jacquemetton.

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A Novel NAD Cofactor Binding Mode in Bacterial IMPDH Explains Inhibitor Selectivity. Andrzej Joachimiak, Magdalena Makowska-Grzyska, Youngchang Kim, Natalia Maltseva, Jerzy Osipiuk, Suresh Kuma Gorla, Mandapati Kavitha, Deviprasad Gollapalli, Lizbeth Hedstrom.

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Transcription Regulation of Hydroxycinnamate Catabolic Gene Expression: Structures of HcaR-Ligand and HcaR-DNA Complexes. Grazyna Joachimiak, Youngchang Kim, Lance Bigelow, Garrett Cobb, Andrzej Joachimiak.

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Overview of New and Improved Software for Molecular Replacement in CCP4. Ronan Keegan, Andrey Lebedev, Ville Uski, Martyn Winn, Jens Thomas, Daniel Rigden, Jaclyn Bibby, Fei Long.

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Bringing “Old” Crystallography Equipment Back to New Life: Upgrading Existing Diffractometers with State-of-the-art Microfocus Sources. Lars Kuttnik, Jorgen Graf, Andre Beerlink, Jorg Wiesmann, Carsten Michaelsen.

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Structural Basis for High Affinity Antibody Recognition of an Intracellular Target. Ho Leung Ng, Niloufar Ataie, Jingyi Xiang, Neal Cheng, Elliott Brea, Wenjie Lu, David Scheinberg, Cheng Liu.

T-24

How X-ray Photons Transform the Active Sites of Proteins: A Study by Single Crystal Spectroscopy Correlated with Macromolecular Crystallography. Feifei Li, E. Sethe Burgie,

Rahul Singh, Lindsay Eltis, Richard Vierstra, Allen Orville.

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Co-crystallization of Dibenzofurane Isomers Without Apparent Molecular Complex Formation. Sergey Lindeman, Shriya Wadumethrige, Rajendra Rathore.

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Lujan Neutron Scattering Center at LANSCE. Anna Llobet.

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The Integration and Shutterless Operations of a New Technology CMOS Detector at ALS Beamline 4.2.2. Jay Nix, Robert Daly.

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Real-time X-ray Diffraction Movies Capture Molecular Details of Contraction. Robert Perz-Edwards, Michael Reedy, Thomas Irving.

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- T-37**
Applications of X-ray Crystallographic Techniques. A Tool to Help Answer Chemical Questions. Richard Staples.
- T-38**
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- T-39**
100 Years of Crystallography: Structural Biology at Merck. Corey Strickland.
- T-40**
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- T-42**
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- T-46**
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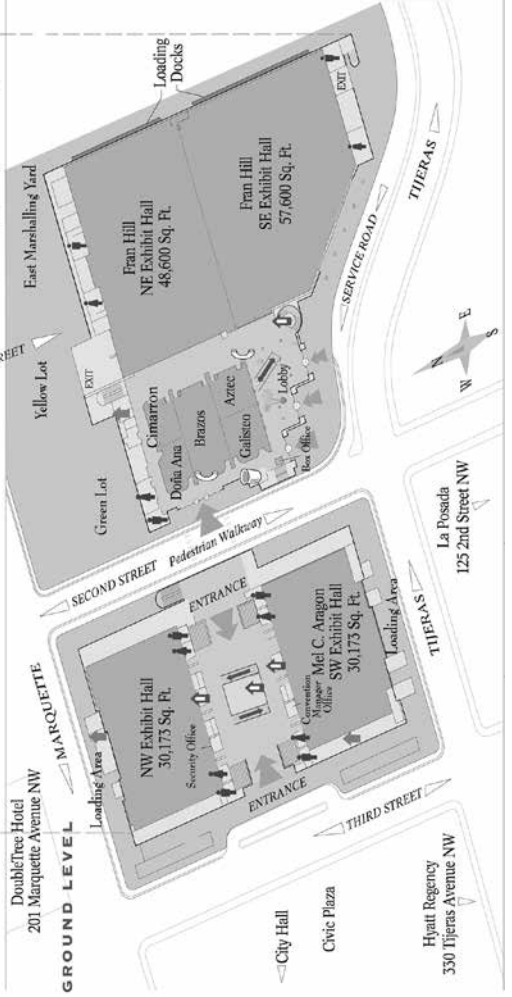
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Albuquerque Convention Center

UPPER LEVEL



EAST COMPLEX
is east of 2nd Street and comprises two levels — upper & ground only



2014 EXHIBIT SHOW - NE EXHIBIT HALL, ALBUQUERQUE CONVENTION CENTER MAY 24 - 27, 2014

SATURDAY - 7:30PM - 10:30PM
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