American Crystallographic Association

66th Annual Meeting

Denver CO

July 22-26, 2016

PROGRAM BOOK

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American Crystallographic Association
Annual Meeting July 22-26, 2016

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SER-CAT	#56
STOE	#6
TA Instruments	#33
TTP LabTech Ltd.	#40,41
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WK.01 - The CSD Python API: A Foundation for Innovation

Chair: **Governors Square 14**
Peter Wood **12:30pm-5:00pm**

Funding provided by Cambridge Crystallographic Data Centre

The CSD Python API workshop is ideal for researchers that have some basic familiarity with the CSD-System, but are interested in learning about more flexible and sophisticated ways to interact with CSD data and functionality; however, anyone is invited to attend. Attendees will not need to be expert in programming or scripting languages, but simply be comfortable with computer systems in general. Our experienced staff will be available to assist with any questions you might have and at the end of the workshop there will be an opportunity to trouble-shoot with the instructors. The instructors will remain for the duration of the ACA conference to provide any additional help and feedback that attendees might appreciate after the workshop.

Almost all ACA attendees will already have access to the CSD Python API through their institution's CSD-System licence, but if attendees do not already have a licence, we can provide short-term workshop licences in advance. Participants will be expected to bring along their own laptops and to have already installed the CSD-System, Python and the CSD Python API on their laptop prior to the workshop.

WK.02 Computational Approaches to the Structural Modelling of Biological Macromolecules using Small-Angle Scattering

Chair: **Governors Square 17**
Kushol Gupta

Funding provided by Wyatt, Technology Corp., Rigaku Americas Corp., Anton Paar

This one-day workshop will focus on computational approaches to structural modelling and analysis. In the first session, a brief reprise of fundamental concepts will be provided, with a focus on pitfalls in data acquisition and reduction that can affect subsequent data analysis and modelling. The remainder of the day will be allocated to the hands-on application of the leading software packages to the analysis of solution scatter. We propose direct participation from the authors of the most prevalent software packages currently used (e.g. ATSAS, SIBYLS, CCP-SAS, FoXs and IMP). Authors will present their software, including the basis for the algorithms employed, and further deliver guided hands-on tutorials for workshop participants. This approach will introduce and train participants on the appropriate application of these tools, including experimental design, model preparation, comparison of structural models using both SAS and complementary information, validation, and most importantly the limitations of interpretation with regards to the biological conclusions that can be made.

Schedule
8:00 am Basic Theory and Methods
- Introduction:what is SAS data good for?
- Theory Essentials: How to get your scattering profiles
- SAXS and SANS: common pitfalls, how to ensure the data is suitable for modelling
- Cross Checks and Validation

9:30 am Coffee Break
10:00 am AT SAS lectures & tutorial
11:30 am Lunch and Discussions
12:30 pm IMP lectures and tutorial
2:30 pm Coffee Break
3:00 pm SIBYLS lectures and tutorial
4:30 pm CCP-SAS lectures and tutorial
6:00 pm Discussion

WK.03 Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials

Chairs: **Governors Square 16**
Tom Grant **9:00am-5:00pm**
Nadia Zatsepin

Funding provided by BioXFEL

Schedule

1. An introduction to serial femtosecond crystallography and how the data differ from conventional crystallography data.

2. Cheetah tutorial: From raw data to useful diffraction patterns.

The first tutorial session will focus on Cheetah (www.desy.de/~barty/cheetah), and will involve the initial analysis and reduction of raw data to a set of clean, usable diffraction patterns in a facility-independent format (HDF5) for further analysis.

3. CrystFEL tutorial: Indexing, integrating, merging, post-refinement and evaluation of serial crystallography data.

The second tutorial session will focus on indexing, integrating and merging the cleaned SFX data using CrystFEL, a software suite created for SFX data analysis (and simulation). The development of CrystFEL is lead by Thomas White (CFEL, DESY), who will be the main instructor for this tutorial, with hands-on support for students from the workshop organizers experienced with CrystFEL: Grant and Zatsepin. The suite is written in C with supporting Perl and shell scripts, and is available as source code under version 3 or later of the GNU General Public License.

WK.04 Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques

Chair: **Auraria Campus**
William Ratcliff

The workshop will be structured as a series of lectures in the field of magnetic neutron scattering presented by organizers and invited speakers (including Branton Campbell, Huibo Cao, and Clarina Dela Cruz), and hands-on sessions where attendees will be assisted by the organizers. Materials will be provided electronically to the students. Students will be required to install software on their computers before the workshop and will be required to bring their laptops for the workshop. They will be required to have access to a Windows operating system.

Schedule

7:45 am Group leaves Sheraton Hotel
8:00 am Registration/Computer Setup
8:30 am Intro to Neutron Diffraction/Refinement
9:15 am Intro to Fullprof
9:45 Coffee Break
10:00 am Hands on exercise in Fullprof
11:30 am Intro to Magnetic Structures
12 pm Lunch
1:00 pm Intro to Magnetic Structures
1:30 pm Intro to Representational Analysis
2:30 pm Representational Analysis
3:00 pm Coffee break
3:15 pm Fullprof Magnetic Structure
4:15 pm Advanced Fullprof
4:45 pm Intro to magnetic space groups in using ISOTROPY software and the Bilbao Crystallographic server.
5:45 pm Wrap Up

Workshop will be held on the campus of the Auraria Higher Education Center, 1068 9th Street Park, Denver.

FRIDAY, JULY 22

WK.05 SHELX Workshop

Chairs: **Governors Square 15**
George Sheldrick
Jens Lübben

Part A: 8:30 am to 12:30 pm
Small molecule and solid state chemistry

George Sheldrick (Göttingen): Space group determination and structure solution with SHELXT
Peter Mueller (MIT): Structure refinement with SHELXL
Bill Clegg (Newcastle): Twinning and absolute structure determination
Claudia Wandtke (Göttingen): shelXle - a GUI for structure determination with SHELX
Daniel Kratzert (Freiburg): DSR - modeling and refinement of disordered structures
Xiaoping Wang (ORNL): refinement of small molecules against neutron data
Ton Spek (Utrecht): SQUEEZE and CheckCIF

Part B: 1:30 to 5:30 pm
Macromolecules

George Sheldrick (Göttingen): Experimental phasing of macromolecules with SHELXC/D/E
Max Nanao (ESRF): RIP and RIPAS phasing with the help of SHELXC/D/E
Andrey Lebedev (CCP4): SHELX in CCP4 and extension of borderline MR solutions with SHELXE
Massimo Sammito (Göttingen): ARCIMBOLDO, BORGES and SHREDDER
Anna Lübben (Göttingen): PDB2INS for setting up macromolecular refinements for SHELXL
Leighton Coates (ORNL): macromolecular refinement against X-ray and neutron data
Jens Lübben (Düsseldorf): R-complete - a better free R?!
Paul Emsley (LMB): Coot for SHELX users

Friday Evening Activities

First Time Attendee and Student Meeting Orientation
05:30-06:30pm **Plaza Ballroom D**

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
07:30pm **Plaza Exhibit**
Must have meeting name badge for entry

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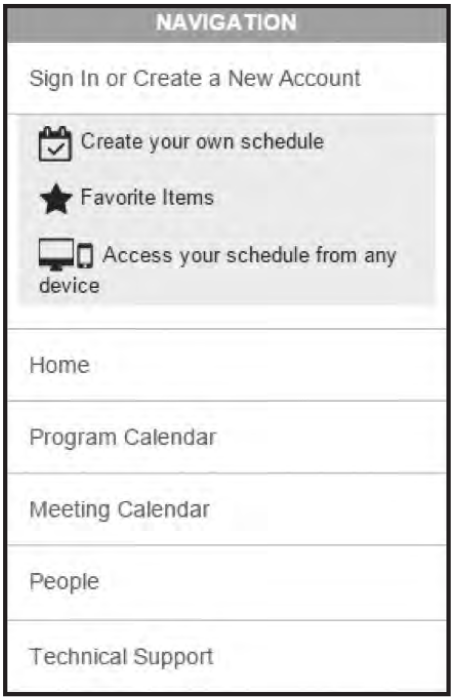

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SATURDAY, JULY 23

Registration Desk	07:30am	Plaza Registration
Speaker Ready Room	8:00am	Plaza Court 1
Council Meeting Room	8:00am	Directors Row F
Exhibit Show	10:00am	Plaza Exhibit
DECTRIS Lunchtime Seminar	12:00 pm	Governors Square 17

AW.01 Trueblood Award and Lecture

T. Terwilliger, Presiding **Plaza Ballroom A, B, C**

8:00 - 8:45am
XFEL Crystal Structure of the Synaptotagmin-1 : SNARE Complex. Axel Brunger, Stanford University

01.01 Poster Preview

Session Chairs: **Governors Square 14**
Louise Dawe and Bill Duax

9:00am 159-SU
Synthesis and Characterization of Novel Low Valent Group 13 Complexes. Lauren Stevens, Samantha DeCarlo, Christopher Snyder, Dennis Mayo, Yu-Sheng Chen, Peter Zavalij, Bryan Eichhorn,

9:08am 164-SA
Charge Density Analysis of 2,5-Dichloro-1,4-benzoquinone (DCBQ) at 20 K. Zhijie Chua, Christopher Gianopoulos, Bartosz Zarychta, Vladimir Zhurov, Alan Pinkerton

9:16am 151-SU
Supramolecular Assembly and a Novel Topology Within a Structurally Diverse Series of Lanthanide p-bromobenzoic Acid-terpyridine Hybrid Materials. August Ridenour, Korey Carter, Ray Butcher, Christopher Cahill.

9:24am 162-MO
Molecular Packing Preferences in "Bridge-Flipped" Isomeric Aryl-2-Pyridylhydrazones and 2-Pyridinecarboxaldehyde Arylhydrazones William Ojala, Kara Kassekert, Lindsey Beard, Charles Ojala.

9:32am 147-MO
High Temperature Nuclear Fuels without Gas Overpressures for Cosmic Deep-Space Explorations. Boris Udovic.

9:40am 20-SU
Dithiazole[4,5-a:5',4'-c]Phenazines as Donors in Co-Crystals with Tetracyanoquinodimethane Derivatives. Bianca Valencia, Yulia A. Getmanenko, Boris Averkiev, Tatiana V. Timofeeva.

9:48am 149-SU
Conductivity of $Cs_{1-x}SixH_2PO_4$ Trough Impedance Spectroscopy: Temperature Dependence Study. Andres Jose Encerrado M., Alan Goos, Ben Deutsch, Israel Martinez, Andrea Montgomery, Victor Gonzalez, Cristian E. Botez.

9:56am Coffee Break

10:30am 152-SA
Prescreening Integral Membrane Crystallization Conditions and Protein Preparations Utilizing FRAP. Eugene Chun, Peng Chen, Ellen Gualtieri, Dmitry Rodionov, Lance Ramsey, Eric Zhao, Wei Liu.

10:38am 145-MO
New *in situ* Capabilities at 17-BM Rapid Acquisition Powder Diffraction Line. Andrey Yakovenko, Wenqian Xu.

10:46am 156SA
Crystal Growth and Phasing made Possible by a Protein Metal Organic Framework (PMOF): Crystals of a Cacodylate-Zinc-His-tag-BRR Complex. Kenneth Satyshur, Anna Baker, Peter Newhouse, Jeffrey Dwulit-Smith, Katrina Forest.

10:54am 160-MO
Humidity Induced Phase Transitions of HEW Lysozyme Investigated by Microcrystalline Powder Diffraction. Thomas Degen, Detlef Beckers, Gwilherm Nenert, Stefanos Saslis, Souzana Logotheti, Fotini Karavassili, Alexandros Valmas, Patras; Irene Margiolaki, Sofia Trampari.

SIG MEETINGS

Industrial	2:00pm	Plaza BallroomABC
Canadian Division	12:00pm	Governors Square 14
Biological Macromolecules	5:00pm	Plaza Ballroom EF
General Interest	5:00pm	Governors Square14
Poster Session SA	5:30pm	Plaza Exhibit

11:02am 158-MO
Structural Genomics Analysis of Cofactor Preference Among Short-Chain Dehydrogenase/Reductases and the Emergence of a Novel SDR Subtype. Stephen Mayclin, Vasilios Marathias, Donald Lorimer, Phillip Pierce, Thomas Edwards, Amy Sullivan, Daniel Haft, Jan Abendroth, Isabelle Phan, Bart Staker, Peter Myler.

11:10am 148SA
Multi-Fluorescent Imaging for Sensitive Protein Crystallization Detection. Ellen Gualtieri, Dmitry Rodionov, Lance Ramsey, Eric Zhao.

11:18am 163SA
Chemical Functionalization of Phenyl-Modified Cadmium Chalcogenide Clusters. Yang Chen, Krishnayan Basuroy, Philip Coppens.

11:26am 150SA
Structure and Dynamics of the Polymyxin-Resistance-associated Response Regulator PmrA in Complex with the Promoter DNA. Chwan-Deng Hsiao.

11:34am 161SA
Characterization and Crystallization of the C-terminal Histidine Phosphatase Domain of Sts-1. Weijie Zhou.

11:42am 155SU
Novel Boronic Acid Inhibitors for the Class D β-Lactamase OXA-1. Alina Morales, Rachel Powers, Joshua Mitchell.

11:50am 154-SA
The Crystal Structure of the Bacteriophage T4 MotA C-terminal Domain in Complex with dsDNA Reveals a Novel Protein-DNA Recognition Motif. Maxime Cuypers, Rosanna Robertson, Brett Waddell, Sivaraja Vaithiyalingam, Kenneth Kreuzer, Deborah Hinton, Stephen White.

02.01 Mineralogical Crystallography

Session Chairs: **Plaza Ballroom D**
Aaron Celestian and Nichole Valdez

9:00am 02.01.01
The Crystal Chemistry of Natural Apatites. John Hughes, Daniel Harlov, Sean Kelly, John Rakovan, Hanna Nekvasil.

9:40am 02.01.02
The High-pressure Orthorhombic to Monoclinic Transition of Lawsonite. Earl O'Bannon, Christine Beavers, Quentin Williams.

10:00am Coffee Break

10:30am 02.01.03
Investigation of the High Temperature Behavior of the Pyroxenes $LiMGe_2O_6$ (M = Cr, V). Anasuya Adibhatla, Gwilherm Nenert, Natalia Dadivanyan.

10:50am 02.01.04
High-Pressure Neutron Diffraction Study of Hydrous Phases. Hongwu Xu, Jinlong Zhu, Jianzhong Zhang, Yusheng Zhao, Donald Hickmott.

11:10am 02.01.05
Incommensurately Modulated Structures of Intermediate Plagioclase Feldspars and their Petrological Implications. Shiyun Jin, Huifang Xu.

11:30am 02.01.06
in situ Ion Exchange in Nanoporous Zirconium Silicates Jason Lively, Aaron Celestian, Bangbo Yan.

03.01.01I Structure-based Drug Design

Session Chairs **Plaza Ballroom A, B, C**
Barry Finzel and Chelsy Prince (Chesterman)

9:00am 03.01.01.02
From Fragment to Treatment for Chronic Lymphocytic Leukemia, the Structure-based Design of BCL-2 Selective venetoclax. Vincent Stoll.

9:30am 03.01.01.03
Fragment-Based Design of BACE Inhibitors as a Potential Therapy for Alzheimer's Disease. Peter Orth.

10:00am Coffee Break

10:30am 03.01.01.04
Structure-Based Drug Design for HIV Integrase Daniel Klein.

11:00am 03.01.01.05
Discovery of an Allosteric Inhibitor of the SUMO-Conjugating E2 Enzyme Ubc9 by Crystallographic Fragment Screening. George Lountos, William M. Hewitt, Katherine Zlotkowski, Samuel D. Dahlhauser, Lindsey B. Saunders, Danielle Needle, Joseph E. Tropea, Chendi Zhan, Guanghong Wei, Buyong Ma, Ruth Nussinov, John S. Schneekloth, Jr., David S. Waugh.

11:20am 03.01.01.06
Structure-based Discovery of Middle East Respiratory Syndrome Coronavirus Fusion Inhibitor. Sheng Ye.

11:40am 03.01.01.07
Crystallographic and Enzymological Studies of Inhibition in Human Norovirus Polymerase Soumya Samanta, Munan Shaik, Francisco Parra, Kenneth Ng.

04.01 Opportunities from New and Improved Sources

Session Chairs: **Governors Square 15**
Sean McSweeney and Bob Sweet

9:00am 04.01.01
Advanced Neutron Research Facilities for Biology at Oak Ridge National Laboratory.
Paul Langan.

9:25 am 04.01.02
Biological X-Ray Crystallography and Scattering Opportunities at the ABBIX Beamlines at the National Synchrotron Light Source –II (NSLS-II). Lonny Berman.

9:40 am 04.01.03
Development of a High-Throughput, High Brightness Macromolecular Crystallography Beamline at the Advanced Light Source.
Corie Ralston, Simon Morton, Jeff Takakuwa, Ken Chow, Charles Swenson, Paul Adams.

10:00am Coffee Break

10:30 am 04.01.04
BioMAX and Structural Biology at MAX IV.
Thomas Ursby, Roberto Appio, Jie Nan, Johan Unge, Mikel Eguiraun, Christopher Ward, Fredrik Bolmsten, Marjolein Thunnissen, Uwe Mueller.

10:50 am 04.01.05
Serial Millisecond Crystallography at the Advanced Photon Source. Jose Manuel Martin Garcia, Nadia Zatsepin, Vadim Cherezov, Uwe Weierstall, Wei Liu, John Spence, Petra Fromme, Robert Fischetti, Craig Ogata, David

Undergraduate Symposium

Sponsored by the Society of Physics Students
Plaza Ballroom D 12:00 - 01:30pm

The ACA invites all undergraduates, graduate students, and their mentors for a reception highlighting undergraduate research on Saturday, July 23 at 12:00pm. Posters prepared on research of undergraduates will be highlighted and refreshments will be provided. The Chief Executive Officer of ACA will give a talk on the use and importance of crystallography to science and engineering.

Kissick, Ganesh Subramanian, Garrett Nelson, Gihan Ketawala, Lan Zhu, Alexander Schaffer, Andrii Ishchenko, Daniel James, Paul Sherrer; Nagarajan Venugopalan, Shenglan Xu.

11:05 am 04.01.06
What if? James Holton.

11:20 am 04.01.07
DIALS – New Software for Diffraction Image Integration. David Waterman, Graeme Winter, James Parkhurst, Luis Fuentes-Montero, Richard Gildea, Markus Gerstel, Aaron Brewster, Nicholas Sauter, Gwyndaf Evans.

11:35 am 04.01.08
New Opportunities for Macromolecular Femtosecond Crystallography at LCLS. Aina Cohen, representing the entire SSRL and LCLS team.

05.01 The Next 100 Years of Powder Diffraction

Session Chairs: Plaza Ballroom E, F
Brian Toby and Andrey Yakovenko

9:00 am 05.01.01
Some Recollections from the Early Days of Neutron and Synchrotron X-ray Powder Diffraction. David E Cox.

9:30 am 05.01.02
High Energy X-ray Powder Diffraction Early Sciences at NSLS II. Sanjit Ghose, Eric Dooryhee.

9:50 am 05.01.03
Future of Neutron Diffraction. Ashifa Huq.

10:10 am Coffee Break

10:30 am 05.01.04
Calibration of the Mars X-ray Powder Diffraction Instrument. David Bish.

10:55 am 05.01.05
Synchrotron Powder Diffraction from the Comfort of Home: Mail-In Program of Beamline 11-BM. Saul Lapidus, Lynn Ribaud.

11:15 am 05.01.06
Thoughts on the Future of Powder Diffraction Inspired by our Work on the Unusual Thermal Expansion and Behavior on Compression of ReO3-type Fluorides. Angus Wilkinson.

11:35 am 05.01.07
Humidity Induced Phase Transitions of HEW Lysozyme Investigated by Microcrystalline Powder Diffraction. Thomas Degen, Detlef Beckers, Gwilherm Nenert, Stefanos Saslis, Souzana Logotheti, Fotini Karavassili Alexandros Valmas, Irene Margiolaki.

11:55 05.01.08
The Power of Powder Crystallography. Suzanna Ward, Amy Sarjeant, Pete Wood, Colin Groom.

03.03.01 Hybrid Method Approaches for Structural Biology

Session Chairs: Plaza Ballroom E, F
Andy Howard and Shuo Qian

1:25 pm 03.03.01
Interplay of Amyloid β Peptide(1–40) and An Anionic Lipid Dimyristoyl-glycero-phosphoglycerol. Shuo Qian, Durgesh Rai, Veerendra Kumar Sharma, Divina Anunciado, Hugh O'Neill, Eugene Mamontov, William Heller, Volker Urban.

1:45 pm 03.03.02
MICAL-1 calponim homology (CH) domain Modulates the Enzyme Methionine-Sulphoxide Oxidase Activity. Mario A. Bianchet, Saif Alqassim, Eitan Borgnia, Marc Nagib, Mauricio Urquiza, L. Mario Amzel.

2:05 pm 03.03.03
Linkage-Specific Conformational Ensembles of Polyubiquitin Chains Revealed by NMR, SANS and Ensemble Structure Modeling. Susan Krueger, Carlos Castañeda, Joseph Curtis, David Fushman.

2:25 pm 03.03.04
Structural Dynamics of Blue Light-sensing Using Flavin (BLUF) Domains. Iva Chitrakar.

2:45 pm 03.03.05
Probing Allosteric Regulation of an Executioner Caspase. Nicholas Vance.

3:00 pm Coffee Break

3:30 pm 03.03.06
Structural Studies of Amyloidogenic Peptides and Proteins. Annette Eva Langkilde, Kyle L Morris, Louise C Serpell, Dmitri I Svergun, Bente Vestergaard.

4:00 pm 03.03.07
Impact of the Crystallization Condition on Importin ß Conformation. Achim Dickmanns, Marcel Tauchert, Clément Hémonnot, Piotr Neumann, Sarah Koester, Ralf Ficner.

4:20 pm 03.03.08
Hybrid Methods of Protein Single Crystal X-ray, Molecular Dynamics and THz Spectroscopy Reveal Functional Importance of Collective Motions of Solvent and Side Chains. Martha Teeter.

4:40 pm 03.03.09
Structural Investigations of the Cellulose Degrading, Multi-domain Enzyme, Cellobiose Dehydrogenase. Annette Bodenheimer.

01.02 Using Standard Tools & Methods in Non-standard Ways

Session Chairs: **Governors Square 14**
Louise Dawe and Andrey Yakovenko

Funding provided by Rigaku/Oxford Diffection

1:30 pm 01.02.01
2-D Powder XRD Applications with Single Crystal Diffractometers. Bob He, Bruce Noll, Charles Campana,

2:10 pm 01.02.02
Working with CASIS to Utilize the International Space Station – United States National Laboratory. Marc Giulianotti.

2:40 pm 01.02.03
Harnessing the Power of the Cambridge Structural Database in your Own Way: The CSD Python API. Paul Sanschagrin, Seth Wiggin.

3:00 pm Coffee Break

3:30 pm 01.02.04
Beyond Single Crystals - 3D Diffraction for Texture Analysis. Jim Britten, Vicky Jarvis, Weiguang Guan.

4:10 pm 01.02.05
Large Area Photon-Counting Detector - From Single Crystal Diffraction to SAXS. Milan Gembicky, Curtis Moore.

4:30 pm 01.02.06
Using the Tools at Hand (SC-XRD and P-XRD instruments) to Study Whatever Comes my way. Stacey Smith.

02.02 Structure-Property Relationships

Session Chairs: **Plaza Ballroom ABC**
Christine Beavers and Pete Wood

Funding provided by Cambridge Crystallographic Data Centre, STOE

1:30 pm 02.02.01
Raising the (metastable) bar: 100% Photo-Switching in Nitrite Linkage Isomers Approaches Ambient Temperature. Lauren Hatcher.

2:00 pm 02.02.02
Just How Much Does Structure Matter? Combining Simulation and Experiment to Study Gas Adsorption and Insertion. Paul Forster, Keith Lawler, Emily Siska.

2:20 pm 02.02.03
Structure-property Relationships in Bismuth-organic Materials. Karah Knope.

2:40 pm 02.02.04
Chain Conformation, Crystal Packing Arrangements and Physico-chemical Properties of Gemfibrozil Salts. Carl Schwalbe, Miren Ramirez, Barbara Conway, Peter Timmins.

3:00 pm Coffee Break

3:30 pm 02.02.05
Knowledge-based Prediction of Solvate Formation. Laszlo Fabian, Khaled Takieddin.

4:00 pm 02.02.06
Synthesis and Luminescence Properties of Uranyl Hydrolysis Products Containing p-iodobenzoic Acid. Mikaela Pyrch, Robert Surbella III, Christopher Cahill.

4:20 pm 02.02.07
Visualizing Structure-property Relationships through Chemical Pressure Analysis. Danny Fredrickson, Joshua Engelkemier.

4:40 pm 02.02.08
Synthesis, Crystal Structure and Electrical Properties of a Layered Strontium Manganese vanadate. Victoria Soghomonian, Qifan Yuan, Carla Slebodnick, Elinor Spencer.

03.02 What to do with SAS Data?

Session Chairs: **Governors Square 15**
Alex Hexemer and Annette Bodenheimer

1:30 pm 03.02.01
A Novel Method to Extract Solvent Information from Small-angle X-ray Scattering Data. David Case, Lois Pollack, Suzette Pabit, Hung Nguyen.

2:00 pm 03.02.02
Recent Updates to the UltraScan SOlution MOdeler (US-SOMO) HPLC-SAXS Data Analysis Module. Emre Brookes, Patrice Vachette, Javier Pérez, Mattia Rocco.

2:30 pm 03.02.03
Shape Determination from Small Angle Scattering Data Corrupted with Narrow Band Noise by Indirect Fourier Transformation Method. Youngha Hwang.

3:00 pm Coffee Break

3:30 pm 03.02.04
Predicting Data Quality in Biological Small-angle Solution Scattering Experiments. Richard Gillilan, Chenzheng Wang, Devin Bougie, Yuexia Lin.

4:00 pm 03.02.05
Quantifying Radiation Damage in Small-Angle X-ray Scattering. Jesse Hopkins, Robert Thorne.

4:30 PM Discussion

05.02 Magnetic Entanglement and Complex Magnetic Materials

Session Chairs: **Plaza Ballroom D**
Branton Campbell and Anna Llobet

1:30 pm 05.02.01
A Novel Route to Quantum Spin Liquids: Bond-directional Magnetic Anisotropies in a Strongly Spin-orbit Coupled iridate, Na2IrO3 Sae Hwan Chun.

2:00 pm 05.02.02
Helical Bunching and Symmetry Lowering Inducing Multiferroicity in Chiral Fe Langasite. Virginie Simonet, Laura Chaix, Rafik Ballou, Andres Cano, Sylvain Petit, Sophie Debrion, Eric Ressouche, Louis-Pierre Regnault, Pascal Lejay, Evan Constable, Claire Colin, Andrej Zorko, Valerio Scagnoli,

2:30 pm 05.02.03
Using Neutrons to Looks at Topological Properties in Materials. David A. Tennant.

3:00 pm Coffee Break

3:30 pm 05.02.04
Magnetostructural Relationship in the Tetrahedral Spin-chain Oxide $CsCoO_2$. Naveed Zafar Ali.

3:50 pm 05.02.05
Exotic Magnetic Orders in Novel Low-dimensional Transition Metal Vanadates. Ovidiu Garlea, Liurukara D. Sanjeewa, Michael A.

McGuire, Colin McMillen, Huibo Cao, Joseph Kolis.

4:10 pm 05.02.06
Crystal and Magnetic Structure of α-$RuCl_3$ Huibo Cao, Arnab Banerjee, Jiaqiang Yan, Craig A. Bridges, Mark D. Lumsden, David G. Mandrus, David A. Tennant, Bryan C. Chakoumakos, Stephen E. Nagler.

4:30 pm 05.02.07
Neutron Diffraction in new Multiferroic Molecular Magnet. Javier Campo, José Alberto Rodriguez Velamazan, Oscar Fabelo, Angel Millan, Laurent Chapon.

4:50 pm 05.02.08
Complex Magnetism and Metal-Insulator Transitions in Hollandite Transition Metal Oxides. Amber Larson, Pouya Motakef, Jeffrey Lynn, Efrain Rodriguez.

01.03 Diversity and Inclusion Evening Session

Session Chairs: Governors Square 14
Lisa Mueller, Ana Gonzalez, Oluwatoyin Asojo

7:30 pm 01.03.01
Engaging All Students in Real Science…. through Modeling. Tim Herman, Shuchismita Dutta, Margaret Franzen.

7:50 pm 01.03.02
Increasing Diversity in STEM, the Case for LGBTQ+ Faculty, Students, and Staff. Benny Chan.

8:10 pm 01.03.03
Crystallography - A Lesson in Disability Inclusion. Bradley Hintze.

8:30 pm 01.03.04
Lessons Learned: 15 years of Crystallography Research with High School and Undergraduate Students. Oluwatoyin Asojo.

2016 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. 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 SIGs. Students who are selected receive a monetary award of $250 and a certificate to be presented at the beginning of their lecture.

Congratulations to the 2016 Etter Lecturers:

BioMac..... Stefan Imseng, Univ. of Basel 03.04.01
Fiber Diffraction ..... Brendan Sullivan, Purdue Univ. 05.06.06
General Interest ..... . Jens Luebben, HeinrichHeineUniv. 01.11.01.09
Industrial..... Mikaela Pyrch, George Washington Univ.....02.02.06
Light Sources..... Charles Bury, Univ. of Oxford 04.05.03
Materials Science..... Daniel Mast, Univ. of Nevada Las Vegas 05.03.06
Neutron Scattering ... Amber Larson, Univ. of Maryland.....05.02.08
Powder Diffraction .... Dan Taylor, Univ. of Maryland 05.07.06
Service..... Claudia Wandtke, Univ. Goettingen..... 01.11.01.04
Small Molecule..... Victoria Hall, Georgetown Univ. 2.04.01.03
Young Scientist ..... Jose Olmos, Rice Univ. 01.04.08

Registration Desk	07:30am	Plaza Registration
Speaker Ready Room	8:00am	Plaza Court 1
Council Meeting Room	8:00am	Directors Row F
Exhibit Show	10:00am	Plaza Exhibit
CCDC Luncheon	12:00pm	Directors Row H
Rigaku Lunch & Learn	12:00pm	Majestic Ballroom
SIG MEETINGS		
Fiber Diffraction	12:00pm	Plaza BallroomB
Joint Materials, Neutron & Powder	12:00pm	Governors Square 15
Young Scientists	12:00pm	Plaza Ballroom EF
Light Sources	5:00pm	Governors Square 15
Poster Session SU	5:30pm	Plaza Exhibit
Bruker Networking Mixer (ticket reqeuired)	8:00pm	Marlowe's Restaurant

AW.02 Etter Early Career Award Presentation & Lecture

Tom Terwilliger, Presiding **Plaza Ballrom EF**

08:00-08:45AM **AW.02.01**

Watching Crystals Work: Structural Dynamics of Metal-organic Frameworks. Jason Benedict, Univ. at Buffalo SUNY

01.04 Etter Early Career Session

Session Chairs: **Plaza Ballroom E, F**
Stacy Vinokur and Martin Donakowski

9:00 am 01.04.01
Single Crystal Investigation of Thermochromic Organic Semiconductor Butoxyphenyl N-Substituted Naphthalene Diimide. Madushani Dharmarwardana, Jeremiah. J Gassensmith.

9:17 am 01.04.02
Determining the Overall Structure and Composition of Complex Thin Films from Local Structure and Composition Measurements. Gavin Mitchson, Jeffrey Ditto, Keenan Woods, Devin Merrill, Catherine Page, David Johnson.

9:34 am 01.04.03
Unraveling the Mechanism of Transition Metal Sulfide Conversion Electrodes with Local Structure Methods. Vicky Doan-Nguyen, Joshua Bocarlsy, Kamila Wiaderek, Olaf Borkiewicz, Karena W. Chapman, Peter Chupas, Ram Seshadri.

9:51 am 01.04.04
Experimental and Theoretical Charge Density Analysis of 1-(2,3-Tichlorophenyl)piperazine. Arshad Mehmood, Benjamin Janesko, Yulia Sevryugina.

10:08 am Coffee Break

10:38 am 01.04.05
Topal-Fresco DNA Base Pairs in the PDB and Lessons in Low Frequency Observations
Bradley Hintze, David Richardson, Jane Richardson, Hashim Al Hashimi, Isaac Kimsey.

10:55 am 01.04.06
Understanding hHint1-Mediated Prodrug Activation. Kimberly Maize, Rachit Shah, Alex Strom, Carston Wagner, Barry Finzel.

11:12 am 01.04.07
Zyrtec – Plasma Transport. Katarzyna Handing, Ivan Shabalin, Karol Szlachta, Karolina Majorek, Wladek Minor.

11:29 am 01.04.08
Structure-Based Enzymology with an X-ray Free Electron Laser. Jose Olmos, Christopher Kupitz, David Xu, Dominik Oberthür, Kanupriya Pande, Jason Tenboer, Suraj Pandey, George Phillips, Marius Schmidt.

01.05.01 General Interest I

Session Chairs: **Governors Square 14**
Stacey Smith and Graciela Diaz

9:00 am 01.05.01.02
Experiences with SAD Structure Determination of Proteins in an Undergraduate Biophysics Laboratory Course. Douglas Juers.

9:20 am 01.05.01.03
Teaching with the Case Study Method to Promote Active Learning in a Small Molecule Crystallography Course for Chemistry Students Shao-Liang Zheng, Michael Campbell, Tamara Powers.

9:40 am 01.05.01.03
Role Play: Real Life Scenarios for Learning and Employability. Simon Coles.

10:00 am Coffee Break

10:30 am 01.05.01.04
Structural Layers in High-Z' Molecular Crystals Carolyn Brock.

10:50 am 01.05.01.05
Accessing the CCDC World Through your Platform: Third-Party Software Integrations Erin Davis, Paul Sanschagrin.

11:10 am 01.05.01.06
Current Status of the Liquid-Metal-Jet X-ray Source Technology including Diffraction and SAXS Applications. Emil Espes, Björn Hansson, Oscar Hemberg, Mikael Otendal, Göran Johansson, Per Takman, Tomi Tuohimaa,

11:30 am 01.05.01.07
PILATUS3 R CdTe Large-area Detectors for Laboratory Applications. Marcus Mueller.

11:50 am 01.05.01.08
Modern CPAD Detector Technology for Higher Energy X-rays. Michael Ruf, Holger Ott, Tobias Stuerzer.

04.02 Surfaces and Interfaces

Session Chairs: **Governors Square 15**
Marian Szebenyi and Kevin Yager

9:00 am 04.02.01
Structure and *in-situ* Processing of Nanostructured Thin Films based on Functional Soft Materials. Detlef-M. Smilgies.

9:30 am 04.02.02
Subnanometer Ligand Asymmetry in Nanoparticle Membranes Probed by Grazing Incidence X-ray Scattering. Zhang Jiang, Jinbo He, Sanket A. Deshmukh, Pongsakorn Kanjanaboos, Ganesh Kamath, Yifan Wang, Subramanian KR.S. Sankaranarayanan, Jin Wang, Heinrich M. Jaeger, Xiao-min Lin.

10:00 am Coffee Break

10:30 am 04.02.03
Photothermal Assembly of Block Copolymers Kevin Yager.

10:50 am 04.02.04
Understanding and Controlling the Preferential Orientation of Metal Halide Perovskite Thin Films for High Performance Solar Cells. Joshua Choi, Benjamin Foley, Alexander Chen, Detlef-M. Smilgies.

11:10 am 04.02.05
New Surface-Optical System of Monocrystalline p-type <100> Si for Si-based micro/or nano Devices at Room Temperature. Kifah Qasim Saleh.

11:30 am 04.02.06
in situ X-ray Analysis of Thin Film Growth John Smedley.

05.03 Crystallography in Solid State Chemistry

Session Chairs: **Plaza Ballroom D**
Danny Fredrickson and Kirill Kovnir

Funding provided by Mosaic Distribution LLC, Rigaku/Oxford Diffraction

9:00 am 05.03.01
Piezoelectrics: Putting the "Squeeze" on New Materials. Michelle Dolgos.

9:30 am 05.03.02
Bibridged Chloridocadmate Chains With, and Without, Hydrogen Bonding. Marcus Bond.

9:50 am 05.03.03
Twinning, Incommensurabilities and General Bad Behaviour How New Methods, Sources and Detectors Allow the Study of Nature's Dirty Little Secrets. Sven Lidin.

10:20 am Coffee Break

10:50 am 05.03.04
Investigation of Aggregation Induced Phosphorescence in a Purely Organic Material by In-House Monochromatic Time-Resolved Diffraction. Krishnayan Basuroy, Sounak Sarkar, Harini ST, Tayur Guru Row, Jason Benedict, Philip Coppens.

11:10 am 05.03.05
Solving Crystal Structures of Inorganic Solids using *ab initio*-assisted Powder Diffraction Jakoah Brgoch.

11:40 am 05.03.06
New High Pressure Phase Diagram for Molybdenum and Rhenium Dioixide. Daniel Mast, Barbara Lavina, Emily Siska, Paul Forster.

TR.01 Transactions Symposium

Session Chairs: Plaza Ballroom A,B,C
Jason Benedict and Arwen Pearson

9:00 am TR.01.01
The Dramatic Rise of Dynamic Crystallography Over The Years. Philip Coppens.

9:30 am TR.01.02
Serendipp, Structural Dynamics and Pyrophosphatases. Craig Wilkinson, Kun-Mou Li, Keni Vidilaseris, Jia-Yin Tsai, Esko Oksanen, Lars Jeuken, Yuh-Ju Sun, Adrian Goldman.

10:00 am Coffee Break

10:30 am TR.01.03
Molecular Engineering of Nano-optomechanical Transducers. Jacqueline Cole.

11:05 am TR.01.04
Dynamic Imaging with X-rays from an Atomistic Perspective. Linda Young, Phay Ho, Christopher Knight, Miklos Tegze, Gyula Faigel.

11:40 am TR.01.05
PATH: A Computational Algorithm that Rapidly Identifies Protein Conformational Transition States and Transition Pathways. Srinivas Niranj Chandrasekaran.

12:00 pm Lunch Beak

1:30 pm TR.01.06
Ultrafast Structural Dynamics in Proteins. Marius Schmidt.

2:05 pm TR.01.07
Imaging Ultrafast Excited State Pathways in Transition Metal Complexes by X-ray Transient Absorption and Scattering Using X-ray Free Electron Laser Source. Lin Chen.

2:40 pm TR.01.08
Combining Multi-mutant and Modular Thermodynamic Cycles to Measure Energetic Coupling Networks in Enzyme Catalysis. Charles Carter, Niranj Chandrasekaran, Violetta Weinreb, Li Li, Tishan Williams.

3:00 pm Coffee Break

3:30 pm TR.01.09
Rubies in the Smoke: Multi-dataset Methods for the Extraction of Weak Signal in X-ray Crystallography. Nicholas Pearce, Sebastian Kelm, Jiye Shi, Charlotte Deane, Frank von Delft.

4:00 pm TR.01.10
Beating Darwin-Bragg Losses in Lab-based Ultrafast X-ray Experiments. Wilfred Fullagar, Jens Uhlig, Hide Tatsuno, Alireza Honarfar, Amal El Nahhas, Villy Sundström, Mikko Palosaari, Kimmo Kinnunen, Ilari Maasilta, Luis Miaja-Avila, Galen O'Neil, Young Joe, Daniel Swetz, Joel Ullom.

4:30 pm TR.01.11
Time Resolved Serial Protein Crystallography in Ultra-Thin Microfluidic Devices. Sarah Perry, Shuo Sui, Yuxi Wang, Christos Dimitrakopoulos, Vukica Srajer, Robert Henning.

01.10 High Impact Crystallographic Education

Session Chairs: **Governors Square 14**
Bruce Foxman and Kraig Wheeler

Funding provided by Crystallographic Resources, Inc.

1:30 pm 01.10.01
Teaching Crystallography with Innovative Tools. Gervais Chapuis.

2:00 pm 01.10.02
What do you Mean "Less Than"? VSEPR Geometry Predictions and Small Molecule Structures. Louise Dawe, Marlon Bridge, Jeffrey Dinsmore, Negeen Foroughian.

2:20 pm 01.10.03
The Utilization of Macromolecular Graphics Programs in Undergraduate Education. Paul Cook

2:40 pm 01.10.04
Teaching New Students the Origins and Use of the Lattice Types. Larry R. Falvello.

3:00 pm Coffee Break

3:30 pm 01.10.05
Web-Based Resources for Teaching Crystallographic Symmetry. Dean Johnston.

3:55 pm 01.10.06
Teaching Crystallography in 2016: Stand Alone 'Give-and-take' in Tutorials and Existing Software. Bruce Foxman.

4:15 pm 01.10.07
Bite-Sized Learning and Teaching Resources for Post-16 Chemistry Using the Cambridge Structural Database. Peter Hoare.

4:35 pm 01.10.08
Education from 824,520 Crystal Structures. Amy Sarjeant, Pete Wood, Suzanna Ward, Colin Groom.

03.04 Molecular Machines

Session Chairs: **Plaza Ballroom E, F**
Eric Montemayor and Aaron Robart

Funding provided by FEI, Integrated DNA Technologies, MiTiGen

1:30 pm 03.04.01
Architecture of Human mTOR Complex 1. Stefan Imseng, Christopher Herbert Stanley Aylett, Evelyn Sauer, Daniel Böhringer, Michael N. Hall, Nenad Ban, Timm Maier.

2:00 pm 03.04.02
Structural Analysis of the Dynamic Schizosaccharomyces Pombe Spliceosome using Single PCarticle cryo-electron Microscopy. Melanie Ohi, Yoshimasa Takizawa, Elad Binshtein, Scott Collier, Pawel Penczek.

2:30 pm 03.04.03
Constructed to Deconstruct: The 26S Proteasome as a Coordinated Degradation Machine. Andreas Martin, Evan Worden, Jared Bard, Corey Dambacher, Mark Herzik, Erik Jonsson, Gabriel Lander.

3:00 pm Coffee Break

3:30 pm 03.04.04
Crystal Structure of Yeast acetyl-CoA Carboxylase. Jia Wei, Liang Tong.

4:00 pm 03.04.05
Strand Acrobatics by a DNA Transpososome. Fred Dyda, Andrea Voth, Nancy Craig, Alison Hickman.

4:30 pm 03.04.06
Structure of the Human Pot1-TPP1 Complex. Cory Rice, Duncan Baird, Tzanko Doukov, Louise Showe, Emmanuel Skordalakes.

04.03 Multiple Crystal Techniques

Session Chairs: **Governors Square 15**
Steve Ginell and Ana Gonzalez

1:30 pm 04.03.01
Efficient Data Collection using Multiple Crys-

tals in High Density Grids. Aina Cohen, Elizabeth Baxter, Jinhu Song, Christopher Barnes, Guillermo Calero, Scott McPhillips.

2:00 pm 04.03.02
Approaches to the Acquisition and Analysis of Nano/microcrystal Synchrotron Data. Gwyndaf Evans, Jose Trincao, Anna Warren, Pierre Aller, James Foadi, David Waterman.

2:30 pm 04.03.03
XFEL Diffraction with Fixed Target Devices: Data Collection and Processing. Artem Lyubimov.

3:00 pm Coffee Break

3:30 pm 04.03.04
An Acoustic Array System for Sample Delivery in Serial Macromolecular Crystallography
Peter Docker, Paul Topham, Mark Prince, Danny Axford, Christian Burton, Gwyndaf Evans, Jim Kay, Dave Stuart, Robert Morris, Michael Newton, Andrew Edwards.

3:50 pm 04.03.05
Technologies for Optimizing Data Collection from Multiple Crystals. Robert Thorne.

4:10 pm 04.03.06
Probing the Limits of Native SAD Phasing. Aaron Finke, Guanya Peng, Tobias Weinert, May Marsh, Laura Vera, Vincent Olieric, Meitian Wang.

4:30 pm 04.03.07
Overcoming Non-isomorphism with Fancy Math. James Holton.

05.04 Novel Methods for Emerging Science

Session Chairs: **Plaza Ballroom D**
Katie Page and Joe Reibenspies

1:30 pm 05.04.01
An out of this World Method to Row Large Volume Protein Crystals Suitable for Neutron Crystallography. Joseph Ng, Michelle Morris, Anuj Singhal, Leighton Coates, Marc Pusey, Jorge Barcena, Juan Manuel Garcia-Ruiz.

1:55 pm 05.04.02
Sample Extractor for Serial Crystallography at XFELs and Synchrotron Sources. Irimpan Mathews, Aina Cohen, Michael Soltis.

2:15 pm 05.04.03
What ChemMatCARS can do for you in Advanced Crystallography? Yu-Sheng Chen.

2:35 pm 05.04.04
Innovations in Two-Dimensional XRD. Bob He.

3:00 pm Coffee Break

3:20 pm 05.04.05
Amorphous Semiconductors Under Pressure: Enabling Controlled Synthesis of Metastable Crystalline Phases by Complementary *ex situ* and *in situ* Characterization. Bianca Haberl, Jamie J. Molaison, Luke L. Daemen, Joerg C. Neuefeind, Reinhard Boehler.

3:40 pm 05.04.06
Applications of Synchrotron X-ray Scattering in Studies of Supramolecules and Nanomaterials: Structure and Kinetics. Xiaobing Zuo.

4:00 pm 05.04.07
in situ Spatial Structural Characterization of Meso Scale Structures Using Xrays. Julien Lhermitte.

4:20 pm 05.04.08
Reactivity, Polymorphism, and Intermediates in Kinetically Controlled Solid State Metathesis Reactions. Andrew Martinolich, Joshua Kurzman, James Neilson.

4:40 pm 05.04.09
A Quantum Leap in High Magnetic Field Neutron Scattering. Collin Broholm.

01.03 Diversity and Inclusion Evening Session

Chairs: **Governors Square 14**
Ana Gonzalez
Oluwatoyin Asojo **7:30pm**

This session includes talks on successful strategies for approaching diversity issues (e.g. inclusion, retention, stereotype threat) either through training, mentoring or research, and for engaging diverse populations through outreach using crystallography.

02.03 Would You Publish This?

Session Chairs: **Governors Square 14**
Brian Dolinar , Danielle Gray and Louise Dawe

Funding provided by Crystallographic Resources, Inc.

7:30 pm 02.03.01
The Difficult, Tedious, and Successful(?) Structure Solution and Refinement of an Unusual Charge-Transfer Complex. Aaron Finke.

7:40 pm 02.03.02
How Powder Diffraction Reminded Me About What's Important. Christine Beavers, Daniel Sun, Norman Su.

7:50 pm 02.03.03
Putting the "Squeeze" on? Removing Heavy Solvents from Organic Cages. Danielle Gray, Timothy Moneypenny, Semin Lee, Jeffrey Moore.

8:00 pm 02.03.04
Ten Years, Nine Coppers, Six Ligands, Three Enablers, and One White Whale. Louise Dawe.

8:10 pm 02.03.05
Would You Publish This? Not Before Running This Script! Paul Sanschagrin, Amy Sarjeant, Pete Wood, Andrew Maloney.

BRUKER YSSIG Networking Mixer

High energy fun, great food and some of the most exciting venues make the mixer a great place to connect with scientists ranging in experience and disciplines. The Sunday night mixer is one of the meeting's most popular events and is **FREE** to registered Students & Postdocs ***(ticket required; pick one up at the Registration Desk)*** and $30 for all others. The mixer will be held at Marlowe's Restaurant, 501 16th Street , http://www.marlowesdenver.com/ . Mixer begins at 8:00pm and is sponsored in part, by Bruker, AXS.

Registration Desk	07:30am	Plaza Registration
Speaker Ready Room	8:00am	Plaza Court 1
Council Meeting Room	8:00am	Directors Row F
Exhibit Show	10:00am	Plaza Exhibit
SIG MEETINGS		
Joint Service & Small Molecule	12:00pm	Plaza Ballroom ABC
Small Angle Scattering	12:00pm	Plaza Ballroom D
Business Meeting for ACA Members	05:00pm	Plaza Ballroom EF
Poster Session MO	05:30pm	Plaza Exhibit

AW.03 Bau Award and Lecture

T. Terwilliger, Presiding **Plaza Ballroom A,B,C**

8:00 AM-8:45 AM **Benno Schoenborn**

01.09 Engaging Undergraduates with Crystallographic Research

Session Chairs: **Governors Square 14**
Rachel Powers and Joe Tanski

9:00 am 01.09.01
Establishing a Framework for Success in Undergraduate Crystallographic Research. Rachel Powers.

9:20 am 01.09.02
Crystallographic Studies Carried out by High-school and Undergraduate Students in Mérida, Venezuela. Graciela Diaz de Delgado, María Cecilia Dávila, Astrid Guadalupe Mora, Miguel Alejandro Ramírez, Julio Abraham Trejo, José Miguel Delgado.

9:40 am 01.09.03
Teaching Chemistry of Crystals: Emphasis on Chemical Features. Alexander Nazarenko.

10:00 am Coffee Break

10:20 am 01.09.04
Crystallography for Undergraduate Research Universities through Collaboration. Richard Staples, Shannon Biross.

10:40 am 01.09.05
Crystallography in the Undergraduate Setting: Strategies for Diffractometer Acquisition and Success in Research Involving X-ray Crystallography with Undergraduate Students. Joe Tanski.

11:00 am 01.09.06
Hands-On Research with Advanced Characterization Instruments: An Undergraduate Practical Exploring Polymorphism. Simon Coles, Lucy Mapp.

11:20 am 01.09.07
Undergraduates Using Crystallography to Characterize Lanthanide Coordination Complexes Lauren DePue, Alex Bard, Richard Jones, Joe Espinoza, Bailey Bouley, Courtney Thomas, Colton D'Ambra, Jason Ross.

11:40 am 01.09.08
Crystallography in Chemistry Labs Supported by X-ray Powder Diffractometer. Karl Hagen.

02.05 Cool Structures

Session Chairs: **Governors Square 15**
Karah Knope and Xiaoping Wang

9:00 am Introductory Remarks

9:05 am 02.05.01
Phase Transitions of a Nucleic Acid Hydrate over a Broad Temperature Range (100K – 273K). Elizabeth Koch, Kelly McKenna, Jennifer Swift.

9:25 am 02.05.02
Universality of Double-Q magnetic Ordering in the Hole-doped 122 Iron-based Superonductors Keith Taddei, Jared Allred, Daniel Bugaris, Saul Lapidus, Matthew Krogstad, Ryan Stadel, Duck Chung, Mercouri Kanatzidis, Stephan Rosenkranz, Raymond Osborn, Omar Chmaissem.

9:40 am 02.05.03
Crystallographic Characterization of Bound

Dinitrogen to an Iron–sulfur–carbon Site. Brandon Mercado, Ilija Coric, Patrick Holland.

10:00 am Coffee Break

10:30 am 02.05.04
Structural Redetermination of Nanosized Capped 145-Metal-Atom Three-Shell Icosahedral $Pd_{145}(CO)_{72}(PEt_3)_{30}$ Obtained from $Pd_{10}(CO)_{12}(PEt_3)_6$ Precursor: Crystallographic Establishment of its Carbonyl Composition and Resulting Implications. Lawrence Dahl, Jeremiah Erickson, Nguyet Tran, Evgueni Mednikov, Sergei Ivanov.

10:50 am 02.05.05
Molecular Dynamics from Slow Diffraction Experiments: Information from a Single-crystal-to-single-crystal Diels–Alder Reaction. Sanaz Khorasani, Delbert Botes, Manuel Fernandes, Demetrius Levendis.

11:05 am 02.05.06
Polymorph Selectivity and Morphology Effects of Diphenylurea on Functionalized Substrates. Marina Solomos, Serena Seshadri, Christina Capacci-Daniel, Jennifer Swift.

11:20 am 02.05.07
A Reversible Solid-to-solid Phase Transition in a Molecular Solid Involving Z' of 12. Stacy Vinokur, Ilia Guzei, Lu Liu, Jennifer Schomaker.

11:35 am 02.05.08
A Calixarene-Based Johnson-Type (J17) Hexadecahedral Cage. Xinxin Hang, Bing Liu, Xiaofei Zhu, Haitao Han, Wuping Liao, Yunling Liu, Chunhua Hu.

11:50 am 02.05.09
Elementary Research: Gases, MOFs & the CSD. Pete Wood, Amy Sarjeant, Andrey Yakovenko, Suzanna Ward, Colin Groom.

03.05 Crystal Sample Preparation: A Crystal is Just the Start!

Session Chairs: **Plaza Ballroom E,F**
Surajit Banerjee and Iva Chitrakar

Funding provided by Molecular Dimensions, TTP LabTech Ltd.

9:00 am 03.05.01
Dehydration and cation replacement dramatically improve crystals of large RNAs. Adrian Ferre-D'Amare.

9:20 am 03.05.02
Microseed Matrix-screening (rMMS): Introduction, Theory, Practice and a New Technique for Membrane Protein Crystallization in LCP. Patrick Shaw Stewart.

9:40 am 03.05.03
Unfolded Proteins Don't Crystallise: What can be Done to Help Proteins Stay Folded? Janet Newman, Marko Ristic, Nicolas Rosa, Shane A. Seabrook.

10:00 am Coffee Break

10:30 am 03.05.04
Towards Automating Dehydration Experiments by Understanding the Underlying Processes. Matthew Bowler.

10:55 am 03.05.05
Methods Development for Cryo- and Variable Temperature Crystallography. David Moreau, Hakan Atakisi, Robert Thorne.

11:15 am 03.05.06
Improvement of Protein Crystal Quality by the Multi-step Soaking Method. Miki Senda, Masanori Hatakeyama, Koh Takeuchi, Toshiya Senda.

11:35 am 03.05.07
I Have a Protein Crystal: What Now? Elspeth Garman.

05.06 Recent Advances in Fiber Diffraction

Session Chairs: **Plaza Ballroom D**
Paul Langan and Joe Orgel

9:00 am 05.06.01
Untangling the Threads of Cellulose Mercerization. Paul Langan, Daisuke Sawada, Yoshiharu Nishiyama, Riddih Shah, Trevor Forsyth, Hugh O'Neill, Masahisa Wada.

9:30 am 05.06.02
Thick Filament Compliance in Actively Contracting Skeletal Muscle. Weikang Ma, Balazs Kiss, Eun-Jeong Lee, Henk Granzier, Thomas Irving.

10:00 am Coffee Break

10:30 am 05.06.03
Detection of Load-Induced Structural Changes to Neurons and the Brain using X-ray Diffraction. Joe Orgel, Rama Madhurapantula.

11:00 am 05.06.04
Studies on the Structural Changes from Non-enzymatic Glycation in type I Collagen. Rama Sashank Madhurapantula, Joe Orgel.

11:20 am 05.06.05
Molecular Interactions in an α-chitin/Hydrazine Complex. Daisuke Sawada, Yu Ogawa, Yoshiharu Nishiyama, Eiji Togawa, Satoshi Kimura, Paul Langan.

11:40 am 05.06.06
X-ray Microscopy Analysis of the Cuprizone Model for Multiple Sclerosis Suggests Copper Deficiency Does not Cause Demyelinatio. Brendan Sullivan, Olga Antipova, Yulia Pushkar.

02.04.01 Advances in Supramolecular Chemistry

Session Chairs: **Plaza Ballroom A,B,C**
Heba Abourahma and Kraig Wheeler

Funding provided by Alkermes, Inc., Moderna Therapeutics

9:00 am 02.04.01.02
Practical Applications of Supramolecular Chemistry. Christer Aakeroy.

9:40 am 02.04.01.03
Uric Acid Cocrystals. Victoria Hall, Jennifer Swift.

10:00 am Coffee Break

10:30 am 02.04.01.04
Rational Design of Metal-Organic Supercontainers as Enzyme Mimics. Zhenqiang (Rick) Wang.

11:10 am 02.04.01.05
Harnessing Uranyl Oxo Atoms in the Supramolecular Assembly of Hybrid Materials. Korey Carter, Mark Kalaj, Christopher Cahill.

11:30 am 02.04.01.06
Biomacromolecular Crystallography Methods for Synthetic Abiologial Molecules. Balasubramanian Venkatakrishnan, Abhishek Singharoy, Yun Liu, Christopher Mayne, Semin Lee, Chun-Hsing Chen, Adam Zlotnick, Klaus Schulten, Amar Flood.

11:45 am 02.04.01.07
Structural Analysis of Extremely Confined Gases Inside a Lipophilic Cage Molecule. Gracia El-Ayle.

12:00 pm Lunch Break

1:30 pm 02.04.02.01
Solid State Dehydration of a Nucleic Acid Hydrate. Jennifer Swift, Elizabeth Koch.

2:10 pm 02.04.02.02
Exploring the Shape Space of Quasiracemic Materials. Kraig Wheeler, Jacqueline Spaniol,

Grant Lakeland, Brian Bourne.

2:30 pm 02.04.02.03
Targeting a Supramolecular Motif by Tuning Hydrogen-bond Donor and Acceptor Power. Marijana Đaković, Ivan Kodrin, Boris-Marko Kukovec, Mladen Borovina, Christer Aakeroy.

2:45 pm 02.04.02.04
Different Packing Patterns in the Mixed Donor-acceptor Co-crystals of Trimeric Perfluoro-ortho-phenylene Mercury with Benzo[1,2-b:6,5-b']dithiophene-,5-dione derivatives. Raul Castaneda, Marina S. Fonari, Chad Risko, Yulia A. Getmanenko, Tatiana V. Timofeeva.

3:00 pm Coffee Break

3:30 pm 02.04.02.05
Digital Design of Pharmaceutical Solids. Susan Reutzel-Edens.

4:10 pm 02.04.02.06
Computational Methods in Crystal Engineering: Polymorphism, Prediction (and design?). Graeme Day.

01.12 Things We No Longer Need to Know

Session Chairs: Governors Square 14
Carla Slebodnick and Charlotte Stern

Funding provided by Crystallographic Resources, Inc., Rigaku/Oxford Diffection

1:30 pm 01.12.01
The Next Generation of X-ray Structural Biologists: Button Pushers or Crystallographers?. John P. Rose, Zheng-Qing (Albert) Fu, John Chrzas, Bi-Cheng Wang.

1:50 pm 01.12.02
FORTRAN? Robert Von Dreele.

2:10 pm 01.12.03
"Things We No Longer Need to Know" - Mastering the Art of Good Diffraction Experiments. Mathias Meyer.

2:30 pm 01.12.04
Things We No Longer Need to Know: Setting up Data Collections with the CAD4 Diffractometer. Paul D. Boyle.

2:45 pm 01.12.05
3D Single Crystal Diffraction at Sub-atomic Resolution: How This is Done at the ORNL Spallation Neutron Source. Xiaoping Wang.

3:00 pm Coffee Break

3:30 pm 01.12.06
Did You Know? Jim Ibers.

3:50 pm 01.12.07
The Reciprocal Lattice in Introductory Crystallography. Larry R. Falvello.

4:05 pm 01.12.09
Some Reflections on Symmetry. William Clegg.

4:25 pm 01.12.09
Things We No Longer Need To Know: Point Group Diagrams. Carla Slebodnick.

4:45 pm 01.12.10
Transforming your World – A Tool for Visualizing Matrix Transformations. Amy Sarjeant, Greg Shields, Pete Wood.

03.01.02 Structure-based Drug Design II

Session Chairs: Governors Square 15
Chelsy Chesterman and Barry Finzel

1:30 pm 03.01.02.01
Structure and Characterization of a Highly Potent and Selective mGlu2 Receptor Agonist LY2812223. Jing Wang, James Monn, Frances Lu, Margaret Kearins, David Clawson, Shane Atwell, Aiping Zhang, Marijane Russell.

2:00 pm 03.01.02.02
Allosteric Activators of AMP-Activated Pro-

tein Kinase (AMPK) for the Treatment of Diabetic Nephropathy. Matthew Calabrese.

2:30 pm 03.01.02.03
At Play in the Briar Patch of Epigenetics. Jim Kiefer.

3:00 pm Coffee Break

3:30 pm 03.01.02.04
Challenges in Designing Inhibitors that Block Carbohydrate-recognition and Associated Biological Functions of Lectins. Helen Blanchard.

4:00 pm 03.01.02.05
"Seriously Sweet": A Structural Guided Approach to Selective Inhibitor Design Toward the Cancer Related Carbonic Anhydrase IX, using Artificial Sweeteners. Akilah Murray, Brian Mahon, Robert McKenna.

4:20 pm 03.01.02.06
Why is Quantum Mechanics (QM)-driven Protein Refinement Crucial in Structure Based Drug Design? Lance Westerhoff, Oleg Borbulevych.

4:40 pm 03.01.02.07
Designing Better Drugs from Small Molecule Structures. Colin Groom, Erin Davis.

03.06 Cryo Electron Microscopy and Electron Diffraction

Session Chairs: Plaza Ballroom E,F
Sangita Sinha and David Belnap

Funding provided by FEI

1:30 pm 03.06.01
The Cryo-TEM Revolution. David Belnap.

2:00 pm 03.06.02
Cryo-EM Structural Studies Mapping Antibody Common Epitopes and Observing pH Induced Conformational Changes of Adeno-Associated Virus Capsids. Robert McKenna, Yu-Shan Tseng, Bridget Lins, Kennon Smith, Paul Chipman, Brittney Gurda, Justin Kurian, Antonette Bennett, Mandy Janssen, Giovanni Cardone, Timothy Baker, Mavis Agbandje-McKenna.

2:30 pm 03.06.03
Integration of X-ray and Electron Microscopy Data to Determine the Structure and Function of a CRISPR RNA-guided Surveillance Complex. Ryan Jackson, Airlie McCoy, Thomas Terwilliger, Randy Read, Blake Wiedenheft.

3:00 pm Coffee Break

3:30 pm 03.06.04
MicroED Opens a New Era for Structural Biology of Biological Macromolecules. Tamir Gonen.

4:30 pm 03.06.05
Structural Architecture of the Autophagy Apecific Class III Phosphatidyl Inositol 3-kinase Complex. Sulochanadevi Baskaran, Goran Stjepanovic, Lars-Anders Carlson, Patricia Grob, Eva Nogales, James Hurley.

4:45 pm 03.06.06
Chemically Functionalized Carbon Films for cryoEM Imaging. Qiu-Xing Jiang, Marc Llaguno, Gaya Yadav.

05.07 *in-situ* and En Operando Methods

Session Chairs: Plaza Ballroom D
Vicky Doan-Nguyen and Ashifa Huq

Funding provided by DECTRIS

1:30 pm 05.07.01
Energy Dispersive X-ray Diffraction (EDXRD) for i*n-situ* Characterization of Battery Systems. Amy Marschilok, Kevin Kirshenbaum, David Bock, Alexander Brady, Zhong Zhong, Kenneth Takeuchi, Esther Takeuchi.

2:00 pm 05.07.02
in situ Small-angle Neutron Scattering of Mesoporous Electrode Materials. Craig A.

Bridges, Xiaoguang Sun, Lilin He, Sheng Dai.

2:18 pm 05.07.03
Panoramic Synthesis of Bulk Inorganic Materials. Daniel Shoemaker.

2:48 pm Coffee Break

3:18 pm 05.07.04
Searching for Ti-clusters in $Mg_{0.7}Ti_{0.3}$ Thin Film. Hyunjeong Kim, Kohta Asano, Kouji Sakaki, Yumiko Nakamura, Akihiko Machida, Naoyuki Maejima, Tetsu Watanuki, Herman Schreuders, Bernard Dam.

3:36 pm 05.07.05
In-situ Isotope-Contrasted Stroboscopic Studies of the Local Atomistic Structure of Catalytic Materials. Daniel Olds, Arnold Päcklar, Katie Page, Peter Peterson, James Neilson.

4:06 pm 05.07.06
Oxygen Storage Properties of $La_{1-x}Sr_xFeO_{3-\delta}$ for Chemical-looping Reactions with *in-situ* Synchrotron X-ray and Neutron Diffraction. Daniel D. Taylor, Nathaniel J. Schreiber, Benjamin D. Levitas, Pamela S. Whitfield, Wenqian Xu, Efrain Rodriguez.

4:24 pm 05.07.07
High-Pressure Single-Crystal Structures of the Hybrid Perovskites $(CH_3NH_3)PbBr_3$ and $(CH_3NH_3)PbI_3$. Christine Beavers, Adam Jaffe, Hemamala Karunadasa.

4:42 pm 05.07.08
High Pressure Single-crystal Diffraction at HPCAT. Dmitry Popov, Rui Li, Changyong Park, Curtis Kenney-Benson, Guoyin Shen.

01.08 Career Development

Chairs: **Governors Square 14**
George Lountos
Martin Donakowski **7:30 pm**

Funding provided by Anatrace, Sigma Aldrich

Brad Conrad, Director of Society of Physics Students

Conrad will talk broadly to an open audience about presenting one's studies and research effectively in a resume/CV and interview. Afterwards, this session will feature resume/CV critiques and mock interviews (by preschedule only) for scientists beginning their careers. Effective communication of one's skills and abilities to a broad audience is a necessary skill but one that is frequently not discussed within an academic's career. To address this, this professional development session will bring together experts of varied career paths to work one-on-one with young scientists to examine how they can improve their written and verbal communication skills to potential employers.

Business Meeting for all ACA Members

5:00pm
Plaza Ballroom EF

All are welcome and strongly encouraged to attend

Registration Desk	07:30am	Plaza Registration
Speaker Ready Room	8:00am	Plaza Court 1
Council Meeting Room	8:00am	Directors Row F
Annual Awards Banquet (ticket required) cash bar-6:30pm, dinner-7:30pm		Plaza Ballroom

AW.04 Fankuchen Award and Lecture

T. Terwilliger, Presiding **Plaza Ballroom A,B,C**

8:00-8:45am **AW.04.01**
Travels in Protein Crystallography.
Elspeth Garman, University of Oxford.

02.06 Making Sense of Diffuse Scattering

Session Chairs: **Governors Square 14**
Jim Britten and Christina Hoffman

9:00 am 02.06.01
Interpreting Diffuse Scattering in Functional Materials. James Neilson, Joshua Kurzman.

9:30 am 02.06.02
Diffuse Scattering in the High Tc Superconductor, $HgBa_2CuO_{4+\delta}$ .Thomas R Welberry.

10:00 am Coffee Break

10:30 am 02.06.03
Investigation of Local Order in Cadmium Cyanide with 3D-ΔPDF Method. Arkadiy Simonov.

10:55 am 02.06.04
Diffuse Scattering from Relaxor PMN-xPT Matthew Krogstad, Peter Gehring, Jacob Ruff, Feng Ye, Zuo-Guang Ye, Stephan Rosenkranz, Raymond Osborn, Daniel Phelan.

11:20 am 02.06.05
Structure and Phase Content Quantification of Manganese Oxide Conformal Thin Films on 3D Electrodes with Total Scattering Analyses. Martin Donakowski, Jean M. Wallace, Megan B. Sassin, Karena W. Chapman, Joseph F. Parker, Jeffrey W. Long, Debra R. Rolison.

11:40 am 02.06.06
Recent Progress of CORELLI: The Elastic Diffuse Scattering Spectrometer at SNS Yaohua Liu, Feng Ye.

04.05 Radiation Damage

Session Chairs: **Plaza Ballroom E,F**
Elspeth Garman and Gerd Rosenbaum

9:00 am 04.05.01
Radiation Damage in Protein Crystallography at X-ray Free-electron Lasers. Karol Nass.

9:30 am 04.05.02
Initial Observations of Radiation Damage in MicroED. Johan Hattne, Dan Shi, Francis Reyes, Jason de la Cruz, Tamir Gonen.

10:00 am Coffee Break

10:30 am 04.05.03
Tracking Specific Radiation Damage in Macromolecular X-ray Crystallography. Charles Bury, Ian Carmichael, John McGeehan, Elspeth Garman.

11:00 am 04.05.04
Dynamic Sampling Image Reconstruction for Automated Diffraction-Based Protein Crystal Positioning. Garth J. Simpson, Nicole M. Scarborough, G. M. Dilshan Godaliyadda, Dong Hye Ye, Azhad Chowdhury, Michael J. Sheedlo, David J. Kissick, Shijie Zhang, Justin A. Newman, Robert F. Fischetti, Chittaranjan Das, Charles A. Bouman.

11:20 am 04.05.05
Structure Solution in the Presence of Radiation Damage. Dominika Borek, Zbyszek Dauter, Marcin Cymborowski, Wladek Minor, Zbyszek Otwinowski.

11:40 am 04.05.06
Radiation Damage in *de novo* Structure Determination Using Fixed-Target Serial Synchrotron Crystallography. Kazuya Hasegawa, Keitaro Yamashita, Kunio Hirata, Go Ueno, Hideo Ago, Tomohiro Murai, Toru Nakatsu, Masaki Yamamoto, Takashi Kumasaka.

03.07.01 Hot Structures I

Session Chairs: Governors Square 15
Betsy Goldsmith and Kimberly Stanek

9:00 am 03.07.01.02
Discovery of a GTP Sensor with a Structural Reverse Genetic Approach. Toshiya Senda, Koh Takeuchi, Miki Senda, Atsuo Sasaki.

9:20 am 03.07.01.03
Bile Salt Receptor Complex Activates a Pathogenic Type III Secretion System. Diana R Tomchick, Peng Li, Giomar Rivera-Cancel, Lisa N Kinch, Dor Salomon, Nick V Grishin, Kim Orth.

9:40 am 03.07.01.04
Structural Basis for Non-canonical Substrate Recognition of Cofilin/ADF Proteins by LIM Kinases. Titus Boggon.

10:00 am Coffee Break

10:30 am 03.07.01.05
Structure, Inhibition and Regulation of a Two-pore Channel TPC1. Alexander Kintzer, Robert Stroud.

10:50 am 03.07.01.06
Structural Insights into CRM1 Interaction with FG-repeat Proteins of the Nuclear Pore Complex. Ralf Ficner, Thomas Monecke, Sarah Port, Manfred Weiss, Ralph Kehlenbach, Achim Dickmanns.

11:10 am 03.07.01.07
Structure of Malaria Vaccine Target CelTOS Reveals its Function and Mechanism of Mediating the Exit of Malaria Parasites From Cells During Host and Vector Cell Traversal. John Jimah, Nichole Salinas, Monica Sala-Rabanal, Nathaniel Jones, L. David Sibley, Colin Nichols, Paul Schlesinger, Niraj Tolia.

11:30 am 03.07.01.08
AcrH-AopB Chaperone-Translocator Complex Structure Reveals a Role for Membrane Hairpins in T3SS Translocon Assembly. Jobichen Chacko, Yu-Keung Henry Mok, J Sivaraman.

05.09 SAS and Integrative Approaches to Complex Structures

Session Chairs: Plaza Ballroom D
Kushol Gupta and Jan Ilavsky

Funding provided by Molmex Scientific, Inc.

9:00 am 05.09.01
Toward "Damascus colloids": Developing Thermal Processing Strategies for Colloidal Gel. Matthew Helgeson.

9:40 am 05.09.02
Structure-based Identification of ATG14 Residues Essential for Starvation-Induced Autophagy. Sangita Sinha, Yang Mei, Minfei Su, Christopher Colbert.

10:05 am Coffee Break

10:35 am 05.09.03
Time-Resolved SAXS with Low Sample Consumption. Thomas Weiss, Tsutomu Matsui, Ivan Rajkovic, Ping Liu.

11:05 am 05.09.04
The Role of Small-Angle Scattering in an Integrated Approach to Characterizing Ageing Kinetics in Advanced Alloys. Andrew Allen, Fan Zhang, Lyle Levine, Jan Ilavsky.

11:45 am 05.09.05
Complex Modeling of Nanostructure in Quantized-growth CdSe Nanoparticles. Pavol Juhas, Alexander N. Beecher, Jonathan S. Owen, Simon J.L. Billinge.

12:10 pm 05.09.06
Characterization of Amorphous High-Surface Area Magnesium Carbonate (Upsalite) Using Laboratory Diffractometer. Céleste Reiss, Olga Narygina, Marco Sommariva, Sara Frykstrand, Johan Forsgren.

01.11.01 Standard Practices in Crystallography II: Structure Refinement and Validation

Session Chair: Plaza Ballroom A, B, C
Peter Mueller

9:00 am 01.11.01.02
Bayesian Library for the Analysis of Neutron Diffraction Data. William Ratcliff, Steven Disseler, Joseph Lesniewski, Dylan Quintana.

9:20 am 01.11.01.03
When Alternative Layer Stackings Cause Commensurate Structures to Co-Exist the Interpretation of the Diffraction Data May Not Be Unique. A. David Rae, Supanimit Chiampanichayakul, Michael S. Sherburn, Anthony C. Willis.

9:40 am 01.11.01.04
Identification of Unknown Metal Atoms in Coordination Compounds. Claudia M. Wandtke, Matthias Weil, Jim Simpson, Birger Dittrich.

10:00 am Coffee Break

10:30 am 01.11.01.05
Model-building using cryo-EM and Crystallographic Maps. Thomas Terwilliger, Paul Adams, Li-Wei Hung, Pavel Afonine, Oleg Sobolev.

11:00 am 01.11.01.06
Strategies to Address Challenging Macromolecular Structural Projects in the Context of an Academic Service Laboratory. Diana R Tomchick.

11:20 am 01.11.01.07
Validation of Macromolecular Structures. Paul Adams, Pavel Afonine, Bradley Hintze, Christopher Williams, Nigel Moriarty, Oleg Sobolev, Peter Zwart, Thomas Terwilliger, Randy Read, David Richardson, Jane Richardson.

11:50 am Lunch Break

1:30 pm 01.11.01.08
Use (and abuse) of Restraints in Structure Refinement. Peter Müller.

1:50 pm 01.11.01.09
An Enhanced Hirshfeld Test - Validating Atomic Vibrations in Crystal Structures. Jens Luebben, Birger Dittrich, George M. Sheldrick.

2:15 pm 01.11.01.10
DSR - Modelling Disorder with new GUIs for ShelXle and Olex2. Daniel Kratzert.

2:40 pm 01.11.01.11
Patterns of Residual Electron Density that Persist in Well-Determined Crystal Structures of Iridium Compounds. Thomas Emge.

3:00 pm Coffee Break

3:30 pm 01.11.01.12
OH...HO Clashes in Recently Published Structures. Carl Schwalbe.

3:50 pm 01.11.01.13
What is Needed for Proper Structure Validation and How to Interprete and Act upon Validation ALERTS. Anthony Spek.

4:20 pm 01.11.01.14
Crystallographic Algorithms for Multiple-CPU Computers. George M. Sheldrick.

01.05.02 General Interest II

Session Chairs: Governors Square 14
Stacey Smith and Graciela Diaz

1:30 pm 01.05.02.01
NSLS-II Biomedical Beamlines for Microcrystallography, FMX, and for Highly Automated Advanced Data Collections. Jean

Jakoncic, Martin Fuchs, Wuxian Shi, Edwin Lazo, Alexei Soares, Dileep Bhogadi, Herbert J. Bernstein, Stuart Myers, Bruno Martins, John Skinner, Lonny Berman, Bob Sweet, Dieter Schneider, Sean McSweeney.

1:50 pm 01.05.02.02
UGA-APS Native SAD Pilot Program at SER-CAT 22BM for General Users. Bi-Cheng Wang, John Rose, John Chrzas, Lirong Chen, Palani Kandavelu, Dayong Zhou, Unmesh Chinte, Zheng-Qing (Albert) Fu, Zhongmin Jin, James Fait, Gerd Rosenbaum, Denny Mills.

2:10 pm 01.05.02.03
Current Status of Microfocus X-ray Sources for Chemical and Biological Crystallography. Juergen Graf, Tobias Stuerzer, Holger Ott, Andreas Kleine, Joerg Wiesmann, Carsten Michaelsen.

2:30 pm 01.05.02.04
Capability and Quality Evaluation of High-Speed Detectors. Zheng-Qing (Albert) Fu, John Chrzas, John P. Rose, Bi-Cheng Wang.

2:50 pm 01.05.02.05
Computing Infrastructure, Software Optimization for High Data Rate MX, and Real Time Analysis. Herbert J. Bernstein, Kaden Badalian, Jean Jakoncic, Edwin Lazo, Sean McSweeney, Wuxian Shi, Alexei Soares, Bob Sweet.

3:10 pm Coffee Break

3:30 pm 01.05.02.06
Low-cost Home-built Imager for Protein Crystal Screening. Thayumanasamy Somasundaram, Michael Zawrotny.

3:50 pm 01.05.02.07
CCP4 Release 7.0. Charles Ballard, Andrey Lebedev.

4:10 pm 01.05.02.08
PDB2INS - An Interface to SHELXL Refinements of Macromolecules. Anna V. Luebben, Jens Luebben, George M. Sheldrick.

4:30 pm 01.05.02.09
Primordial Proteins had No Cysteines, Tryptophans, or Methionines, Started with a Valine, and Used No Codons Ending in Adenine. William Duax, Matthew Szarzanowicz, John P Scaduto, Sanjay Connare.

4:50 pm 01.05.02.10
Structural Analysis of Diverse Members of the Cyclic Amide Hydrolase Family of Toblerone Fold Enzymes. Thomas Peat.

03.07.02 Hot Structures II

Session Chairs: **Governors Square 15**
David Lodowski and George Lountos

Funding provided by Beryllium

1:30 pm 03.07.02.01
A Role for SETMAR in Gene Regulation: Insights from Crystal Structures of the DNA-binding Domain in Complex with DNA? Qiujia Chen, Millie M. Georgiadis.

1:50 pm 03.07.02.02
Crystal Structures and RNA-binding Properties of Two Hfq Homologs from *Aquifex aeolicus*. Kimberly Stanek, Peter Randolph, Jennifer Patterson, Cameron Mura.

2:10 pm 03.07.02.03
Structural and Biochemical Characterization of the Frequency-interacting RNA Helicase from *Neurospora crassa*. Yalemi Morales, Jacqueline Johnson, Sean Johnson.

2:30 pm 03.07.02.04
Recognition of a Bacterial Alarmone Through Long-Distance Association of Two Riboswitch Domains. Christopher Jones, Adrian Ferré-D'Amaré.

2:50 pm Coffee Break

3:30 pm 03.07.02.05
Apo Structures of the Adenine Riboswitch Aptamer Domain Determined Using an X-

Ray Free Electron Laser. Jason Stagno, Yu Liu, Yuba Bhandari, Chelsie Conrad, Subrata Panja, Monalisa Swain, Lixin Fan, Garrett Nelson, Chufeng Li, Derek Wendel, Thomas White, Anton Barty, Ryan Tuckey, Marzena Dyba, Sergey Tarasov, Uwe Weierstall, Nadia Zatsepin, Thomas Grant, Charles Schwieters, Jinwei Zhang, Adrian Ferre-D'Amare, Petra Fromme, David Draper, Kemin Tan, Xiaobing Zuo, Xinhua Ji, John Spence, Sarah Woodson, Yun-Xing Wang.

3:50 pm 03.07.02.06
Pairing and Conformational Plasticity of the U6 Small Nuclear Ribonucleoprotein's Internal Stem Loop. Eric Montemayor, Allison Didychuk, Honghong Liao, Panzhou Hu, David Brow, Samuel Butcher.

4:10 pm 03.07.02.07
Structure of MutY Complexed to DNA with a Transition State Mimic Reveals Mechanism and Predicts a Class of Retaining BER Glycosylass. Martin Horvath, Valerie O'Shea, Ryan Woods, Aurea Chu, Sheng Cao, Jody Richards, Sheila David.

4:30 pm 03.07.02.08
Cytochrome c Binds Detergent Hydrocarbons in a Well-defined Pocket. Bruce E. Bowler, Levi J. McClelland, Tung-Chung Mou, Frank G. Whitby, Stephen R. Sprang.

03.08 Structural Enzymology

Session Chairs: **Plaza Ballroom E, F**
Katarzyna Handing and Carrie Wilmot

1:30 pm 03.08.01
Dihydrodipicolinate Reductase as a Target For Development of Antimicrobial Compounds. Maksymilian Chruszcz, Swanandi Pote, Nicholas Mank, Vincent Klapper, Amy Arnette, Linda Shimizu.

2:00 pm 03.08.02
Catalytic Cycle of MenD (SEPHCHC synthase) from the Menaquinone Biosynthesis Pathway Revealed by X-ray Crystallography. Ghader Bashiri, Ehab Jirgis, Jodie Johnston, Esther Bulloch, Laura Nigon, Edward Baker.

2:20 pm 03.08.03
X-ray and Neutron Crystallographic Studies of Protein Kinase A Catalytic Subunit Function. Andrey Kovalevsky, Oksana Gerlits, Amit Das, William Heller, Paul Langan, Susan Taylor.

2:40 pm 03.08.04
XModeScore – A Powerful Method for Determination of Hydrogen Atom Locations And Protonation States in Structural Enzymology. Oleg Borbulevych, Lance Westerhoff.

3:00 pm Coffee Break

3:30 pm 03.08.05
Time-Resolved Molecular Snapshots Reveal an Unprecedented Mechanism for Recognition and Removal of Damaged Bases in DNA Elwood Mullins.

4:00 pm 03.08.06
Oxygen Species at the Active Site of a Fungal Polysaccharide Monooxygenase. William B. O'Dell, Flora Meilleur.

4:20 pm 03.08.07
Chicken or the Egg: The Structural Story of a Fungal Protease and a Corn Chitinase. Marcia M. Chaudet, Todd A. Naumann, Neil P.J. Price, David R. Rose.

4:40 pm 03.08.08
Structure of the HOIP-RBR/E2~ubiquitin/ubiquitin Complex Reveals RBR E3 Ubiquitin Ligase Mechanism and Regulation. Bernhard Lechtenberg, Akhil Rajput, Ruslan Sanishvili, Malgorzata Dobaczewska, Carl Ware, Peter Mace, Stefan Riedl.

05.08 Small Angle Scattering in Broad Spectrum: Chemistry and Morphology in Complex Soft Materials

Session Chairs: **Plaza Ballroom D**
Cheng Wang and Wei Chen

1:30 pm 05.08.01
Neutron Contrast Variation in Soft and Biological Materials. Volker Urban.

2:00 pm 05.08.02
A General Method for Nanoparticles Size Selective Purification using Critical Casimir Forces Studied with Small Angle Neutron Scattering, Hongyu Guo, Gheorghe Stan, Yun Liu.

2:30 pm 05.08.03
Scattering Models, Techniques, and Applications for Resonant Soft X-ray Scattering. Brian Collins.

3:00 pm Coffee Break

3:30 pm 05.08.04
Resonant Soft X-ray Scattering Studies of Helical Liquid Crystals. Chenhui Zhu.

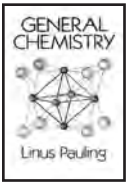
4:00 om 05.08.05
Depth Resolved Spectroscopy From Resonant Reflectivity. Kevin Stone.

4:30 pm 05.08.06
Structure Foundations of High Performance in Polymer Semiconductors. Dean DeLongchamp.

WEDNESDAY, JULY 27

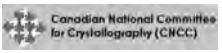
Planning Session for
2017 Spring Meeting in
New Orleans

8:00AM Governors Square 14



Pauling Poster Prizes, Canadian and Poster Prize

The Pauling Poster Prizes were established by the ACA to honor Linus Pauling and are supported by member donations. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each 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, 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 on Structural Dynamics Poster Prize

A prize of $250 is given for excellence in research on structural determination and dynamics of systems, enabled by 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

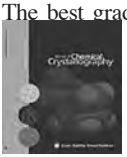
CrystEngComm (published by the Royal Society of Chemistry) is very pleased to sponsor a prize to be awarded to the best graduate or undergraduate poster presentation in the area of crystal engineering/ supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted 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.

Journal of Chemical Crystallography Poster Prize

The best gradudate 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.



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.

Posters

POSTER HANGING INSTRUCTIONS

All posters should be displayed from 10:30 am on Saturday, July 23 until 7:30 pm on Monday, July 25. Please be present at your poster from 5:30 - 7:30 pm on the day to which you are assigned.

1-SU
In-situ Powder Diffraction Studies of Na1.5Gd1.5F6:Yb:Er Upconverting Nanocrystals During Synthesis. A. M. Milinda Abeykoon, Damien Hudry, Eric Dooryhee, Dmytro Nykypanchuk, James H. Dickerson.

2-SU
Understanding Carbonic Anhydrase Inhibition using X-rays, Neutrons, and Molecular Dynamics. Mayank Aggarwal.

3-SA
Substructure Determination for Native-SAD phasing. Ayaka Harada, Yusuke Yamada, Dorothee Libschner, Naohiro Matsugaki, Toshiya Senda.

4-MO
The Jahn-Teller Switch in Partially Deuterated Ammonium Copper Tutton Salt, $(NH_4)_2[Cu(H_2O)_6](SO_4)_2$ Arthur J. Schultz, John A. Schlueter, Venkatesha R. Hathwar, Mads Ry Jørgensen, Bo B. Iversen, Paula M. B. Piccoli, Xiaoping Wang, Christina Hoffman, Andrey Yakovenko, Gregory J. Halder.

5-SU
Structure and Reactivity of Pt(II) Nitrile Complexes. Alberto Albinati, Roberta Bertani, Maurizio Casarin.

6-SA
CCP4 Web services. Andrey Lebedev, Ville Uski, Marcin Wojdyr, David Waterman, Ronan Keegan, Charles Ballard, Eugene Krissinel.

7-MO
An Add-on Device for Automated In Situ Screening. Angela Criswell, Thom Hendrixson, Joseph Ferrara, Zhao Zijian, Cheng Yang, Colin Acheson, Pierre LeMagueres.

8-SU
Photofunctional Zwitterionic Metal-Organic Framework with Tunable Adsorption Properties. Wen An.

9-SA
Structural Insights into Intron RNA Splicing. Aaron Robart, Navtej Toor, Russel Chan, Jessica Peters.

10-SU
Discovery of Novel Antibacterials Targeting the MEP Pathway Using the Crystal Structure of F. tularensis IspD. Arthur Tsang, Schroeder Noble, Nagarajan Pattabiraman, Chinchu Johny, Amanda Haymond, Robin Couch.

11-MO
Structure of Pathogen-related Yeast CAP protein, Pry1 in Complex with a Competitive Inhibitor of Cholesterol Binding. Oluwatoyin Asojo, Alan Kelleher, Elissa M Hudspeth, Rabih Darwiche, Roger Schneiter.

12-SU
Metal-Organic Frameworks as Platforms for the Controlled Nanostructuring of Single Molecule Magnets. Darpandeep Aulakh, Joshua Pyser, Xuan Zhang, Kim Dunbar, Andrey Yakovenko, Mario Wriedt.

13-SA
The Crystal Structure of the Precursors for Polymethine Dyes with Bulky Groups. Boris Averkiev, Logan Wolfel, Yulia A. Getmanenko, Tatiana V. Timofeeva.

14-SU
Crystallographic Insight into Enhanced Catalytic Activity of Carbonic Anhydrase II using "Activating" Ligands for Improved Cognitive Function. Avni Bhatt, Marc Ilies, Robert McKenna.

15-MO
A Modular Plate System For *in situ* Data Collection. Kevin Battaile, Anne Mulichak, Eric Hollabaugh, Eric Zoellner, Lisa Keefe, Benjamin Apker.

16-SA
Nucleocapsid Protein of Human Coronavirus NL63. Bozena Szelazek, Wojciech Kabala, Krzysztof Kus, Michal Zdzalik, Michal Burmistrz, Dominik Florek, Krzysztof Pyrc, Grzegorz Dubin.

19-SA
Strategy for Extensible, Evolving Terminology for Material Science and the PDB. Talapady Bhat.

20-SU
Dithiazole[4,5-a:5',4'-c]Phenazines as Donors in Co-Crystals with Tetracyanoquinodimethane Derivatives. Bianca Valencia, Yulia A. Getmanenko, Boris Averkiev, Tatiana V. Timofeeva.

21-SU
Hard X-ray Scattering Study on the Structure of Si-Dopped Ferric Oxyhydroxides. Olaf Borkiewicz, Gabriela Pieczara, Maciej Manecki, Grzegorz Rzepa.

22-SU
Structure of a Highly Expressed Family 74 Glycoside Hydrolase from the Cellulolytic Bacteria Streptomyces sp. SirexAA-E. Christopher Bianchetti, Adam Kositzke.

23-SA
Double-stranded RNAs with Open Major Grooves from Trypanosome RNA Editing. Blaine Mooers, Akila Venkataramany, Shelly Gulati, Chiedza Kanyumbu, Barat Venkataramany, Kristi Rice, Victoria Mooers, Jugmen Sherpa, Amitranshu Singh, Kyle Cahill.

24-SU
Introduction of Zwitterionic Moieties into Metal-Organic Frameworks via Post Synthetic Modifications. Hubert Bilan, Mario Wriedt.

25-SA
NE-CAT: Crystallography Beamlines for Challenging Structural Biology Research. Surajit Banerjee, Kanagalaghatta Rajashankar, Malcolm Capel, Cynthia Salbego, Leslie Kinsland, Jonathan Schuermann, Narayanasami Sukumar, Igor Kourinov, James Withrow, Anthony Lynch, Steve Ealick, Frank Murphy, David Neau, Kay Perry.

26-MO
New Technologies for X-ray Generation and Detection. Bruce C. Noll, Tobias Stuerzer, Holger Ott, Michael Ruf.

27-SA
Production of IL-24 and its Receptors for Structural Studies. Cem Sonmez, Alexander Wlodawer, Jacel Lubkowski.

28-SU
Mirror Image Crystal Structures of a Self-Assembling 3D DNA Crystal. Chad Simmons, Fei Zhang, Xiaodong Qi, Nour Eddine Fahmi, Yan Liu, Hao Yan.

29-MO
Optimization of Experimental Parameters for Powder Diffraction with PHOTON II Detectors and APEX3 Software. Charles Campana, Victor Young.

30-SA
Insights on the Reactivity and Partial Retro-Diels-Alder Character of Norbornene Compounds Derived from Charge-Density Studies at 20 K. Christopher Gianopoulos, Alan Pinkerton, Bartosz Zarychta, Simone Cenedese, Vladimir Zhurov.

31-SU
Synchrotron X-ray studies of spinels at high pressure, high temperatures in a large volume press.. Christian Lathe, Joern Lauterjung.

32-SU
Non-Trans Peptides: Protect Your Structure. Know the Warning Signs.. Christopher Williams, Bradley Hintze, Lizbeth Videau, Jane

Richardson, David Richardson.

33-MO
High-speed Detectors Enable Synchrotron Serial Crystallography. Clemens Schulze-Briese.

34-SU
Non-classical, Diol-based Inhibition of Carbonic Anhydrase IX as a Potential Breast Cancer Therapy. Carrie Lomelino, Brian Mahon, Claudiu Supuran, Robert McKenna, Mario Sechi.

35-MO
Models for Copper Dynamic Behavior in Doped Cadmium DL-Histidine Crystals: Electron Paramagnetic Resonance and Crystallographic Analysis. Michael Colaneri, Simon Teat, Jacqueline Vitali.

36-MO
Porphyrins for Advanced Materials Science Applications. Lawrence Cook, Winnie Wong-Ng, Greg Brewer.

37-MO
Disruption of a Histidine-Histidine Interaction at the Dimer Interface of Stilbene Synthase Alters Substrate Specificity. Charles Stewart.

38-SA
A Micromanufactured Dynamic Beamstop. Diane Bryant, Andrew Doran, Corie Ralston, Marc Allaire, Simon Morton, John Pepper, Richard Celestre, Steve Dimaggio.

39-SA
Cloning, Expression and Preliminary Purification of Ribosomal protein S12 Methylthiotransferase RimO from *Thermus thermophilus* HB8. Prabhu Damotharan, Jeyakanthan J.

40-MO
Improvement of Protein Crystal Diffraction Quality by High-Pressure Cryocooling. Marian Szebenyi, Qingqiu Huang.

41-SA
Structural Basis for PECAM-1 Homophilic Binding. Dongwen Zhou, Cathy Paddock, Peter Newman, Jieqing Zhu.

42-SU
Methods to Achieve Fast, Precise Single Crystal Data Using Intelligent Design. Eric Reinheimer, Mathias Meyer, Przemyslaw Stec, Fraser White, Joseph Ferrara, Alex Griffin, Pierre LeMagueres.

43-MO
Yes Virginia, There Is Jahn-Teller Distortion in Cu(NO3)2 Hexahydrate. Frank R. Fronczek, Andrew W. Maverick.

44-SA
Crystallization of Carboxy-Terminal ATP-Citrate Lyase. Marie Fraser, Koto Hayakawa, Kristi Ngo, Jinhong Hu, Jillian Rogers.

45-SU
Quantitative Analysis of a Gallbladder Stone using Rietveld Analysis. Prabal Dasgupta.

46-MO
Crystal Structure of the NIST Fab at 2A Resolution. Travis Gallagher, Connor Galvin, Ioannis Karageorgos.

47-MO
Crystallographic Studies of Human Acetylcholinesterase Reactivation by Oximes. Oksana Gerlits, Donald Blumenthal, Palmer Taylor, Andrey Kovalevsky, Mikolai Fajer, Xiaolin Cheng.

48-SU
Pim-1 kinase Complexes with ATP-competitive Inhibitors. Grzegorz Dubin, Jozefina Bogusz, Karol Zrubek, Krzysztof Rembacz, Przemyslaw Golik.

49-SA
Upgrade Program of Macromolecular Crystallography Beamlines at the Photon Factory, Japan. Masahide Hikita, Yusuke Yamada, Naohiro Matsugaki, Ayana Tomita-Sato, Masahiko Hiraki, Toshiya Senda.

51-SA
Crystal Structure of a Thermostable Lipase from Marine Streptomyces. Shulin Hou, Zexin Zhao, Yonghua Wang, Jinsong Liu.

52-SU
Identification of the Inhibition Mechanism of Hydroxycitrate on Human ATP Citrate Lyase through X-ray Crystallography. Jinhong Hu, Marie Fraser, Aruna Komakula.

54-SU
Molecular Shape Directed Crystalline Quasiracemates. Ian Tinsley, Kraig Wheeler.

55-SA
How Many Birds Can One Kill With a Single Stone, or is the Development of a New Shotgun Medicine Possible at All? Yancho Devedjiev.

56-SU
Femtosecond Structural Dynamics in Photoactive Yellow Protein from TR-SFX. Kanupriya Pande.

57-MO
Time Resolved SAXS at the BioCAT Beamline 18 ID at the Advanced Photon Source. Thomas Irving, Osman Bilsel, Sagar Kathuria, Srinivas Chakravarthy.

58-SA
Apo and Co-factor Bound Structures of *Mycobacterium tuberculosis* Acetolactate Synthase, ilvB1. Adam Salazar, Cory Thurman, James Sacchettini.

59-SU
Proton Conduction and Chemical Stability of the High-Temperature Cubic CsH_2PO_4 Modification. Israel Martinez, Victor Gonzalez, Cristian Botez, Alan Goose.

60-MO
Expression, Purification and Enzymatic Characterization of Dihydroorotase from *Methanococcus jannaschii*. Jacqueline Vitali, Aditya Singh, Michael Colaneri.

61-SU
DIALS: Handling Pixel Outliers in Background Modelling. James Parkhurst, David Waterman, Luis Fuentes-Montero, Richard Gildea, Gwyndaf Evans, Garib Murshudov, Graeme Winter.

62-SA
Structural Basis for the Complexity of Site II-Mediated Neutralization of Respiratory Syncytial Virus. Jarrod Mousa, Alexander Sevy, Bruno Correia, Jessica Finn, Oleksandr Kalyuzhniy, Gabriela Alvarado, Xiaolin Wen, John Bates, Theodore Jardetzky, Hannah King, William Schief, Leah Loernic, Melanie Ohi, James Crowe, Rachel Fong, Jens Meiler, Marion Sauer, Benjamin Doranz.

63-SU
Automated Rigid Body Segmentation. Jens Luebben, Birger Dittrich, George M. Sheldrick.

64-MO
Crystallographic Insights into the Structure-Activity Relationships of Diazaborine Enoyl-ACP Reductase Inhibitors. Jessica Vey, H. Howard Xu, Cheryl Jordan, Braddock Sandoval, Damian Gilling, Michael Groziak.

65-MO
MXCuBE3: A Web-based Beamline Control Software for BIOMAX at MAX IV. Jie Nan, Mikel Eguiraun, Fredrik Bolmsten, Antonio Milan, Matias Guijarro, Marcus Oscarsson, Daniele Sanctis, Uwe Mueller, Marjolein MGM Thunnissen.

66-SA
Synthesis, Charterization, and Application of Ferrocene Complexes as Estrogen's Pentant Groups for Breast Cancer Treatment: an Approach to Design Novel Metal-Based Therapeutic Drugs. José A. Carmona-Negrón, Enrique Meléndez, William J. Bauer, Eddie Snell, Arnold L. Rheingold, Alberto Santana, Belinda Pastrana-Ríos.

Posters

67-SA
Structural Model for a Novel Protein From The Clam *Lucina pectinata*. Josiris D. Rodriguez-Perez, Juan Lopez-Garriga.

68-MO
Improving X-ray Data Quality via Humid Manipulation and Transfer of Macromolecular Crystals. Douglas Juers.

69-SU
Extended Range Ultra Small-angle X-ray, Small-angle, and Wide-angle Scattering for Materials Characterization. Jan Ilavsky, Fan Zhang, Lyle Levine, Ross Andrews, Andrew Allen.

70-SU
Elucidating the Structural Basis of Interaction Between the Viral BHRF1 and Pro-apoptotic BID. Karen Glover, Samuel Wyatt, Sangita Sinha.

71-SA
New Compression Algorithms for Macromolecular Crystallographic Diffraction Images II. Kaden Badalian, Herbert J. Bernstein.

72-MO
Structural Insights into Energy Storage Materials Using Hard X-Rays. Kamila Wiaderek, Peter Chupas, Olaf Borkiewicz, Karena W. Chapman.

73-MO
A Seven-Space Representation of Lattices Based on Sorted Delaunay Reduction. Lawrence C. Andrews, Herbert J. Bernstein.

74-SA
Structural Transformations of Copper Isophthalate-Based Kagome Frameworks Upon Dehydration. Laura McCormick, Simon Teat, Russell Morris, Matthew McPherson, Samuel Morris, David Cordes, Alexandra Slawin.

75-SA
Mono-, Di, and Tetrabromo Naphthalene Diimides: Single Crystal X-Ray Structural Analysis and Application as Acceptor in Donor-Acceptor Co-Crystals. James Foster, Yulia A. Getmanenko, Boris Averkiev, Tatiana V. Timofeeva.

76-MO
Structural Insights into the Transamination Mechanism of Aminotransferase CrmG in Caerulomycin Biosynthesis. Jinsong Liu, Jinxin Xu, Yiguang Zhu, Zhan Feng, Changsheng Zhang.

77-MO
The Small-Angle X-Ray Scattering Core Facility Of Center For Cancer Research Of National Cancer Institute. Lixin Fan, Yun-Xing Wang.

79-MO
Structure and Function of KstR from *M. tuberculosis*: Anecdotes in Crystal Optimization, Automation, and Undergraduate Research. Larissa Podust, Hugues Ouellet.

80-SA
Phasing Macromolecular Crystal Structure with Selenourea. Zhipu Luo, Zbigniew Dauter.

81-SA
Scotch Tape Facilitates Taking High Quality Pictures Through Microscope With Smartphone. Zhipu Luo, Zbigniew Dauter, Milosz Ruszkowski.

82-MO
IUCr – Supporting "Crystallography Around the World". Marvin Hackert, Gautam Desiraju, Masaki Takata, Santiago Garcia-Granda, Luc Van Meervelt, A. Mike Glazer, Michele Zema, J. Mitchell Guss, Brian McMahon, Samar Hasnain, Hanna Dabkowska, Radomir Kuzel, Michael Dacombe, Andrea Sharpe, Wulf Depmeier, Peter Strickland.

83-MO
In-situ and Time-Resolved Atomic Pair Distribution Function Measurements in Hydrogen Gas Environment at BL22XU in SPring-8. Naoyuki Maejima, Akihiko Machida, Tetsu

Watanuki, Hyunjeong Kim, Kouji Sakaki, Yumiko Nakamura.

84-SU
Crystallization of a TonB Dependent Transporter from Hypervirulent *Klebsiella pneumoniae*. Melissa Pinard, christine jao, Susan buchanan, Istvan Botos.

85-SA
A Data Dictionary for Archiving Integrative/Hybrid Models. Helen M. Berman, John Westbrook, Brinda Vallat, Ben Webb, Andrej Sali.

86-MO
Structural Modeling of C/EBPβ– Cyclin D1 Interactions. Maria Miller.

87-SU
BioSAXS-2000 AUTO: New Features Of SAXSlab 3.1 and the Automatic Sample Changer. Mark Del Campo, Angela Criswell, Colin Acheson, Thom Hendrixson, Katsunari Sasaki.

88-MO
Structure of the Lutein-Binding Domain of Human STARD3 with Phase Extension to 1.74 Å and Model of a Complex with Lutein. Martin Horvath, Binxing Li, Evan George, Quang Tran, Paul Bernstein.

89-SA
Solving Protein Structures Without a Model Or Experimental Phases. Massimo D. Sammito, Claudia L. Millán-Nebot, Rafael J. Borges, Andrey Nascimento, George M. Sheldrick, Isabel Usón.

90-SA
Crystal Structures of Plant N-Methyltransferase Complexes Reveal New Insights into Substrate Recognition and Catalytic Mechanism. Miguel Torres, Xue Chen, Luiz Eugenio, Jeremy Morris, Kenneth Ng, Elesha Hoffarth, Juila Savtchouk, Peter Facchini.

91-MO
Expanding the Limits of In-House Data Collection with the METALJET X-ray Source. Matthew Benning, Séverine Freisz.

92-SA
Phasing of Synchrotron Serial Crystallographic Data by Isomorphous Replacement. Max Nanao.

93-MO
A Novel Binding Motif of the Carbapenem Drug Ertapenem in a Class D β-lactamase OXA-24/40. Joshua Mitchell, Rachel Powers.

94-MO
Routine Fast Fragment Screening in Crystals at Diamond's XChem Facility. Myron Smith.

95-SA
X-ray Analysis for the Ternary ZrO2-Y2O3-Nb2O5 used as Thermal Barrier Coating. Nara Guimaraes, Danieli Aparecida Reis.

96-MO
Positive Residual Density in Organic Molecules: Can We Fit It? Alexander Nazarenko.

97-SA
Mechanistic Insight into a Novel Metal-dependent DMSP-Lyase. Nicholas Schnicker, Mishtu Dey.

98-SU
Membrane Lipids As Energy Stress Signal via RsbQ/P in *Bacillus subtilis*. Nipawan Nuemket, Takashi Kumasaka, Kazuki Omichi.

99-SA
XFEL Still Shots and Multi-crystal Data Merging. Nicholas Sauter, Aaron Brewster, Iris Young.

100-MO
A method for High-Throughput, Low Volume Soaking of Protein Crystals in Rapid Screening fragment libraries. Paul Thaw, David Hargreaves.

101-SU
Biochemical Basis of the Interaction between

HIV-1 Vpu and the Clathrin Adaptor Protein Complexes AP-1 and AP-2. Rajendra Singh, Xiaofei Xia, Charlotte Stoneham, Yong Xiong, John Guatelli.

102-MO
Recent Developments at the Beamline for Biological Small Angle X-ray Scattering BL4-2 at SSRL. Ivan Rajkovic, Tsutomu Matsui, Ping Liu, Thomas Weiss.

103-SU
CRISPR RNA-guided DNA Interference in *Escherichia coli*. Ryan Jackson, Sarah Golden, Paul van Erp, Airlie McCoy, Thomas Terwilliger, Randy Read, Blake Wiedenheft, Joshua Carter.

104-SA
Thermal Contraction of Cryoprotectant Solutions for Optimized Protein Crystal Cryoprotection. Robert Thorne, Hakan Atakisi, Chen Shen, Ethan Julius, Timothy Tyree, David Moreau.

105-SU
Actinide Hybrid Materials: Supramolecular assembly and periodic trends. Robert Surbella III, Jochen Autschbach, Ginger Sigmon, Peter Burns, Jon Schwantes, Christopher Cahill, Kristi Pellegrini, Bruce McNamara, Lucas Ducati.

106-MO
Conserved Structural Core within Bovine Antibody Ultralong CDR H3s. Robyn Stanfield, Ian Wilson, Vaughn Smider.

107-SA
Targeting the SIX1-EYA Transcriptional Complex for Anti-Cancer Therapy Using Structure Guided and High Throughput Approaches. Rui Zhao.

108-SU
Temperature Dependent Reversible Phase Transition for a Ni(II) Complex. Nigam Rath, Jason Schultz, Liviu Mirica, Charles Campana.

109-SU
Purification and Crystallization of Two-Component Flavin Monooxygenase Systems. Liliana Gonzalez-Osorio, Jessica Vey, Samatar Jirde, Gilberto Mendez, Kellee Eberle, Bilal Madha, Jacki Manoukian, Richard Lengkong, Casper Wong.

111-MO
RCSB Protein Data Bank: Views of Structural Biology for Basic and Applied Research. Stephen K. Burley, Jesse Woo, Chunxiao Bi, Huanwang Yang, Cole Christie, Jasmine Young, Rachel Kramer Green, Christine Zardecki, Tara Kalro, Helen M. Berman, Andreas Prli_, Peter Rose, Chris Randle, Zukang Feng, John Westbrook.

112-SU
Comparison of structures and Functions of 2-methylcitrate Synthase (mcsA) from *Aspergillus fumigatus* and Citrate Synthase (hCS) from *Homo sapiens*. Caleb Schlachter, Vincent Klapper, Taylor Radford, Maksymilian Chruszcz.

113-SA
Pressure Dependency of CO2 Sorption in Metal-Organic Frameworks. Samuel Marks, Karina Riascos-Rodriquez, Arturo Henandez-Maldonado, Paul Evans.

114-SA
A Series of Crystalline Solids Composed of 2-Aminopyridines and Glutaric Acid: Similarities and Structural Diversity. Shabarinath Bejagam, Kathryn Storms, Sergiu Draguta, Marina S. Fonari, Tatiana V. Timofeeva.

115-MO
Is Mail-In Crystallography at the CLS right for you? Shaunivan Labiuk, James Gorin, Kathryn Janzen, Michel Fodje, Pawel Grochulski.

116-SA
Structural Insights into the Specific Recognition of Lys48-linked Tri-ubiquitin Chains by the AIRAPL Protein. Simin Rahighi, Ilana

Braunstein, Tsutomu Matsui, Thomas Weiss, Ariel Stanhil, Soichi Wakatsuki.

117-SA
Patterned Crystallization on Unpatterned Substrates. Serena Seshadri, Marina Solomos, Jennifer Swift.

118-SU
Radiation response and annealing behavior of A_2TiO_5 (A = Nd, Gd, and Yb). Sulgiye Park.

119-SA
Crystal Structure of Glycogen Debranching Enzyme and Insights into its Catalysis and Disease-Causing Mutations. Song Xiang, Liting Zhai, Lingling Feng, Lin Xia, Huiyong Yin.

120-MO
In Crystallo Capture of a Covalent Intermediate in the UDP-Galactopyranose Mutase Reaction. Jack Tanner.

121-SU
Preliminary Neutron Diffraction Experiments of Manganese Catalase using iBIX. Taro Yamada, Katsuhiro Kusaka, Naomine Yano, Takaaki Hosoya, Masaki Katagiri.

122-MO
Getting Ahead of Drug Resistance in the Schistosome Parasite. Alex Taylor.

123-SA
Stabilizing Transient Enzyme-substrate interaction of 2OG Oxygenases via Disulphide cross-linking. Thomas Leissing, Rasheduzzaman Chowdhury, Christopher Schofield, Xin Lu.

124-MO
Crystalline Products of CO_2 Capture by Piperazine Aqueous Solutions. Tatiana V. Timofeeva, Antal Sofia, Marina S. Fonari, Raul Castaneda, Carlos Ordonez.

125-SU
Structural and Functional Analysis of the Inner Membrane Protein, YejM, from *Salmonella typhimurium* - an Essential Protein for Cell Growth and Cardiolipin Transport. Uma Gabale, Gene Qian, Elaina Roach, Susanne Ressl.

126-SA
Structural Basis for Assembly and Function of a Heterodimeric Plant Immune Receptor. Li Wan.

127-SA
SCXRD Meets PXRD to Investigate Temperature Induced Polymorphism in a Metal-Organic Framework. Juby Varghese.

128-SU
Anisotropic Ordering in Bulk Covalent Organic Framework Powders. Demetrius A. Vazquez-Molina, Fernando J. Uribe-Romo.

129-SU
Neutron Crystallographic Studies of HIV-1 protease: Drug Binding, Drug Resistance and Proton Transfer. Andrey Kovalevsky, Paul Lanan, Amit Das, Irene Weber, Chen-Hsiang Shen, Matthew Blakeley, Jerry Parks, Jeremy Smith, Kevin Weiss, David Keen, Oksana Gerlits, John Louis, Troy Wymore.

130-MO
Dual Pinhole Mini-beam Collimator Provides Lower Background. Nagarajan Venugopalan, Robert Fischetti, Shenglan Xu, Oleg Makarov, David Kissick.

131-SU
Examining the Effect of Data Redundancy on Small Molecule Structure Refinement. Wayne Pearson.

132-MO
Integrated Synchrotron Biophysics Research at the Case Center for Synchrotron Biosciences. Wuxian Shi, Mark Chance, Jen Bohon, Erik Farquhar, Mike Sullivan.

133-SA
Structural Study of a Glycosyltransferase From A Marine Streptomyces Species. Tingting Xu,

aiang Liu, Liping Gong, Jinsong Liu.

134-SU
Structural Analysis of Arylpiperazinecarborane Derivatives. Yulia Sevryugina, Paulina Gonzalez.

135-MO
Insights into ParB Spreading from the Complex Structure of Spo0J and parS. Yuh-Ju Sun, Bo-Wei Chen.

136-MO
Crystal Structure of the Cyan Fluorescent Protein Cerulean S175G Mutant. Tae-Sung Yoon, Sangwook Park, Sunghyun Kang.

138-SA
Merging Data for Optimal Estimation of Phasing Signals in Multi-Crystal Experiments. Zbyszek Otwinowski, Dominika Borek, Marcin Cymborowski, Wladek Minor.

139-SU
PDB-101: Educational Portal for Molecular Explorations of Biology and Medicine from the RCSB Protein Data Bank. Christine Zardecki, Cole Christie, Stephen K. Burley, Shuchismita Dutta, David S. Goodsell, Robert Lowe, Chris Randle, Wendy Tao, Maria Voigt, Jesse Woo.

141-SA
Improved Pharmacological and Structural Properties of HIV Fusion Inhibitor AP3 over Enfuvirtide. Yun Zhu.

143-SU
Detection and Imaging of Microcrystalline Membrane Proteins using SONICC. Ellen Gualtieri, Lance Ramsey, Eric Zhao, Dmitry Rodionov.

144-MO
Novel Base-Pairing Interactions at the tRNA Wobble Position Crucial for Accurate Reading of the genetic code. Natalia Demeshkina, Marat Yusupov, Gulnara Yusupova, Alexey Rozov, Eric Westhof.

145-MO
New *in situ* Capabilities at 17-BM Rapid Acquisition Powder Diffraction Line. Andrey Yakovenko, Wenqian Xu.

146-SU
Superprotonic Behavior and High-Temperature Dehydration of Phosphate Solid Acids. Benjamin Deutsch, Victor Gonzalez, Alex Price, Heber Martinez, Israel Martinez, Andres Encerrado, Botez Cristian, Alan Goos.

147-MO
High Temperature Nuclear Fuels without Gas Overpressures for Cosmic Deep-Space Explorations. Boris Udovic.

148-SA
Multi-Fluorescent Imaging for Sensitive Protein Crystallization Detection. Lance Ramsey, Ellen Gualtieri, Dmitry Rodionov, Eric Zhao.

149-SU
Conductivity of $Cs_{1-x}SixH_2PO_4$ Trough Impedance Spectroscopy: Temperature Dependence Study. Andres Jose Encerrado M., Alan Goos, Ben Deutsch, Israel Martinez, Andrea Montgomery, Victor Gonzalez, Cristian E. Botez.

150-SA
Structure and Dynamics of the Polymyxin-Resistance-Associated Response Regulator PmrA in Complex with the Promoter DNA. Chwan-Deng Hsiao.

151-SU
Supramolecular Assembly and a Novel Topology Within a Structurally Diverse Series of Lanthanide P-Bromobenzoic Acid-Terpyridine Hybrid Materials. August Ridenour, Ray Butcher, Christopher Cahill, Korey Carter.

152-SA
Prescreening Integral Membrane Crystallization Conditions and Protein Preparations Utilizing FRAP. Ellen Gualtieri, Eugene Chun, Wei Liu, Dmitry Rodionov, Eric Zhao, Peng Chen, Lance Ramsey.

153-SU
Prescreening Membrane Protein Crystallization Conditions with LCP-FRAP. Lance Ramsey, Eric Zhao, Ellen Gualtieri, Dmitry Rodionov.

154-SA
The Crystal Structure of the Bacteriophage T4 MotA C-terminal Domain in Complex with dsDNA Reveals a Novel Protein-DNA Recognition Motif. Maxime Cuypers, Kenneth Kreuzer, Deborah Hinton, Stephen White, Rosanna Robertson, Brett Waddell, Sivaraja Vaithiyalingam.

155-SU
Novel Boronic Acid Inhibitors for the Class D β-Lactamase OXA-1. Alina Morales, Rachel Powers, Joshua Mitchell.

156-SA
Crystal Growth and Phasing made possible by a Protein Metal Organic Framework (PMOF): Crystals of a Cacodylate-Zinc-His-tag-BRR Complex. Kenneth Satyshur, Anna Baker, Peter Newhouse, Jeffrey Dwulit-Smith, Katrina Forest.

157-MO
Structural Basis for Promiscuous PAM Recognition in type I–E Cascade from *E. coli*. Robert Hayes, Scott Bailey, Blake Wiedenheft, Ailong Ke, Yibei Xiao, Fran Ding, Paul B. G. van Erp, Kanagalaghatta Rajashankar.

158-MO
Structural Genomics Analysis of Cofactor Preference Among Short-Chain Dehydrogenase/Reductases and the Emergence of a Novel SDR Subtype. Stephen Mayclin, Vasilios Marathias, Donald Lorimer, Phillip Pierce, Thomas Edwards, Amy Sullivan, Daniel Haft, Jan Abendroth, Isabelle Phan, Bart Staker, Peter Myler.

159-SU
Synthesis and Characterization of Novel Low Valent Group 13 Complexes. Lauren Stevens, Christopher Snyder, Samantha DeCarlo, Dennis Mayo, Yu-Sheng Chen, Peter Zavalij, Bryan Eichhorn.

161-SA
Characterization and Crystallization of the C-terminal Histidine Phosphatase Domain of Sts-1. Weijie Zhou.

162-MO
Molecular Packing Preferences in “Bridge-Flipped” Isomeric Aryl-2-Pyridylhydrazones and 2-Pyridinecarboxaldehyde Arylhydrazones. William Ojala, Kara Kassekert, Lindsey Beard, Charles Ojala.

163-SA
Chemical Functionalization of Phenyl-Modified Cadmium Chalcogenide Clusters. Yang Chen, Krishnayan Basuroy, Philip Coppens.

164-SA
Charge Density Analysis of 2,5-Dichloro-1,4-benzoquinone (DCBQ) at 20 K. Zhijie Chua, Alan Pinkerton, Vladimir Zhurov, Christopher Gianopoulos, Bartosz Zarychta.

Presenting Author Index

Aakeroy, Christer.....02.04.01.02
Abeykoon, A.M.Milinda.....1-SU
Adams, Paul.....01.11.01.07
Adibhatla, Anasuya.....02.01.03
Aggarwal, Mayank.....2-SU
Albinati, Alberto.....5-SU
Ali, Naveed Zafar.....05.02.04
Allen, Andrew.....05.09.04
An, Wen.....8-SU
Andrews, Lawrence C.....73-MO
Asojo, Oluwatoyin.....11-MO
Asojo, Oluwatoyin.....01.03.04
Aulakh, Darpandeep.....12-SU
Averkiev, Boris.....13-SA
Badalian, Kaden.....71-SA
Ballard, Charles.....01.05.02.07
Banerjee, Surajit.....25-SA
Bashiri, Ghader.....03.08.02
Baskaran, Sulochanadevi 03.06.05
Basuroy, Krishnayan.....05.03.04
Battaile, Kevin.....15-MO
Beavers, Christine.....02.03.02
Beavers, Christine.....05.07.07
Bejagam, Shabarinath.....114-SA
Belnap, David.....03.06.01
Benedict, Jason.....AW.02.01
Benning, Matthew.....91-MO
Berman, Helen M.....85-SA
Berman, Lonny.....04.01.02
Bernstein, Herbert J.....01.05.02.05
Bhat, Talapady.....19-SA
Bhatt, Avni.....14-SU
Bianchet, Mario A.....03.03.02
Bianchetti, Christopher.....22-SU
Bilan, Hubert.....24-SU
Bish, David.....05.01.04
Blanchard, Helen.....03.01.02.04
Bodenheimer, Annette.....03.03.09
Boggon, Titus.....03.07.01.04
Bond, Marcus.....05.03.02
Borbulevych, Oleg.....03.08.04
Borek, Dominika.....04.05.05
Borkiewicz, Olaf.....21-SU
Bowler, Matthew.....03.05.04
Bowler, Bruce E.....03.07.02.08
Boyle, Paul D.....01.12.04
Brgoch, Jakoah.....05.03.05
Bridges, Craig A.....05.07.02
Britten, Jim.....01.02.04
Brock, Carolyn.....01.05.01.04
Broholm, Collin.....05.04.09
Brookes, Emre.....03.02.02
Brunger, Axel.....AW.01.01
Bryant, Diane.....38-SA
Burley, Stephen K.....111-MO
Burton, Christian.....04.03.04
Bury, Charles.....04.05.03
Calabrese, Matthew.....03.01.02.02
Campana, Charles.....29-MO
Campo, Javier.....05.02.07
Cao, Huibo.....05.02.06
Carmona-Negrón, José.....66-SA
Carter, Charles.....TR.01.08
Carter, Korey.....02.04.01.05
Case, David.....03.02.01
Castaneda, Raul.....02.04.02.04
Chacko, Jobichen.....03.07.01.08
Chan, Benny.....01.03.02
Chandrasekaran, S. N.....TR.01.05
Chapuis, Gervais.....01.10.01
Chaudet, Marcia M.....03.08.07
Chen, Qiujia.....03.07.02.01
Chen, Lin.....TR.01.07
Chen, Yu-Sheng.....05.04.03
Chen, Yang.....163-SA
Chitrakar, Iva.....03.03.04
Choi, Joshua.....04.02.04
Chruszcz, Maksymilian.....03.08.01
Chua, Zhijie.....164-SA
Chun, Sae Hwan.....05.02.01
Clegg, William.....01.12.08
Cohen, Aina.....04.03.01
Cohen, Aina.....04.01.08
Colaneri, Michael.....35-MO
Cole, Jacqueline.....TR.01.03
Coles, Simon.....01.05.01.03
Coles, Simon.....01.09.06
Collins, Brian.....05.08.03
Cook, Lawrence.....36-MO
Cook, Paul.....01.10.03
Coppens, Philip.....TR.01.01
Cox, David E.....05.01.01
Criswell, Angela.....7-MO
Cuypers, Maxime.....154-SA
Dahl, Lawrence.....02.05.04
Đaković Marijana.....02.04.02.03
Damotharan, Prabhu.....39-SA
Dasgupta, Prabal.....45-SU

Davis, Erin 01.05.01.05
Dawe, Louise 01.10.02
Dawe, Louise 02.03.04
Day, Graeme 02.04.02.06
Degen, Thomas 05.01.07
Del Campo, Mark 87-SU
DeLongchamp, Dean 05.08.06
Demeshkina, Natalia 144-MO
DePue, Lauren 01.09.07
Deutsch, Benjamin 146-SU
Devedjiev, Yancho 55-SA
Dharmarwardana, M. 01.04.01
Diaz de Delgado, Graciela 01.09.02
Dickmanns, Achim 03.03.07
Doan-Nguyen, Vicky 01.04.03
Dolgos, Michelle 05.03.01
Donakowski, Martin 02.06.05
Duax, William 01.05.02.09
Dubin, Grzegorz 48-SU
Dyda, Fred 03.04.05
El-Ayle, Gracia 02.04.01.07
Emge, Thomas 01.11.01.11
Encerrado M., A. J. 149-SU
Espes, Emil 01.05.01.06
Evans, Gwyndaf 04.03.02
Fabian, Laszlo 02.02.05
Falvello, Larry R. 01.12.07
Falvello, Larry R. 01.10.04
Fan, Lixin 77-MO
Ferre-D'Amare, Adrian 03.05.01
Ficner, Ralf 03.07.01.06
Finke, Aaron 02.03.01
Finke, Aaron 04.03.06
Forster, Paul 02.02.02
Foster, James 75-SA
Foxman, Bruce 01.10.06
Fraser, Marie 44-SA
Fredrickson, Danny 02.02.07
Fronczek, Frank R. 43-MO
Fu, Zheng-Qing (Albert) 01.05.02.04
Fullagar, Wilfred TR.01.10
Gabale, Uma 125-SU
Gallagher, Travis 46-MO
Garlea, Ovidiu 05.02.05
Garman, Elspeth AW.04.01
Garman, Elspeth 03.05.07
Gembicky, Milan 01.02.05
Gerlits, Oksana 47-MO
Ghose, Sanjit 05.01.02
Gianopoulos, Christopher 30-SA
Gillilan, Richard 03.02.04
Giulianotti, Marc 01.02.02
Glover, Karen 70-SU
Goldman, Adrian TR.01.02
Gonen, Tamir 03.06.04
Gonzalez-Osorio, Liliana 109-SU
Graf, Juergen 01.05.02.03
Gray, Danielle 02.03.03
Groom, Colin 03.01.02.07
Gualtieri, Ellen 152-SA
Gualtieri, Ellen 143-SU
Guimaraes, Nara 95-SA
Guo, Hongyu 05.08.02
Haberl, Bianca 05.04.05
Hackert, Marvin 82-MO
Hagen, Karl 01.09.08
Hall, Victoria 02.04.01.03
Handing, Katarzyna 01.04.07
Harada, Ayaka 3-SA
Hasegawa, Kazuya 04.05.06
Hatcher, Lauren 02.02.01
Hattne, Johan 04.05.02
Hayes, Robert 157-MO
He, Bob 01.02.01
He, Bob 05.04.04
Helgeson, Matthew 05.09.01
Herman, TIm 01.03.01
Hikita, Masahide 49-SA
Hintze, Bradley 01.04.05
Hintze, Bradley 01.03.03
Hoare, Peter 01.10.07
Holton, James 04.03.07
Holton, James 04.01.06
Hopkins, Jesse 03.02.05
Horvath, Martin 88-MO
Horvath, Martin 03.07.02.07
Hou, Shulin 51-SA
Hsiao, Chwan-Deng 150-SA
Hu, Chunhua 02.05.08
Hu, Jinhong 52-SU
Hughes, John 02.01.01
Huq, Ashifa 05.01.03
Hwang, Youngha 03.02.03
Ibers, Jim 01.12.06
Ilavsky, Jan 69-SU
Imseng, Stefan 03.04.01
Irving, Thomas 57-MO
Jackson, Ryan 03.06.03

Presenting Author Index

Jackson, Ryan 103-SU
Jakoncic, Jean 01.05.02.01
Jiang, Zhang 04.02.02
Jiang, Qiu-Xing 03.06.06
Jimah, John 03.07.01.07
Jin, Shiyun 02.01.05
Johnston, Dean 01.10.05
Jones, Christopher 03.07.02.04
Juers, Douglas 01.05.01.02
Juers, Douglas 68-MO
Juhas, Pavol 05.09.05
Khorasani, Sanaz 02.05.05
Kiefer, Jim 03.01.02.03
Kim, Hyunjeong 05.07.04
Kintzer, Alexander 03.07.01.05
Klein, Daniel 03.01.01.04
Knope, Karah 02.02.03
Koch, Elizabeth 02.05.01
Kovalevsky, Andrey 03.08.03
Kovalevsky, Andrey 129-SU
Kratzert, Daniel 01.11.01.10
Krogstad, Matthew 02.06.04
Krueger, Susan 03.03.03
Labiuk, Shaunivan 115-MO
Langan, Paul 04.01.01
Langan, Paul 05.06.01
Langkilde, Annette Eva 03.03.06
Lapidus, Saul 05.01.05
Larson, Amber 05.02.08
Lathe, Christian 31-SU
Lebedev, Andrey 6-SA
Lechtenberg, Bernhard 03.08.08
Leissing, Thomas 123-SA
Lhermitte, Julien 05.04.07
Lidin, Sven 05.03.03
Liu, Yaohua 02.06.06
Liu, Jinsong 76-MO
Lively, Jason 02.01.06
Lomelino, Carrie 34-SU
Lountos, George 03.01.01.05
Luebben, Jens 63-SU
Luebben, Anna V. 01.05.02.08
Luebben, Jens 01.11.01.09
Luo, Zhipu 81-SA
Luo, Zhipu 80-SA
Lyubimov, Artem 04.03.03
Ma, Weikang 05.06.02
Madhurapantula, R. S 05.06.04
Maejima, Naoyuki 83-MO
Maize, Kimberly 01.04.06
Marks, Samuel 113-SA
Marschilok, Amy 05.07.01
Martin, Andreas 03.04.03
Martin Garcia, J. M. 04.01.05
Martinez, Israel 59-SU
Mast, Daniel 05.03.06
Mathews, Irimpan 05.04.02
Mayclin, Stephen 158-MO
McCormick, Laura 74-SA
McKenna, Robert 03.06.02
Mehmood, Arshad 01.04.04
Mercado, Brandon 02.05.03
Meyer, Mathias 01.12.03
Miller, Maria 86-MO
Mitchell, Joshua 93-MO
Mitchson, Gavin 01.04.02
Montemayor, Eric 03.07.02.06
Mooers, Blaine 23-SA
Morales, Alina 155-SU
Morales, Yalemi 03.07.02.03
Moreau, David 03.05.05
Mousa, Jarrod 62-SA
Mueller, Marcus 01.05.01.07
Müller, Peter 01.11.01.08
Mullins, Elwood 03.08.05
Murray, Akilah 03.01.02.05
Nan, Jie 65-MO
Nanao, Max 92-SA
Nass, Karol 04.05.01
Nazarenko, Alexander 01.09.03
Nazarenko, Alexander 96-MO
Neilson, James 02.06.01
Neilson, James 05.07.05
Neilson, James 05.04.08
Newman, Janet 03.05.03
Ng, Joseph 05.04.01
Noll, Bruce C. 26-MO
Nuemket, Nipawan 98-SU
O'Bannon, Earl 02.01.02
O'Dell, William B. 03.08.06
Ohi, Melanie 03.04.02
Ojala, William 162-MO
Olmos, Jose 01.04.08
Orgel, Joe 05.06.03
Orth, Peter 03.01.01.03
Otwinowski, Zbyszek 138-SA
Pande, Kanupriya 56-SU
Park, Sulgiye 118-SU

Parkhurst, James 61-SU
Pearce, Nicholas TR.01.09
Pearson, Wayne 131-SU
Peat, Thomas.....01.05.02.10
Perry, Sarah TR.01.11
Pinard, Melissa 84-SU
Podust, Larissa 79-MO
Popov, Dmitry.....05.07.08
Powers, Rachel 01.09.01
Pyrch, Mikaela.....02.02.06
Qasim Saleh, Kifah 04.02.05
Qian, Shuo.....03.03.01
Rae, A. David.....01.11.01.03
Rahighi, Simin 116-SA
Rajkovic, Ivan 102-MO
Ralston, Corie 04.01.03
Ramsey, Lance.....153-SU
Ramsey, Lance.....148-SA
Ratcliff, William 01.11.01.02
Rath, Nigam 108-SU
Reinheimer, Eric 42-SU
Reiss, Céleste 05.09.06
Reutzel-Edens, Susan.....02.04.02.05
Ridenour, August 151-SU
Robart, Aaron.....9-SA
Rodriguez-Perez, Josiris.....67-SA
Rose, John P. 01.12.01
Ruf, Michael 01.05.01.08
Salazar, Adam 58-SA
Samanta, Soumya 03.01.01.07
Sammito, Massimo D. 89-SA
Sanschagrin, Paul 01.02.03
Sanschagrin, Paul 02.03.05
Sarjeant, Amy 01.12.10
Sarjeant, Amy 01.10.08
Satyshur, Kenneth.....156-SA
Sauter, Nicholas 99-SA
Schlachter, Caleb 112-SU
Schmidt, Marius TR.01.06
Schnicker, Nicholas 97-SA
Schultz, Arthur J. 4-MO
Schulze-Briese, Clemens 33-MO
Schwalbe, Carl.....01.11.01.12
Schwalbe, Carl.....02.02.04
Senda, Miki 03.05.06
Senda, Toshiya 03.07.01.02
Seshadri, Serena.....117-SA
Sevryugina, Yulia.....134-SU
Shaw Stewart, Patrick 03.05.02
Sheldrick, George M. 01.11.01.14
Shi, Wuxian.....132-MO
Shoemaker, Daniel 05.07.03
Simmons, Chad 28-SU
Simonet, Virginie.....05.02.02
Simonov, Arkadiy.....02.06.03
Simpson, Garth J. 04.05.04
Singh, Rajendra 101-SU
Sinha, Sangita 05.09.02
Skordalakes, Emmanuel 03.04.06
Slebodnick, Carla 01.12.09
Smedley, John 04.02.06
Smilgies, Detlef-M. 04.02.01
Smith, Stacey 01.02.06
Smith, Myron.....94-MO
Soghomonian, Victoria.....02.02.08
Solomos, Marina 02.05.06
Somasundaram, T. 01.05.02.06
Sonmez, Cem.....27-SA
Spek, Anthony 01.11.01.13
Stagno, Jason 03.07.02.05
Stanek, Kimberly.....03.07.02.02
Stanfield, Robyn 106-MO
Staples, Richard 01.09.04
Stevens, Lauren 159-SU
Stewart, Charles.....37-MO
Stoll, Vincent.....03.01.01.02
Stone, Kevin.....05.08.05
Sullivan, Brendan 05.06.06
Sun, Yuh-Ju 135-MO
Surbella III, Robert 105-SU
Swift, Jennifer.....02.04.02.01
Szebenyi, Marian.....40-MO
Szelazek, Bozena.....16-SA
Taddei, Keith.....02.05.02
Tanner, Jack.....120-MO
Tanski, Joe.....01.09.05
Taylor, Alex.....122-MO
Taylor, Daniel D. 05.07.06
Teeter, Martha 03.03.08
Tennant, David A.....05.02.03
Terwilliger, Thomas 01.11.01.05
Thaw, Paul.....100-MO
Thorne, Robert.....04.03.05
Thorne, Robert.....104-SA
Timofeeva, Tatiana V.....124-MO
Tinsley, Ian 54-SU
Tomchick, Diana R.....03.07.01.03
Tomchick, Diana R.....01.11.01.06

Presenting Author Index

Torres, Miguel....90-SA
Tsang, Arthur....10-SU
Udovic, Boris....147-MO
Urban, Volker....05.08.01
Ursby, Thomas....04.01.04
Valencia, Bianca....20-SU
Vance, Nicholas....03.03.05
Varghese, Juby....127-SA
Vazquez-Molina, D....128-SU
Venkatakrishnan, B....02.04.01.06
Venugopalan, Nagarajan....130-MO
Vey, Jessica....64-MO
Vinokur, Stacy....02.05.07
Vitali, Jacqueline....60-MO
Von Dreele, Robert....01.12.02
Wan, Li....126-SA
Wandtke, Claudia M....01.11.01.04
Wang, Zhenqiang (Rick)....02.04.01.04
Wang, Jing....03.01.02.01
Wang, Bi-Cheng....01.05.02.02
Wang, Xiaoping....01.12.05
Ward, Suzanna....05.01.08
Waterman, David....04.01.07
Wei, Jia....03.04.04
Weiss, Thomas....05.09.03
Welberry, Thomas R....02.06.02
Westerhoff, Lance....03.01.02.06
Wheeler, Kraig....02.04.02.02
Wiaderek, Kamila....72-MO
Wilkinson, Angus....05.01.06
Williams, Christopher....32-SU
Wood, Pete....02.05.09
Xiang, Song....119-SA
Xu, Tingting....133-SA
Xu, Hongwu....02.01.04
Yager, Kevin....04.02.03
Yakovenko, Andrey....145-MO
Yamada, Taro....121-SU
Ye, Sheng....03.01.01.06
Yoon, Tae-Sung....136-MO
York, Joseph....01.08.01
Young, Linda....TR.01.04
Zardecki, Christine....139-SU
Zhao, Rui....107-SA
Zheng, Shao-Liang....01.05.01.03
Zhou, Weijie....161-SA
Zhou, Dongwen....41-SA
Zhu, Yun....141-SA
Zhu, Chenhui....05.08.04
Zuo, Xiaobing....05.04.06

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About the ACA

The American Crystallographic Association, Inc. (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 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 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 have 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. ACA is a member society of the American Institute of Physics (AIP) and an Regional Associate Member of the International Union of Crystallography.

The total international membership of ACA is about 1,000 with meetings held annually. There are 12 Scientific Interest Groups (SIGs) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Light Sources, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, and Young Scientists. A special division for members residing in Canada is also active. 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.

MARK YOUR CALENDAR

Future ACA Meetings:

2017
New Orleans, Louisiana
Friday May 26 - Tuesday May 30

2018
Toronto, Ontario, Canada
Friday July 20 - Tuesday July 24

Program at a Glance

Friday

Morning

WK.02	Computational Approaches to the Structural Modelling of Biological Macromolecules using SAS	GS17
WK.03	Serial Crystallography Data Analysis with Cheetah and CrystFEL	GS16
WK.04	Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques (off site)	Auraria Campus
WK.05	SHELX Workshop - Part A: Sm Mol & Solid State Chemistry	GS15

Afternoon

WK.01	The CSD Python API: A Foundation for Innovation	GS14
WK.02	Computational Approaches to the Structural Modelling of Biological Macromolecules using SAS	GS17
WK.03	Serial Crystallography Data Analysis with Cheetah and CrystFEL	GS16
WK.04	Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques (off site)	Auraria Campus
WK.05	SHELX Workshop - Part B: Macromolecules	GS15

Evening

Student Orientation	**5:30pm**	**PBD**
Opening Reception and Exhibit Show	**7:30pm**	**Plaza Exhibit**

Saturday

Morning

AW.01	Trueblood Award & Lecture - Axel Brunger	PBABC
01.01	Poster Preview	GS14
02.01	Mineralogical Crystallography	PBD
03.01.01	Structure-based Drug Design - I	PBABC
04.01	Opportunities from New and Improved Sources	GS15
05.01	The Next 100 Years of Powder Diffraction	PBEF

Afternoon

Undergraduate Symposium	12:00pm	PBD
Processing SAXS Data with RAW: An Overview and Hands-On Tutorial		GS15
DECTRIS Lunchtime Seminar		GS17
01.02	Using Standard Tools & Methods in Non-standard Ways	GS14
02.02	Structure-Property Relationships	PBABC
03.02	What to do with SAS Data?	GS15
03.03	Hybrid Method Approaches for Structural Biology	PBEF
05.02	Magnetic Entanglement and Complex Magnetic Materials	PBD

Evening

SIG MEETINGS

Industrial	12:00pm	PBABC
Canadian Division	12:00pm	GS14
Biological Macromolecules	5:00pm	PBEF
General Interest	5:00pm	GS14

Poster Session I	**5:30pm**	**Plaza Exhibit**
01.03 Diversity & Inclusion	7:30pm	GS14

Sunday

Morning

AW.02	Etter Early Career Award & Lecture - Jason Benedict	PBEF
TR.01	Transactions Symposium - Structural Dynamics	PBABC
01.04	Etter Early Career Session	PBEF
01.05.01	General Interest - I	GS14
04.02	Surfaces and Interfaces	GS15
05.03	Crystallography in Solid State Chemistry	PBD

Afternoon

Rigaku Lunch & Learn	12:00pm	Majestic Ballroom
CCDC Luncheon	12:00pm	Directors Row H
TR.02	Transactions Symposium - Structural Dynamics	PBABC
01.10	High Impact Crystallographic Education	GS14
03.04	Molecular Machines	PBEF
04.03	Multiple Crystal Techniques	GS15
05.04	Novel Methods for Emerging Science	PBD

Evening

SIG MEETINGS

Light Sources	5:00pm	GS15
Fiber Diffraction	12:00pm	PDB
Joint Materials, Neutron & Powder	12:00pm	GS15
Young Scientists	12:00pm	PBEF

Poster Session II	**5:30pm**	**Plaza Exhibit**
02.03 Would You Publish This?	7:30pm	GS14
Bruker Networking Mixer	8:00pm	Marlowe's Restaurant

Monday

Morning

AW.03	Bau Award and Lecture - Benno Schoenborn	PBABC
01.09	Engaging Undergraduates with Crystallographic Research	GS14
02.04.01	Advances in Supramolecular Chemistry	PBABC
02.05	Cool Structures	GS15
03.05	Crystal Sample Preparation: A crystal is just the start!	PBEF
05.06	Recent Advances in Fiber Diffraction	PBD

Afternoon

01.12	Things We No Longer Need to Know	GS14
02.04.02	Advances in Supramolecular Chemistry	PBABC
03.01.02	Structure-based Drug Design - II	GS15
03.06	Cryo Electron Microscopy and Electron Diffraction	PBEF
05.07	In-situ and En Operando Methods	PBD

Evening

SIG MEETINGS

Joint Service & Small Molecule PBABC	12:00pm	

Business Meeting for all ACA Members	5:00pm	PBEF
Poster Session III	**5:30pm**	**Plaza Exhibit**
01.08 Career Development	7:30pm	GS14

Tuesday

Morning

AW.04	Fankuchen Award and Lecture - Elspeth Garman	PBABC
01.11.01	Standard Practices II: Structure Refinement & Validation	PBABC
02.06	Making Sense of Diffuse Scattering	GS14
03.07.01	Hot Structures - I	GS15
04.05	Radiation Damage	PBEF
05.09	SAS and Integrative Approaches to Complex Structures	PBD

Afternoon

01.05.02	General Interest - II	GS14
01.11.02	Standard Practices II Structure Refinement and Validation	PBABC
03.07.02	Hot Structures - II	GS15
03.08	Structural Enzymology	PBEF
05.08	SAS with Resonant X-rays in Broad Spectrum: Chemistry and Morphology in Complex Soft Materials	PBD

Evening

Annual Awards Banquet — **PBABC**

Cash Bar 6:30pm **Dinner 7:30pm**
(ticket required)

Planning Session for 2017 Meeting in New Orleans
GS14

2016 EXHIBIT SHOW **Plaza Exhibit Foyer**
Friday 7:30pm-10:30pm
Saturday, Sunday, Monday, 10:00am-7:30pm

KEY TO ROOMS

PBABC = Plaza Ballroom A,B,C
PBD = Plaza Ballroom D
PBEF = Plaza Ballroom E,F
GS14 = Governors Square 14
GS15 = Governors Square 15
GS16 = Governors Square 16
GS17 = Governors Square 17
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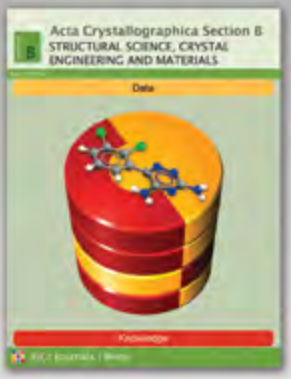

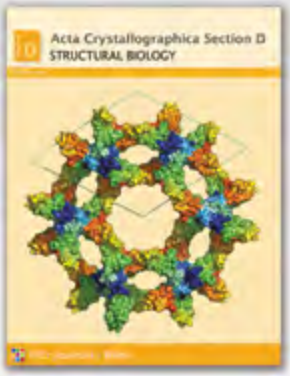

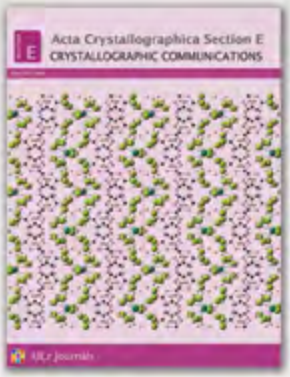

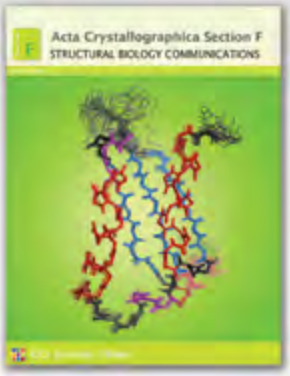

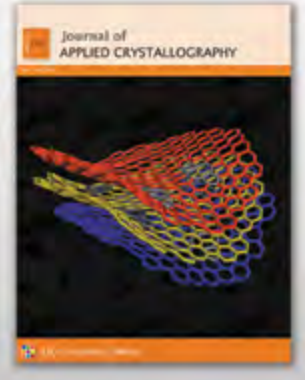

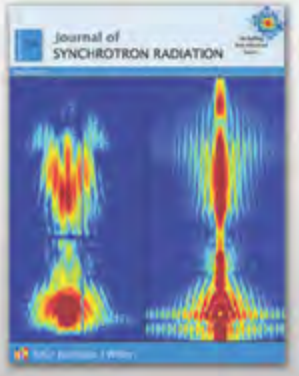

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