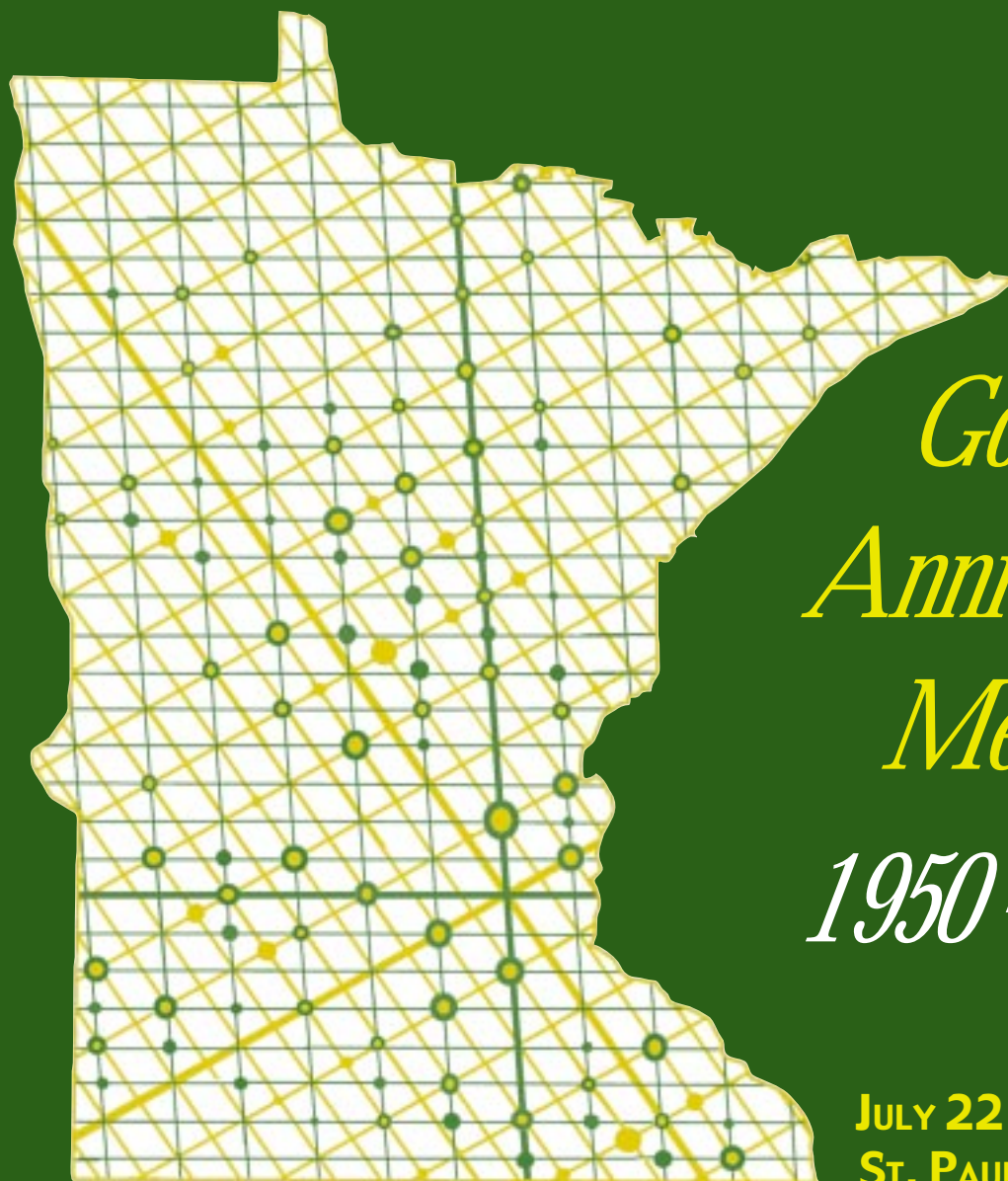


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*Golden
Anniversary
Meeting
1950 - 2000*

**JULY 22 - 27, 2000
ST. PAUL, MINNESOTA**

ACA 2000



**AMERICAN
CRYSTALLOGRAPHIC
ASSOCIATION**

*Golden Anniversary
Meeting*

**JULY 22 - 27, 2000
ST. PAUL, MINNESOTA**

Program Committee

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Doyle Britton
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Contributors

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BioCryst Pharmaceuticals, Inc.
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WK01 SHELX for Twins and Macromolecular Structures

Kellogg Room-Radisson Hotel Chair: George Sheldrick

A. Introduction, phasing etc. Chair: Duncan McRee08:30 - 08:45 George Sheldrick
Historical introduction to SHELX08:45 - 09:10 George Sheldrick
Dual-space *ab initio* direct methods (SHELXD)09:10 - 09:35 Thomas Schneider
MAD phasing09:35 - 10:00 Louis Farrugia
The WinGX user interface

10:00 - 10:20 Discussion

10:20 - 10:35 Coffee Break

B. Structure refinement Chair: Ethan Merritt10:35 - 11:00 Dale Tronrud
Introduction to refinement; solvent model11:00 - 11:20 George Sheldrick
Restraints and constraints11:20 - 11:45 Bill Clegg
Weak data, disorder and other problems in small molecules11:45 - 12:10 Thomas Schneider
Disorder in macromolecules

12:10 - 12:30 Discussion

12:30 - 1:30 Buffet lunch

C. Twinning Chair: Thomas Schneider01:30 - 01:45 Regine Herbst-Irmer
Racemic twinning and the Flack parameter01:45 - 02:10 Regine Herbst-Irmer
Merohedral twins02:10 - 02:35 Victor Young
Non-merohedral twins02:35 - 03:00 Hartmut Luecke
Twinning in proteins and the perils of ignoring it

03:00 - 03:20 Discussion

03:20 - 03:35 Coffee Break

D. Errors, validation and anisotropic refinement Chair: Bill Clegg03:35 - 04:00 Ton Spek
Small-molecule validation04:00 - 04:20 George Sheldrick
Estimation of parameter errors04:20 - 04:45 Ethan Merritt
Anisotropic refinement of macromolecules04:45 - 05:10 Duncan McRee
Validation of error estimates for metalloproteins

05:10 - 05:30 Discussion

WK02 How to Make Technical PresentationsWabasha Room-Radisson Hotel Chair: Eric Chen
08:30 - 12:00

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of oral presentations, this workshop is designed to introduce the art behind a successful technical oral presentation.

The objectives of this workshop are to teach students to:

- Conceive the theme of an oral presentation
- Gauge the audience before the presentation
- Fit the presentation into an allotted time
- Interact with the audience during the presentation
- Answer questions from the audience at the end

This workshop is intended for graduate students in physics and materials science, for scientists and engineers in crystallography, for technical supervisors and managers in corporate America.

WK03 Use and Application of the Cambridge Structural DatabaseWabasha Room-Radisson Hotel Chair: Steve Maginn
01:30-05:30

This 1/2-day workshop is aimed at any researcher who uses the Cambridge Structural Database (CSD) in their work, or indeed at anyone wishing to learn about the CSD. Infrequent users will gain an insight into the full range and power of applications of the CSD, and even more experienced users will discover new ways to approach problems. Presentations on the content and use of the database will be mixed in with demonstrations of the new CSD search software ConQuest and the knowledge-based library IsoStar.

Opening Reception
06:30 - 10:00pm
Science Museum of Minnesota
120 West Kellogg St.

Opening Ceremony

Room A

08:00-08:30 Connie Chidester, President, Presiding

01.01 Battery Materials: Amorphous Carbons and Polymer Electrolytes

Rooms 4,5,6 Chair: Jackie Johnson

08:30-09:15 **01.01.01**

Fundamental NMR Investigations of Conduction Ions in Anode and Electrolyte Materials Using the Near Electrode Imager. Rex E. Gerald, II, Robert J. Klingler, Jerome W. Rathke.

09:15-10:00 **01.01.02**

Thin-Film Techniques for Ceramic Lithium-Ion Batteries. Joop Schoonman.

10:00-10:30 Coffee Break.

10:30-11:15 **01.01.03**

Large Scale Atomistic Simulations of Amorphous Polymers and Ceramic/Polymer Interfaces on Parallel Computers. Priya Vashishta, Rajiv Kalia, Aiichiro Nakano, Satyavani Vemparala, Philip Walsh.

11:15-12:00 **01.01.04**

Novel Electrolyte Materials for Secondary Batteries and Other Electrochemical Devices. Doug MacFarlane.

12:00-01:30 Lunch Break.

01:30-02:00 **01.01.05**

Crystallographic Studies of Lead-Acid Battery Materials. Joseph Pluth, Ian Steele.

02:00-02:45 **01.01.06**

Electrolytes with High Cation Transport Number and Conductivity for Lithium Battery Applications. Austin Angell, Giaoguang Sun, Marcello Videa, Wu Xu.

02:45-03:30 **01.01.07**

Solid State NMR Studies of Ion Transport Mechanisms in Semicrystalline and Amorphous Polymer Electrolytes. Steve Greenbaum, Song Ho Chung, Yifeng Wang, Dina Golodnitsky, Emanuel Peled, Luigi Persi, Bruno Scrosati.

03:30-04:00 Coffee Break.

04:00-04:45 **01.01.08**

Using Crystallography to Understand Polymer Electrolytes. Yuri G. Andreev, Peter G. Bruce.

04:45-05:30 **01.01.09**

Neutron Scattering Studies of the Structure and Dynamics of Carbon Anode Materials. Peter Papanek.

05:30-06:00 **Amorphous Materials SIG Meeting**

02.01 Hot New Structures

Room A

Chair: Cele Abad-Zapatero

08:30-08:32

Opening Remarks. Cele Abad-Zapatero.

08:32-08:54

02.01.01

Hypothetical Proteins from Haemophilus Influenzae: Two New Structures Implying Methyltransferase Function. Kap Lim, Hong Zhang, Alexandra Tempczyk, Nicklas Bonander, John Toedt, Andrew Howard, Edward Eisenstein, Osnat Herzberg.

08:54-09:16

02.01.02

"Purple" Lipoxygenase - X-Ray Analysis of Complexes with Three Different Peroxides. Ewa Skrzypczak-Jankun, P.A. Brault, R. Bross, M.O. Funk, N.P. McCabe, J. Jankun.

09:16-09:38

02.01.03

Crystal Structure of Glucose-6-Phosphate Isomerase from *Bacillus stearothermophilus* at 1.93Å Resolution. J. K. Mohana Rao, N. Nandhagopal, Alexander Wlodawer.

09:38-10:00

02.01.04

Three Dimensional Structure of an Ig-like NK Cell Receptor in Complex with a Class I MHC Ligand. Jeffrey Boyington, Shawn Motyka, Andrew Brooks, Peter Sun.

10:00-10:30

Coffee Break.

10:30-10:52

02.01.05

The Mitochondrial Transcription Factor sc-mtFB Structure Offers Insights into Mitochondrial Transcription. Florian D. Schubot, Chun-Jung Chen, John P. Rose, Bi-Cheng Wang.

10:52-11:14

02.01.06

The Anti-Hypertensive ANP Receptor Binding Domain Structure Reveals Dual Allosteric Control. Focco Van Den Akker, Xiulun Zhang, Masaru Miyagi, Zuewen Huo, Kunio S. Misono, Vivien C. Yee.

11:14-11:36

02.01.07

A Purine Biosynthesis Bifunctional Enzyme at 1.75Å Resolution: A Target for Anti-Cancer Therapy. Samantha E. Greasley, Dennis Wolan, Patricia Horton, Stephen J. Benkovic, G. Peter Beardsley, Ian A. Wilson.

11:36-11:58

02.01.08

The Asymmetric Nucleosome. Joel Harp, B. Leif Hanson, David Timm, Gerard Bunick.

02.02 Ultra-High Resolution Macromolecular Crystallography

Room B

Chair: Paula Fitzgerald

08:30-08:35

Opening Remarks. Paula Fitzgerald.

08:35-09:00

02.02.01

Strategies for Collecting and Processing Extremely High Resolution Macromolecular Diffraction Data. Peter Kuhn, S. Michael Soltis.

09:00-09:30

02.02.02

Resolving Mechanistic Issues in Serine Proteases Using <1.0 Å Crystallographic Data. Richard Bott, Grant Ganshaw, Mike Soltis, Peter Kuhn, Mark Knapp.

09:30-10:00

02.02.03

The 1.2Å High Resolution Crystal Structure Unveils How Bacteria Form Crosslinks in Their Peptidoglycan Cell Wall. Michael A. McDonough, Wenlin Lee, Lakshmi Kotra, Zhi-Hong Lee, Yoshifumi Takeda, Shahriar Mobashery, Judith A. Kelly.

10:00-10:30 Coffee Break.

10:30-11:00 **02.02.04**
Crystal Structure Studies of Chorismate Lyase from *E. coli*. Travis Gallagher, Carrie Stover, Martin Mayhew, Marcia Holden.

11:00-11:30 **02.02.05**
Insights Into the Mechanism of an Aldolase Enzyme Determined at Ultra-High Resolution. Andreas Heine, John Luz, Grace DeSantis, Chi-Huey Wong, Ian Wilson.

11:30-12:00 **02.02.06**
Ultra-High Resolution Studies of Human Carbonic Anhydrase Inhibitor Complexes. Craig A. Behnke, Isolde Le Trong, Jeff Godden, Jürgen Bajorath,

08.01 Advances in Small Angle Scattering Instrumentation and Data Analysis

Rooms 2,3 Chair: Harry Brumberger

08:30-09:00 **08.01.01**
Near Surface Small Angle Neutron Scattering: Techniques and Applications. Paul Butler, William Hamilton.

09:00-09:30 **08.01.06**
Neutron Scattering Instrumentation Upgrades at the Oak Ridge High Flux Isotope Reactor. Gerard J. Bunick, George D. Wignall.

09:30-10:00 **08.01.03**
Evaluation of Small-Angle Scattering Data from Interacting Systems. Otto Glatter, Gerhard Fritz, Alexander Bergmann.

10:00-10:30 Coffee Break.

10:30-11:00 **08.01.04**
SAS Data Analysis: The State of the Art. Dmitri Svergun.

11:00-11:30 **08.01.05**
The Neutron Bonse-Hart Diffractometer for USANS at NIST. John Barker, Charles Glinka.

11:30-12:00 **08.01.02**
Quantitative Characterization of Multicomponent Microstructures with Anomalous Small-Angle Scattering. Pete R. Jemian.

Poster Preview I

Rooms 4,5,6 Chair: Jeff Habel

12:00-12:05 **P010**
Powder Diffraction Analysis of $\text{Sr}_2\text{AlTaO}_6$, $\text{Sr}_{2-x}\text{Al}_{1-x}\text{Ta}_{1+x}\text{O}_6$ and $\text{Sr}_2\text{Al}_{1-x}\text{Ta}_{1+x}\text{O}_{6-2x}\text{F}_{2x}$ ($x=0.01-0.10$): An Attempt to Control the Antiphase Boundary Concentration. Paris Barnes, Patrick M. Woodward.

12:05-12:10 **P022**
Mutational Dominance and Cooperativity in Aldehyde Dehydrogenase. Heather Breen, Thomas Hurley.

12:10-12:15 **P055**
Crystal Structure of D-Lactate Dehydrogenase; A Membrane-Associated Respiratory Enzyme. Orly Dym, Ann Pratt, Chien Ho, David Eisenberg.

12:15-12:20 **P106**
Beta-Carbonic Anhydrase Active Site Architecture is a Mirror Image of that of Alpha-Carbonic Anhydrases. Mathew S. Kimber, Emil F. Pai.

12:20-12:25 **P115**
1,2,3,4,4A,12A-Hexahydro-5,5-Dimethyl-1-H-[2] Benzopyrano[3,2-C]Coumarin. Ramodasan Krishna, Devadasan Velmurugan, Shanmuga Sundara Raj, Hoog Kun Fun, Shanmuga Sundaram, Nathan Raghu, S.Narasinga Rao.

12:25-12:30 **P121**
Peculiarities of Anomalous Behavior of PMN Crystal Atoms in the Temperature Region of 183-203 K. Alla R. Lebedinskaya, Mikhail F. Kupriyanov.

12:30-12:35 **P133**
The Prediction of the Crystal Structures of Perovskites Using the Software Program SPuDS. Michael Lufaso, Patrick Woodward.

12:35-12:40 **P148**
Understanding the Rules of Protein: RNA Interactions. Jeffrey Myers, James Allers, Yousif Shamoo.

12:40-12:45 **P166**
Probing the Local Structure of Doped Manganites Using the Atomic Pair Distribution Function. Thomas Proffen, Simon Billinge, Valeri Petkov.

12:45-12:50 **P196**
High Resolution Crystal Structure of Isocitrate Dehydrogenase from *Bacillus subtilis*. Satinder K. Singh, David C. LaPorte, Leonard J. Banaszak.

12:50-12:55 **P208**
Polymorphous Crystallization and Diffraction of Chorismate Lyase from *E. coli*. Carrie Stover, Martin P. Mayhew, Marcia J. Holden, D. Travis Gallagher.

12:55-01:00 **P229**
Crystal Structure Analysis of 6H,6Ah,7H,12Bh,13H-Bis[1] Benzopyrano[4,3-B:4'3' D]Pyran-13-One. Devadasan Velmurugan, Ramodasan Krishna, S.Narasinga Rao, S. Shanmuga Sundara Raj, Hoog Kun Fun, M. Shanmuga Sundaram, R. Raghunathan.

04.01 General Interest I

Room B Chair: Lieselotte Templeton

01:30-02:00 **04.01.01**
Crystallographic Groupoids: Past, Present, and Future. Carroll K. Johnson.

02:00-02:30 **04.01.02**
A Two-Spring Model of Chemical Bonding. I.D. Brown.

02:30-03:00 **04.01.03**
A New Class of Conducting Solids: Phenalenyl-Based Neutral Radicals as Intrinsic Molecular Metals. Wally Cordes, T. M. Barclay, R. C. Haddon, X. Chi, M. E. Itkris, A. A. Pinkerton, R. T. Oakley, Kristin Kirschbaum.

03:00-03:30 **04.01.04**
Erc₂N@C80 and a Progress Report on the Crystal Structures of Endohedral Fullerenes. Marilyn Olmstead, Alan Balch, Ana Bettencourt-Dias.

03:30-04:00 Coffee Break.

04:00-04:30 **04.01.05**
Packing of 1:1 Tert-Butylcalix[4]arene Inclusion Compounds. Gary Enright, Eric Brouwer, Chris Ratcliffe, John Ripmeester, Kostia Udachin.

04:30-05:00 **04.01.06**
Generalizations Drawn from a Collection of Crystals Having Z' > 1. Carolyn P. Brock, Brian O. Patrick.

05:00-05:30 **04.01.07**
Disorder - A Crystallographic Enigma. Judith L. Flippen-Anderson, Jeffrey R. Deschamps, Richard D. Gilardi, Clifford George.

08.02 Materials Structure at Long Length Scales: Recent Discoveries

Rooms 2,3 Chair: Thomas Rieker

01:30-02:00 **08.02.01**
Assessing Orientation Texture in Small-Angle Scattering. John D. Barnes.

02:00-02:30 **08.02.02**
Real-Time Ultra-SAXS Studies of "Crazing" in a Rubbery Polymer. J. David Londono, A. Jagota, S. Bennison, R. Davidson.

02:30-03:00 **08.02.03**
Small Angle Neutron Scattering from Ultrathin Polymer Films. Sanat Kumar.

03:00-03:30 **08.02.04**
Polymerization of Rod-Like Micelles. Steven Kline.

03:30-04:00 Coffee Break.

04:00-04:30 **08.02.05**
Small and Wide Angle Scattering of Disc Shaped Surfactant Aggregates. B. Deme, M. Dubois, Th. Gulik-Kryzwicki, Th. Zemb.

04:30-05:00 **08.02.06**
Synchrotron Small-Angle X-Ray Scattering Studies of Tertiary RNA Folding. Pappannan Thiagarajan, Xingwang Fang, Kenneth Littrell, Soenke Seifert, Xiao-jing Yang, Stephen Henderson, Tao Pan, Tobin Sosnick.

05:00-05:30 **08.02.07**
Anisotropic USAXS and SANS Studies of Microcracking in Textured Ceramic Materials. Andrew J. Allen, Edwin R. Fuller Jr., Gabrielle G. Long, Jan Ilavsky, Pete R. Jemian.

05:30-06:00 **Small Angle Scattering SIG Meeting**

02.03 Drug Design

Room A Chairs: William Stallings & Bruce Jacobson

01:30-02:00 **02.03.01**
Structure-based Design and Structural Genomics in Drug Discovery. Patricia C. Weber, Michael Cable, Thierry Fischmann, Alan Hruza, Charles Lesburg, Andrew Prongay, Paul Reichert, Corey Strickland, Shane Taremi, William Windsor, Zhen Wu, Nanhua Yao.

02:00-02:30 **02.03.02**
Rational Design of Electrophilic Diazeniumdiolates for Pharmacologic Delivery of Nitric Oxide. Xinhua Ji, Aloka Srinivasan, Joseph E. Saavedra, Larry K. Keefer, Ajai Pal, Xun Hu, Shivendra V. Singh.

02:30-03:00 **02.03.03**
Human Liver Glycogen Phosphorylase Inhibitors Bind at a New Allosteric Site. Virginia Rath, Mark Ammirati, Dennis Danley, Jennifer Ekstrom, Michael Gibbs, Thomas Hynes, Kirk McPherson, Thanh Olson, Judith Treadway, Dennis Hoover.

03:00-03:30 **02.03.04**
Structurally-Biased Combinatorial Design of Antivirals. James Hogle.

03:30-04:00 Coffee Break.

04:00-04:30 **02.03.05**
Structure Assisted Design of Human Rhinovirus 3C Protease Inhibitors. D.A. Matthews, P.S. Dragovich, S.E. Webber, S.A. Fuhrman, A.K. Patick, T.J. Prins, J.T. Marakovits, J.W. Meador, R.A. Ferre, S.T. Worland.

04:30-05:00 **02.03.06**
Design of Transthyretin Amyloid Inhibitor. James C. Sacchetti, Thomas Klabunde, H. Michael Petrassi, Craig Smith, Hans Purkey, Jeffery W. Kelly.

05:00-05:30 **02.03.07**
CrystalLEAD™: A Method for Discovering Novel Lead Compounds Using X-Ray Crystallography as a Screen Tool. Vicki Nienaber, Paul Richardson, Vered Klinghofer, Jennifer Bouska, Vincent Giranda, Jonathan Greer.

05:30-06:00 **Bio Mac SIG Meeting**

Exhibit Show	10:00-07:30	Exhibit Hall A
MSC User Lunch	12:00	Rooms 7,8
CCDC User Meeting	12:00	Room 9
Bio Mac SIG Meeting	05:30	Room A
Small Molecule SIG Meeting	05:30	Room B
Amorphous Materials SIG Meeting	05:30	Rooms 4,5,6
Small Angle Scattering SIG Meeting	05:30	Rooms 2,3
Poster Session I	05:30-07:30	Exhibit Hall A
Mentor/Mentee Dinner	07:30	Radisson Lobby
Service Crystallography & Small Molecule SIG Dinner	07:30	Radisson Lobby
MSC Fun Run	07:30	

**TR.00 Transactions Symposium:
Using Crystallography to Understand
Enzyme Mechanism**

Rooms A,B Chair: Douglas Ohlendorf

08:30-09:00 **TR.00.01**
The Control of Cofactor Chemistry by Protein Structure. Dagmar Ringe.

09:00-09:30 **TR.00.02**
Structural Pathway of Metal-Dependent Phosphoryl Transfer in the Active Site of EcoRV Endonuclease. John Perona, Nancy Horton, My Sam, Bernard Connolly.

09:30-10:00 **TR.00.03**
Three TrpRS Conformations Stabilize a Dynamic, Dissociative Transition-State. Charles W. Carter, Jr., Valya Ilyin, Yuhui Yin, Pascal Retailleau, Xin Huang.

10:00-10:30 Coffee Break.

10:30-11:00 **TR.00.04**
Enzymatic Decarboxylation. Steven E. Ealick.

11:00-11:30 **TR.00.05**
The Structure and Mechanism of Beta-Lactamase. Osnat Herzberg.

11:30-12:00 **TR.00.06**
The Structure and Mechanism of MJ0109 Gene Product - A Bifunctional Enzyme from *M. jannaschii*. Boguslaw Stec, Kenneth A. Johnson, Hongying Yang, Liangjing Chen, Mary F. Roberts.

12:00-02:00 Lunch Break.

Chair: Dagmar Ringe

02:00-02:30 **TR.00.07**
Biomimetic Approaches for Understanding Metalloenzyme Mechanisms. Lawrence Que.

02:30-03:00 **TR.00.08**
Structural Studies of Acinetobacter Strain ADP1 Protocatechuate 3,4-Dioxygenase at 2.2Å Resolution. Douglas H. Ohlendorf, Matthew W. Vetting, David A. D'Argenio, L. Nicholas Ornston.

03:00-03:30 **TR.00.09**
Structural Studies on the Mechanism of 2-Oxoglutarate Oxygenases. Christopher J. Schofield, Jack E. Baldwin, Ian Clifton, Karl Harlos, Li Ching Hsueh, Matthew D. Lloyd, Colin Mckinnon, Jingshan Ren, David K. Stammers, Zhihong Zhang.

03:30-04:00 Coffee Break.

04:00-04:30 **TR.00.10**
Arginase, a Manganese Metalloenzyme Implicated in Erectile Dysfunction. David Christianson.

04:30-05:00 **TR.00.11**
A Twelve Year Journey Towards Identifying the Catalytic Base in UDP-Galactose 4-Epimerase. Hazel M. Holden.

05:00-05:30 **TR.00.12**
Inactive Enzyme in Catalytically Active Crystal? A Case Study of Glycerol Phosphorylation by Glycerol Kinase. Chen Mao, Ozer Zahide, Min Zhou, Fatih Uckun.

05:30 ACA Business Meeting

Rooms A,B

05.01 New Science Using New Neutron Sources and Instruments

Rooms 2,3 Chair: Brian Toby

08:30-09:00 **05.01.01**
Investigation of Hybrid Bilayer Membranes by Neutron Reflectometry Using Phase Determination and Inversion. C.F. Majkrzak, N.F. Berk, S. Krueger, J.A. Dura, M. Tarek, D. Tobias, V. Silin, C.W. Meuse, J. Woodward, A.L. Plant.

09:00-09:30 **05.01.02**
Hydration of a Single Monolayer of Cytochrome c Vectorially-Oriented at a Soft Interface via Neutron Interferometry. Kent Blasie, Larry Kneller, Ann Edwards, Erik Nordgren, Norman Berk, Susan Krueger, Charles Majkrzak.

09:30-10:00 **05.01.03**
Leveraging Information from Small-Angle Scattering for Structural Studies of Biomolecular Interactions. Jill Trehwella.

10:00-10:30 Coffee Break.

10:30-11:00 **05.01.04**
Phase Transitions and Phase Segregation in $(A_{0.5}Ln_{0.5})MnO_3$ (A = Sr, Ca; Ln = Lanthanide ion) and $(Ca_{1-x}Bi_x)MnO_3$ Perovskites. Patrick Woodward, P. N. Santhosh, Joshua Goldberger, Tom Vogt.

11:00-11:25 **05.01.05**
Crystal Structures in the Perovskite Series $Sr_nFe_nO_{3n-1}$ ($n = 2, 4, 8, \text{ and } \infty$). Jason Hodges, James Jorgensen, X. Xiong, Bogdan Dabrowski.

11:25-11:50 **05.01.06**
Neutron Crystallography of the Amblygonite $(LiAlPO_4F)$ - Montebasite $(LiAlPO_4OH)$ Solid Solution. Bryan Chakoumakos, Lee Groat.

11:50 - 12:00 P122
Temperature- and Humidity-Dependent Cation Relocation in Zeolites: Pb-RHO. Yongjae Lee, Glover A. Jones, Jonathan Hanson, Andrea Freitag, John B. Parise, John Z. Larese, David R. Corbin, Volker Kahlenberg.

12:00-2:00 Lunch Break.

12:00 **Neutron Scattering SIG Meeting**

Chair: Bryan Chakoumakos

02:00-02:30 **05.01.07**
Inelastic Neutron Scattering: A Versatile Probe of Dynamics. Dan Neumann.

02:30-03:00 **05.01.08**
Combined Neutron Scattering and First-Principles Studies of Novel Solids. Taner Yildirim.

03:00-03:30 **05.01.09**
Solving Impurity Structures Using Inelastic Neutron Scattering. Collin Broholm.

03:30-04:00 Coffee Break.

04:00-04:30 **05.01.10**
The Local Structure-Function Relationship in Partially Ordered Materials: The Essential Role of Neutrons. Simon J. L. Billinge.

04:30-05:00 **05.01.11**
The Determination of the Structure of Solutes by Neutron Diffraction with Isotopic Substitution. John F. C. Turner, Alan Soper.

05:00-05:30 Moderated Discussion: Diffraction Instrumentation at the Spallation Neutron Source.

09.01 Cool Structures

Rooms 4,5,6 Chair: Curt Haltiwanger

08:30-08:45 **09.01.01**

Hydrogen Bonding Analysis of PETT Derivatives that Inhibit HIV-1 Reverse Transcriptase. Elise A. Sudbeck, Jason D. Jennissen, Taracad K. Venkatachalam, Fatih M. Uckun.

08:45-09:00 **09.01.02**

Unusual Hydrogen Bonding in Quinoline Carboxylic Acid Compounds. Amy Narducci, Gudrun Trescher, Curtis Haltiwanger, Jeffery Axten, Robert Daines, William Kingsbury.

09:00-09:15 **09.01.03**

Strychnine Resolutions of Substituted Mandelic Acids. Robert Gould, Iain Mackay, Malcolm Walkinshaw.

09:15-09:30 **09.01.04**

Octanitrocubane - A Highly Energetic Molecule. Richard Gilardi.

09:30-09:45 **09.01.05**

Between a Rock and a Hard Place: Structural Studies on Two Polymorphs of a Novel Inhibitor of LpPLA₂. Royston C.B. Copley.

09:45-10:00 **09.01.06**

Structural Studies of Glycosylamines. Summer E. Hanson, William H. Ojala, Joanne M. Ostman, Charles R. Ojala.

10:00-10:30 Coffee Break.

10:30-10:45 **09.01.07**

Dimolybdenum Bis(*S,S,S*-triosopropoxyamine). A Blue Compound with an Unusual Mo-Mo Triple Bond. De-Dong Wu, Malcolm Chisholm, John Huffman.

10:45-11:00 **09.01.08**

The Structural Chemistry of NX₄PF₆ (X= H, D). Robert Hammond, Ian Swainson.

11:00-11:15 **09.01.09**

A Novel Organotellurate(IV) - Molecular Analog of Pac-Man? Kristin Kirschbaum, Helene Citeau, Olaf Conrad, Dean Giolando.

11:15-11:30 **09.01.10**

The Devil is in the Details: The Structure Determination of a 5-fold Mercury Substituted Sandwich Complex with Close Hg-Hg van der Waals Contacts and Contamination from a 4-fold Substituted Constituent. Bruce Noll, Thierry Brotin, Gregory Kottas, Josef Michl.

11:30-11:45 **09.01.11**

Amine and Amino Alcohol Complexes of Copper(II) Hexafluoroacetylacetonate, Cu(Hfac)₂, the Sequel. Frank Fronczek, Damon Billodeaux, Zuzanna Cygan, Mona Bufaroosha, Emily Maverick, Andrew Maverick.

11:45-12:00 **09.01.12**

Electrocrystallization and Characterization of the First Doubly Ring-Oxidized Phthalocyanine. Anna Gardberg, Peter Doan, Brian Hoffman, James Ibers.

Poster Preview II

Rooms 4,5,6 Chair: Jeff Habel

12:00-12:05 **P026**

Diffraction Studies of Potexviruses. Christopher Bunick, Greg Ferrell, Amy Kendall, Winston Chapman, Mitzi Reams, Nicholas Fletcher, Lisa Keen, Gerald Stubbs.

12:05-12:10 **P080**

Structural Similarities Between Influenza Matrix Protein M1 and HIV Matrix and Capsid Proteins: An Evolutionary Link Between Negative-Stranded RNA Viruses and Retroviruses. Audray Harris, Ming Luo.

12:10-12:15 **P083**

Control of Transport in Crystal Growth Using Restrictive Geometry Crystallization. Anna Holmes, Liqing Chen, Joseph D. Ng, Edward J. Meehan, Robert J. Naumann

12:15-12:20 **P089**

Perturbations of NADPH-Cytochrome P450 Oxidoreductase: Implications for Pi-Pi Orbital Overlap. Paul Hubbard, Rosemary Paschke, Anna Shen, Charles Kasper, Jung-Ja Kim.

12:20-12:25 **P098**

Crystal Structure of an Engineered Monomeric Form of IL-10 Complexed to an Anti-IL10 Fab. Kristopher Josephson, Brandi Curry, Walter Leigh, Walter Mark.

12:25-12:30 **P122**

Temperature- and Humidity-Dependent Cation Relocation in Zeolites: Pb-RHO. Yongjae Lee, Glover A. Jones, Jonathan Hanson, Andrea Freitag, John B. Parise, John Z. Larese, David R. Corbin, Volker Kahlenberg.

12:30-12:35 **P128**

High Resolution Views of Protein Farnesyltransferase Substrate and Product Complexes. Steve Long, Kimberly Terry, Lorena Beese.

12:35-12:40 **P143**

Reaching 0.66Å Resolution with a 36 kDa Enzymatic Complex. Andre Mitschler, Ruslan Sanishvili, Andrzej Joachimiak, Eduardo Howard, Patrick Barth, Valerie Lamour, Michael Van Zandt, Evelyn Sibley, Dino Moras, Alberto Podjarny.

12:40-12:45 **P152**

Structure-Based Design of Conjugated Styryl Ketones as Candidate Cytotoxic and Anticancer Agents. Eliud O. Oloo, Jonathan R. Dimmock, Maniyan P. Padmanilayam, Lata Prasad, J. Wilson Quail.

12:45-12:50 **P155**

X-Ray Crystal Structure of Two Biphenyl Compounds. A. Subbaiah Pade, Devadasan Velmurugan, S.Narasinga Rao.

12:50-12:55 **P170**

Crystal Structure Analysis of Tetrahydro Chromeno [4',3,3,4] Pyrano [3-2C] Alpha-Naphtho Coumarin. S.Narasinga Rao, Ramodasan Krishna, Kandan Mani, Nathan Raghu.

12:55-01:00 **P206**

Pyruvate Dehydrogenase Kinase: Echo of the Past. Nic Steussy, Melissa Bowker-Kinley, Kirill Popov, Robert A. Harris, Jean Hamilton.

Buerger Award Presentation and Lecture

Rooms A,B Connie Chidester Presiding

01:00-02:00
Then and Now – Reflections of a Mature Discipline. Lyle Jensen.

04.01 General Interest II

Rooms 4,5,6 Chair: Carroll Johnson

02:00-02:30 **04.01.08**
Modern High-Pressure Measurements with a CCD System. Michael Ruf, Eric Hovestreydt, Ludger Häming.

02:30-03:00 **04.01.09**
Using Anomalous Scattering Data in Phases Refinement via Sayre Equations. Jeffrey Roach, Pascal Carter, David Sayre, Charles W. Carter.

03:00-03:30 **04.01.10**
Find Additional Symmetry, Correct Space Groups and Initiate Searches of the CSD Database from XSELL. Robert A. Sparks, Stephen Christian.

03:30-04:00 Coffee Break.

04:00-04:30 **04.01.11**
Non-Merohedral Twins - Experiences with GEMINI and SHELXL. Regine Herbst-Irmer.

04:30-05:00 **04.01.12**
The W.M. Keck Foundation Center for Molecular Structure in the California State University. Katherine Kantardjieff.

05:00-05:30 **04.01.13**
Teaching Diffraction Using Computer Simulations Over the Internet. Thomas Proffen, S. J. L. Billinge, R. B. Neder.

02.04 Protein Nucleic Acid Interactions

Rooms A,B Chair: Cynthia Wolberger

08:30-09:00 **02.04.01**
Unraveling the Mechanism of a Hexameric DNA Helicase. Tom Ellenberger.

09:00-09:30 **02.04.02**
Structural Characterization of a Universally Conserved Protein-RNA Interaction from the Signal Recognition Particle. Robert T. Batey, Robert P. Rambo, Louise J. Lucast, Brian Rha, Jennifer A. Doudna.

09:30-10:00 **02.04.03**
A New RNA-Binding Motif Found in the Structure of Heat Shock Protein-15Kd.. Bart Staker, Philipp Korber, James Bardwell, Mark Saper.

10:00-10:30 Coffee Break.

10:30-11:00 **02.04.04**
DNA-protein Interactions in Mismatch Repair. Wei Yang, Murray Junop, Hon Ling, Changill Ban, Galina Obmolova, Peggy Hsieh.

11:00-11:30 **02.04.05**
The DNA-Binding Domain of the Intron-Encoded Endonuclease I-Tevi Harbors Three Different DNA-Binding Motifs. Patrick Van Roey, Christopher A. Waddling, Kristin M. Fox, Marlene Belfort, Victoria Derbyshire.

11:30-12:00 **02.04.06**
DNA Interactions and Conformational Changes in Type IA DNA Topoisomerases. Alfonso Mondragon, Anita Changela, Hadar Feinberg.

07.01 Service Crystallography at Synchrotrons

Rooms 4,5,6 Chair: James Britten

08:30-09:00 **07.01.01**
Courier-Based Data Collection Extends the Scope of Macromolecular Crystallography at the NSLS. Robert M. Sweet, Michael Becker, John M. Skinner.

09:00-09:30 **07.01.02**
Daresbury Analytical Research & Technology Service. Elizabeth MacLean, John Charnock, Susan Slawson, Richard Strange, Elizabeth Towns-Andrews.

09:30-10:00 **07.01.03**
Service Crystallography at Synchrotrons: Small Molecule Single-Crystal Diffraction. William Clegg.

10:00-10:30 Coffee Break.

10:30-11:00 **07.01.04**
Service Crystallography: Broadening the Impact of the APS. Richard Harlow.

11:00-12:00 **07.01.05**
On the Possibility of a Service Component at the ChemMatCARS Facility at the Advanced Photon Source. James Viccaro, David Cookson, Tim Graber, Joseph Pluth.

Exhibit Show	10:00-07:30	Exhibit Hall A
Neutron Scattering SIG Meeting	12:00	Rooms 2,3
Bruker User Lunch	12:00	Rooms 7,8,9
Poster Session II	05:30-07:30	Exhibit Hall A
ACA Business Meeting	05:30	Rooms A,B
MSC Dinner (by invitation only)	06:30	
Quantum Users Meeting	07:00	Radisson Hotel
YSSIG Mixer	08:00	Great Waters Brewery

03.01 Fibers 2K: Twists and Turns for the New Millennium

- Rooms 2,3 Chairs: Dan Kirschner & Barry Farmer
- 08:30-08:35 Introduction.
- 08:35-09:00 **03.01.01**
2D-X-Ray Diffraction on Single Muscle Fibers: A Tool for Studying the Molecular Mechanism of Muscle Contraction. Theresia Kraft, Thomas Mattei, Ante Radocaj, Christoph Nocula, Bernhard Brenner.
- 09:00-09:30 **03.01.02**
Interesting Biological Things You Can Do with Undulator X-Ray Beams. Tom Irving.
- 09:30-10:00 **03.01.03**
Aspects of Disorder in Fiber Diffraction Analysis. Rick Millane, Jon Eads.
- 10:00-10:30 Coffee Break.
- 10:30-11:00 **03.01.04**
In-situ Investigation of the Spinning Process of Orb-weaving Spiders by X-Ray Diffraction Techniques. Christian Riekel.
- 11:00-11:30 **03.01.05**
High-fidelity, Monodisperse Nylon 6 Oligomers: New Turning and Twisting. Edward Atkins.
- 11:30-12:00 Open Discussion.
- 12:00-01:30 **Fiber Diffraction SIG Meeting.**
- 02:00-02:30 **03.01.06**
CCP13 Software Development. Mark Shotton.
- 02:30-03:00 **03.01.07**
Molecular-Level Control of Fibrous Protein Assembly. David L. Kaplan, Sandra Szela, Peter Avtges, Regina Valluzzi, Stefan Winkler, Donna Wilson, Dan Kirschner.
- 03:00-03:30 **03.01.08**
Determination of Sub-micron Orientational Order in Thermotropic Liquid Crystal Polymer Fibers. Jennifer Taylor, M. Libera.
- 03:30-04:00 Coffee Break.
- 04:00-04:30 **03.01.09**
Wide and Small Angle X-Ray Analysis of Poly(ethylen-*co*-octene). John Blackwell, R. Androsch, S.N. Chvalun, B. Wunderlich.
- 04:30-05:00 **03.01.10**
No Abstract. Kenn Gardner.
- 05:00-05:30 **03.01.11**
Ordered Structure Determined via Diffraction Methods in a Series of Chiral Polyesters. Stephen Z.D. Cheng, Christopher Y. Li, Shi Jin, Frank W. Harris, Bernard Lotz.
- 05:30-05:35 Discussion and Conclusion.

Poster Preview III

Rooms 4,5,6 Chair: Jeff Habel

- 12:00-12:05 **P009**
Conformation and Reactivity of Hydrazone Dithioesters of Alpha-N-Heterocyclic Ketones. Steven Baldwin, Margaret Kastner, Brian Williams, Jeremy Pronchik, Eric Ralph, Elizabeth Blank, John Scovill.
- 12:05-12:10 **P027**
Charge Density Distribution on the *endo*- and *exo*- Faces of the Double Bond of bicyclo [2.2.1]heptene Derivatives. P. Burckel, A. Alan Pinkerton.
- 12:10-12:15 **P045**
Structural Comparison of a Glyoxysomal Precursor Protein with its Proteolytically Cleaved Mature Form. Bryan Cox, Leonard Banaszak.
- 12:15-12:20 **P051**
1.9 Å Crystal Structure of an Octamer RNA with Tandem GG/UU Mispairs. Junpeng Deng, Muttaiya Sundaralingam.
- 12:20-12:25 **P072**
Crystal Structure Analysis of 1-Oxa-2-Hydroxy-2(4-Chlorophenyl)-3,3-Dimethoxy Cyclopenta[F]Phenanthrene. Laksmanan Govindasamy, V. Rajakannan, Devadasan Velmurugan, S.Narasinga Rao, Suh Il-Hwan, Jose Binoy.
- 12:25-12:30 **P108**
Important Inter- and Intra- Molecular Contacts in Canavalin Protein Crystal Growth. Natalie Kirkland, M. Elizabeth Green, Edward Snell, Marc Pusey, Joseph D. Ng.
- 12:30-12:35 **P111**
Local Simulated Annealing Refinement with a Real Space Target. Andrew Korostelev, Richard Bertram, Zhi Chen, Eric Blanc, Michael Chapman.
- 12:35-12:40 **P147**
A Structural Genomics Snapshot: Progress Towards the Crystal Structures of Four *Pyrobaculum aerophilum* Proteins. Cameron Mura, David Eisenberg.
- 12:40-12:45 **P156**
Designing Self-Assembling Multimeric Protein Cages and Filaments. Jennifer E. Padilla, Christos Colovos, Todd O. Yeates.
- 12:45-12:50 **P183**
Influences of Detergents and Amphiphiles on the Crystallization of Integral Membrane Proteins. Matthew Rosenow, Craig Magee, JoAnn Williams, James Allen.
- 12:50-12:55 **P225**
A Novel Microporous Niobium Titanate: Structure Solution of an Octahedral Molecular Sieve from a 5 x 8 x 8 Micrometer Twinned Crystal Using Synchrotron X-Ray Sources. Akhilesh Tripathi, John Parise, Nyman May, Tina M. Nenoff.
- 12:55-01:00 **P240**
Toward the Ultra-High Resolution Structure of a *Clostridium histolyticum* Collagen-Binding Domain. Jeffrey Wilson, Joshua Sakon, Osamu Matsushita.

Warren Award Presentation and Lecture

Rooms A,B Connie Chidester, Presiding

01:00-02:00 **WA.00.01**
Crystal Truncation Rods, Ancient and Modern. Ian Robinson.

10.01 Synchrotron Radiation at the Cutting Edge

Room 4,5,6 Chair: Andrzej Joachimiak

02:00-02:25 **10.01.01**
Challenges for Synchrotron Radiation in Biological Crystallography. Thomas Earnest, Carl Cork, Li-Wei Hung, Gerry McDermott, Keith Henderson.

02:25-2:40 **P153**
Robotic Mounting and Alignment of Cryogenic Samples for Unattended X-Ray Data Collection. Jeff Olson, Ron Jones, Jeff Pan, Michael Blum, Jonathan Greer, Sean Merrick, Peter Magdalinos, Steven Muchmore, Vicki Nienaber.

02:40-03:05 **10.01.02**
Large Molecular Structures and Substructures: Pushing the Frontiers with Synchrotron Radiation and X-Ray Detectors. Daniel Thiel.

03:05-03:30 **10.01.03**
Data Collection and Processing via the Internet. W. Minor, M. Cymborowski, Z. Otwinowski.

03:30-04:00 Coffee Break.

04:00-04:30 **10.01.04**
Making the Most of Weak MAD or SAS Data. George M. Sheldrick.

04:30-05:00 **10.01.05**
SAS Phasing: A Powerful Tool for Protein Crystal Structure Determination Is Maturing. Bi-Cheng Wang, C.-J. Chen, Z.-J. Liu, C. Wu, F. Schubot, G. Rosenbaum, E. Vysotski, J. Lee, H. Dailey, J. Ferrara, M. Schiffer, P. Pokkukur, A. Joachimiack, R. Zhang, A. Howard, J. Chrzas, A. Robbins, J. Rose.

05:00-05:30 **10.01.06**
The Structure of Aldose Reductase at 0.66 Å Resolution: Implications for the Catalytic Mechanism. Alberto Podjarny, Eduardo Howard, Raul Cachau, Andre Mitschler, Bernard Chevrier, Valerie Lamour, Andrzej Joachimiak, Ruslan Sanishvili, Michael Van Zandt, Dino Moras.

05:30-06:00 **Synchrotron Radiation SIG Meeting**

02.05 High Throughput Crystallization

Rooms A,B Chair: Gary Gilliland

02:00-02:30 **02.05.01**
Structural Proteomics of an Archaeon. Aled Edwards.

02:30-03:00 **02.05.02**
Growth and Handling of Crystals in High Throughput Production. Alexander McPherson.

03:00-03:30 **02.05.03**
Gearing Up for Structural Genomics: The Challenge of Hundreds of Proteins and Hundreds of Thousands of Crystallization Experiments Per Year. George T. DeTitta, J. Luft, J. Wolfley, R. Collins, M. Bianca, D. Weeks, I. Jurisica, P. Rogers, J. Glasgow, S. Fortier.

03:30-04:00 Coffee Break.

04:00-04:30 **02.05.04**
High Throughput Crystallization Screening for Structural Genomics and Data Mining. Brent Segelke.

04:30-05:00 **02.05.05**
Crystal Monitor: The Relational Database Application for Crystal Growth. Lance Stewart, Hidong Kim.

05:00-05:30 **02.05.06**
Strategies for Dealing with Crystallization Problems Encountered in High Throughput Screening. Gary L. Gilliland, J. G. Nicklas Bonander, Maria Tordova, Jane Ladner.

05:30-06:00 **Service Crystallography SIG Meeting**

Employment Outlook Session

Rooms A,B Chair: Jennifer Garlitz

08:00 Crystallography Jobs in the New Millennium. A panel discussion about what jobs are available, where to get them and how to find them. What type of experience do you need to succeed?

Exhibit Show	10:00-07:30	Exhibit Hall A
Fiber SIG Meeting	12:00	Rooms 2,3
PDB User Lunch	12:00	Rooms 7,8,9
Poster Session III	05:30-07:30	Exhibit Hall A
Service SIG Meeting	05:30	Rooms A,B
Synchrotron SIG Meeting	05:30	Rooms 4,5,6
IUCr SAS Meeting	05:30	Rooms 2,3
50th Anniversary Cruise	07:00	Boat Dock

HH.00 HHMI Contributions to Macromolecular Science

Rooms A,B

Chair: Tom Steitz

08:30-09:00 Introductory Remarks. Tom Steitz.

09:00-09:30 **HH.00.01**
Structural and Functional Insights into the Mechanism of Synaptic Vesicle Fusion. Axel Brunger.

09:30-10:00 **HH.00.02**
The G-Protein Switch: A Matter of Timing. Stephen Sprang.

10:00-10:30 Coffee Break.

10:30-11:00 **HH.00.03**
Structural Mechanism of the Src Kinases. John Kuriyan.

11:00-11:30 **HH.00.04**
X-Ray Crystallographic Studies of Eukaryotic Translation Initiation Factors. Stephen Burley.

11:30-12:00 **HH.00.05**
Structure of the C-terminal Domain of Tup1, a Yeast Transcriptional Corepressor. Cynthia Wolberger, Elizabeth Sprague, Michael Redd, Alexander Johnson.

12:00-01:30 Lunch Break.

01:30-02:00 **HH.00.06**
Mechanisms of Cyclin-Dependent Kinase Regulation. Nikola Pavletich.

02:00-02:30 **HH.00.07**
Protein Crystallography and Tropical Diseases. Wim G.J. Hol, Stephen Suresh, Jerri Bressi, Jungwoo Choe, Kevein Kennedy, Mike Gelb, Fred Buckner, Wes Van Voorhis, Misol Ahn, Claudia Roach, Wendy Minke, Zhongsheng Zhang, Feng Hong, Jason Picken, Ethan Merritt, Christophe Verlind, Erkang Fan.

02:30-03:00 **HH.00.08**
Structure and Function of Cellular and Viral MHC Homologs. Pamela J. Bjorkman.

03:00-03:30 Coffee Break.

03:30-04:00 **HH.00.09**
Structure and Function of the Developmental Signaling Molecule Hedgehog. D.J. Leahy, T.M.T. Hall, J.A. Porter, N. Fuse, T. Maiti, P.A. Beachy.

04:00-04:30 **HH.00.10**
Polar Versus Nonpolar Interactions in the Molecular Recognition by a Receptor for its Highly Polar Ligands: Structural Results. Florante A. Quiocho, Xiaoqun Duan.

04:30-05:00 **HH.00.11**
Structural Biology of Viral Entry. Stephen Harrison.

05:00-05:30 **HH.00.12**
The Structure of the 50S Ribosomal Subunit at 2.7 Å Resolution and its Functional Consequences. T.A. Steitz, N. Ban, P. Nissen, P.B. Moore.

09.02 Crystal Engineering

Dedicated to Peggy Etter

Rooms 4,5,6 Chair: Carol Brock

08:30-09:00 **09.02.01**
Unnatural Crystals - Designed Using a Hydrogen-Bonded Template. James H. Loehlin.

09:00-09:30 **09.02.02**
Organized Molecular Assemblies by Shape Mimicry. Kraig A. Wheeler, Mukta Hendi, Shella Fomulu, Raymond E. Davis.

09:30-10:00 **09.02.03**
Solid State Structure Versus Solid State Reactivity of Aromatic Aldehydes with 2,4-Dinitrophenylhydrazine. Zofia Urbaczyk-Lipkowska.

10:00-10:30 Coffee Break.

10:30-11:00 **09.02.04**
So You Say You Are a Crystal Engineer. What Have You Engineered for Me Lately? Joseph Lauher, Frank Fowler.

11:00-11:30 **09.02.05**
Selective Absorption of Solvent Molecules by Porous Crystal Structures of Hydrophobic Dipeptides. Carl Henrik Görbitz.

11:30-12:00 **09.02.06**
Engineering Crystals of Pharmaceutical Solids. Susan Reutzell-Edens, Julie Bush, Greg Stephenson.

12:00-01:30 Lunch Break.

Chair: Joel Bernstein

01:30-02:00 **09.02.07**
Hydrogen Bonding Involving Metal Halides: Systematic Study and Design of Crystalline Solids. Lee Brammer, Eric Bruton, Juan Mareque Rivas, John Swearingen, Paul Sherwood.

02:00-02:30 **09.02.08**
Some Limitations in Attempted Quasiracemate Formation. Raymond E. Davis, Kraig A. Wheeler, Mukta Hendi, Shella Fomulu.

02:30-03:00 **09.02.09**
Hexagonal Tiling of Tetrachlorodicyanobenzene Isomers. Doyle Britton.

03:00-03:30 **09.02.10**
Removing Centrosymmetric Packing in Nonlinear Optical Materials via Host-Guest Complexation. Ali Rashid, John Stezowski.

03:30-04:00 Coffee Break.

04:00-04:30 **09.02.11**
Solid State Photochemistry of Alpha-Azido Acetophenone Derivatives, Crystal Lattice Influence on Reactivity. Sarah Mandel, Jeanette Krause-Bauer, Anna Gudmundsdottir.

04:30-05:00 **09.02.12**
Structure, Properties, and Reactivity of Some Metal Complexes of Unsaturated Dicarboxylic Acids. Graciela Díaz de Delgado, Alexander Briceño, Jines Contreras, Teresa Gonzalez, Belkis Ramirez.

01.02 Radiation Damage in Materials

Rooms 2,3 Chair: John Kieffer

08:30-09:00 **01.02.01**
Computer Simulation of Radiation Effects in Solids. L. René Corrales, Byeongwon Park.

09:00-09:30 **01.02.02**
Nuclear Glass Behaviour Under Irradiation: Current Status of Research on French Glass. Dominique Ghaleb, Bruno Boizot, Jean Marc Delayw, Abdelkarim Abbas, Guillaume Petite, Yves Serruys, Georges Calas.

09:30-10:00 **01.02.03**
Structure and Phase Stability in Complex Waste Glass Systems. Andrew Buechele, Ian Pegg, Hao Gan, David McKeown, Wing Kot, Isabelle Muller.

10:00-10:30 Coffee Break.

10:30-11:00 **01.02.04**
Dissolution Mechanisms of Neodymium (Nd) in Aluminoborosilicate Glass - Optical Spectroscopic Approach. Hong Li.

11:00-11:30 **01.02.05**
Antistructure and Point Defect Response in the Recovery of Ion-Irradiated Cu₃Au. Robert Averback, C. P. Flynn, Lucun Wei, Y. S. Lee.

11:30-12:00 **01.02.06**
Radiation Embrittlement Assessment in Nuclear Reactor Pressure Vessel Surrogate Materials. Davor Balzar, Donna Hurley, George Alers, G. Robert Odette.

12:00-12:30 **Materials Science SIG Meeting**

George Jeffrey Memorial Session

Rooms 4,5,6 Bryan Craven, Presiding
12:00

01.04 Network Glasses

Rooms 2,3 Chair: Ronald Cappelletti

01:30-02:10 **01.04.01**
Rigidity Transitions, Self-Organization and Network Stress in Glasses. Punit Boolchand, Y. Wang, D. Georgiev, W.J. Bresser.

02:10-02:50 **01.04.02**
Neutron Inelastic Scattering from Ternary Network Glasses: The Se-As-Ge and Se-As-Br Systems. Birgit Effey Schwickert, R.L. Cappelletti.

02:50-03:30 **01.04.03**
Structural Properties of Chalcogenide Glasses and Crystals Determined by Nuclear Magnetic Resonance. P. Craig Taylor.

03:30-04:00 Coffee Break.

04:00-04:40 **01.04.04**
Atomic Vibrations in Network Glasses. Philip B. Allen.

04:40-0:57 **01.04.05**
Cation Coordination in Oxychloride Glasses. Jacqueline Johnson, Diane Holland, P.G. Appleyard, C.E. Johnson.

04:57-05:14 **01.04.06**
Intermediate- and Extended-Range Order in Network Glasses. John Kieffer, Eric Guilbert, Dmitry Nekhayev.

05:14-05:31 **01.04.07**
High-Resolution Structure of Cax/2A1xSi_{1-x}O₂ Glasses (x=0,0.25,0.5,0.67) by High-Energy X-Ray Diffraction. Valeri G. Petkov, S.J.L. Billinge, S.D. Shastri, B. Himmel.

Exhibit Show	10:00-04:00	Exhibit Hall A
Materials Science SIG Meeting	12:00	Rooms 2,3
Canadian Div. Business Meeting	12:00	Rooms A,B
General Interest SIG Meeting	05:30	Rooms A,B
Small Mol. & Service Cr SIG	05:30	Rooms 4,5,6
Young Scientist SIG Meeting	05:30	Rooms 2,3
Annual Awards Banquet		Radisson Hotel
Reception 06:00-7:00		
Dinner 07:00-10:00		

02.06 Problem Structure Determination

Rooms A,B Chair: Wim Hol

08:30-09:00 **02.06.01**
Crystallization and Structure Solution of the U2A/U2B" Protein-RNA Ternary Complex. Stephen Price, Kiyoshi Nagai.

09:00-09:30 **02.06.02**
Structure Determination of Neurexin 1 β : Too Few Seleno-Methionines and Too Many Molecules. Gabby Rudenko, T. Nguyen, T.C. Sudhof, J. Deisenhofer.

09:30-10:00 **02.06.03**
Sixty-Six Se Atoms and 2160 Amino-Acids in the Asymmetric Unit: Structure of AEP-Transaminase. Celia C. H. Chen, Alexander Kim, Hong Zhang, Andrew J. Howard, George M. Sheldrick, Debra Dunaway-Mariano, Osnat Herzberg.

10:00-10:30 Coffee Break.

10:30-11:00 **02.06.04**
Completion of the Tryptophan Biosynthesis Pathway: Problematic MAD on TrpD. Olga Mayans, Andreas Ivens, Kasper Kirschner, Matthias Wilmanns.

11:00-11:30 **02.06.05**
The Assembly of Rab Geranylgeranyltransferase. Hong Zhang, Miguel Seabra, Johann Deisenhofer.

11:30-12:00 **02.06.06**
The Structure of the 50S Ribosomal Subunit at 2.4 Å Resolution and its Functional Consequences. Poul Nissen, Nenad Ban, Jeff Hansen, Peter B. Moore, Thomas A. Steitz.

04.01 General Interest III

Rooms 4,5,6 Chair: I. David Brown

08:30-09:00 **04.01.14**
High Brightness X-Ray Sources - Implementation and Benefits. Graham Fraser, Neil Loxley, John Wall, Mark Taylor, Ladislav Pina, Rene Hudec, Adolf Inneman.

09:00-09:30 **04.01.15**
Macromolecular Data Collection with Cryogenic Helium. Leif Hanson, Joel Harp, Kristin Kirschbaum, Damon Parrish, David Timm, Andrew Howard, Alan Pinkerton, Gerard Bunick.

09:30-10:00 **04.01.16**
Investigations of Sulfur SAS Phasing Using a Rotating Anode CCD Detector System. M. Gary Newton, John P. Rose, Zhi-Jie Liu, Steven Foundling, Robert Sparks, Bi-Cheng Wang.

10:00-10:30 Coffee Break.

10:30-11:00 **04.01.17**
How the CO Acquired Its Bend? George Phillips, Boguslaw Stec.

11:00-11:30 **04.01.18**
Does Improved Data Collection Result in a Better Structure? Jeffrey R. Deschamps, Clifford George, Judith L. Flippen-Anderson.

11:30-12:00 **04.01.19**
Protein Crystal Engineering Using Knowledge-Based Potentials. Jeffrey A. Bell, Ganesh H. Iyer, Swagata Dasgupta, Usha Srinivasan.

Paul Sigler Memorial Session

Rooms A,B Chair: Len Banaszak
12:00

See You Next Year In

Los Angeles, California

July 21 - 26, 2001

Manned Poster Sessions

Session I- Sunday

Session II-Monday

Session III-Tuesday

5:30 p.m. to 7:30 p.m. in Exhibit Hall A

Posters:

Will be up all week on 4ft. x 8ft. boards

Should be assembled before 5:00 p.m. on Sunday

Removed before 12:00p.m. on Thursday

With an underscore are candidates for the Pauling Prize

With an asterik are candidates for the Oxford Low Temperature Prize

P001 Poster Session I

A Student Investigation of the Molecular Recognition Between Sulfa Drugs & Carboxylic Acids By Cocrystallization. Daniel Adsmond, Mark Whittener.

P002 Poster Session II

Strategies to Crystallize the BTB Domain. K. Farid Ahmad, Gilbert G. Privé.

P003 Poster Session III

Expression, Crystallization and Structural Determination of Saposin B: A Sphingolipid Activator Protein. Victoria E. Ahn, Gilbert G. Privé.

P004 Poster Session I

The Structural Biology Center Bending Magnet Beamline 19BM at the APS: Preliminary Results. R.W. Alkire, Gerd Rosenbaum, Norma Duke, Frank J. Rotella, Rich Benn, John Gonczy, Andrzej Joachimiak, Tom Coleman, Istvan Naday.

P005 Poster Session II

Crystal Structure of the Extracellular Mycolyl Transferase "Antigen 85B" from *Mycobacterium tuberculosis*. Daniel Anderson, Guenter Harth, Marcus Horwitz, David Eisenberg.

P006 Poster Session III

Structure Determination of the Pyruvate Dehydrogenase Multienzyme Complex E1 Component from *E. coli*. P. Arjunan, A. Brunskill, K. Chandrasekhar, M. Sax, W. Furey.

P007 Poster Session I

Calcium-Mediated Thermostability in the Subtilisin Superfamily: The Crystal Structure of *Bacillus* Ak.1 Protease at 1.8Å Resolution. Ted Baker, Clyde Smith, Helen Toogood, Heather Baker, Roy Daniel.

P008 Poster Session II

Preliminary Crystallographic Investigation of Thiamin Pyrophosphokinase. L-J Baker, Boli Huang, Robert A. Harris, David E. Timm.

P009 Poster Session III

Conformation and Reactivity of Hydrazone Dithioesters of Alpha-N-Heterocyclic Ketones. Steven Baldwin, Margaret Kastner, Brian Williams, Jeremy Pronchik, Eric Ralph, Elizabeth Blank, John Scovill.

P010 Poster Session I

Powder Diffraction Analysis of Sr_2AlTaO_6 , $Sr_{2-x}Al_{1-x}Ta_{1+x}O_6$ and $Sr_2Al_{1+x}Ta_{1-x}O_{6-2x}F_{2x}$ ($x=0.01-0.10$): An Attempt to Control the Antiphase Boundary Concentration. Paris Barnes, Patrick M. Woodward.

P011 Poster Session II

Polymer Morphology by SAS Using Temperature-Induced Contrast Variation. John D. Barnes.

P012* Poster Session III

Mechanistic Studies of 3-Hydroxyacyl CoA Dehydrogenase. Joe Barycki, Leonard J. Banaszak.

P013 Poster Session I

Structural Study of CobD: The L-Threonine-O-3-phosphate Decarboxylase Involved in Cobalamin Biosynthesis. Cary Bauer, Kevin Brushaber, Cheom-Gil Cheong, Jorge Escalante-Semerena, Ivan Rayment.

P014 Poster Session II

Structure Determination of a *P. aeruginosa* Enzyme in the Biosynthetic Pathway of Alginate. Lesa Beamer, Catherine Regni, Peter Tipton.

P015 Poster Session III

The High Mosaicity Illusion: Revealing the True Physical Characteristics of Macromolecular Crystals. Henry Bellamy, Edward Snell, Jeff Lovelace, Matthew Pocross, Gloria Borgstahl.

P016 Poster Session I

Advancements Toward Automated Crystallographic Refinement of Biomacromolecular Structures. Daniel Berard, Zeljko Dzakula, Sandor Szalma.

P017 Poster Session II

xmlCIF: A Proposal for Faithful Translation Between XML and Extended CIF. Herbert J. Bernstein, Frances C. Bernstein.

P018 Poster Session III

Crystal Structure of Human Alpha-Thrombin with a Factor XIII Peptide. Sanjoy K. Bhattacharya, Chittalakottu Sadasivan, Vivien C. Yee.

P019 Poster Session I

Solvent Structure in a Collagen-Like Model Peptide. Balaji Bhyravbhatla, Donald Caspar.

P020* Poster Session II

Two-(Mg²⁺)-Ion Catalysis in HPPK: Crystal Structure of a Ternary Complex with AMPCPP and 6-Hydroxymethyl-7,8-Dihydropterin at 1.25Å Resolution. Jaroslaw Blaszczyk, Genbin Shi, Honggao Yan, Xinhua Ji.

P021 Poster Session III

Are Microgravity-Grown Insulin Crystals Better Than Those Grown on the Ground? Gloria Borgstahl, Edward Snell, Henry Bellamy, Jeff Lovelace, Walter Pangborn.

P022 Poster Session I

Mutational Dominance and Cooperativity in Aldehyde Dehydrogenase. Heather Breen, Thomas Hurley.

P023* Poster Session II

Supramolecular Rings and Tapes: Accommodating Hydrogen Bonds and Alkyl Chains. Eric Bruton, Lee Brammer.

P024 Poster Session III

Strange New Ligands for Alkali Metal Ions, or Are They? Jeffrey Bryan, Tatiana Levitskaia, Konstantinos Kavallieratos, Benjamin Hay, Richard Sachleben.

P025 Poster Session I

Muvview2: An Improved Graphical Intensity Viewer. Garold Bryant, Barry Finzel.

P026 Poster Session II

Diffraction Studies of Potexviruses. Christopher Bunick, Greg Ferrell, Amy Kendall, Winston Chapman, Mitzi Reams, Nicholas Fletcher, Lisa Keen, Gerald Stubbs.

P027* Poster Session III

Charge Density Distribution on the *endo*- and *exo*-Faces of the Double Bond of bicyclo [2.2.1]heptene Derivatives. P. Burckel, A. Alan Pinkerton.

- P028** Poster Session I
Structural Analysis of Nucleotide-Binding to an Aminoglycoside Phosphotransferase, APH(3')-IIIa. David Burk, Adelaine Leung, Wai-Ching Hon, Albert Berghuis.
- P029** Poster Session II
Solid State Structures of $[M(En)_a](Naphthalene\ Disulphate)_b \cdot H_2O_c \cdot X$: A Unique Example of Crystal Engineering with Structural Isomers. Jiwen Cai, Chenzhu Liao, Xiaopeng Hu, Xiaolong Feng.
- P030** Poster Session III
The Use of an Interactive Reciprocal Lattice Visualization Method for the Analysis of Problem Structures. Charles Campana, Mark Pressprich, Stephen Christian, Ward Robinson.
- P031** Poster Session I
High-Resolution Structures of Amicyanin Compared at Room Temperature and 100 K. Chris Carrell, Zhi-Wei Chen, Louise Cunane, Rosemary Durley, F. Scott Mathews.
- P032** Poster Session II
Quinocytocrome C: An Intramolecular Electron Transfer Complex. Zhi-Wei Chen, F. Scott Mathews, Kazunobu Matsushita, Tetsuo Yamashita, Hirohide Toyama, Osao Adachi, Henry D. Bellamy.
- P033*** Poster Session III
Low Resolution Sulfur "Super Atom" SAS Phasing of Macromolecules Containing Disulfid Bonds. Chun-Jung Chen, John P. Rose, Gerold Rosenbaum, Bi-Cheng Wang.
- P034** Poster Session I
Crystal Structure of 4a-OH-Tetrahydropterin Dehydratase/DCoH Complexed with a Substrate Analog. Liqing Chen, Pamela H. Roberts, Edward J. Meehan, Katherine L. Gross, Steven W. Bailey, June E. Ayling.
- P035** Poster Session II
Chemical Bonding in Energetic Materials: TNDP and Beta-NTO. Yu-Sheng Chen, Elizabeth A. Zhurova, A. Alan Pinkerton.
- P036** Poster Session III
The Three-Dimensional Structures of Nicotinate Mononucleotide:5,6-Dimethylbenzimidazole Phosphoribosyltransferase (CobT) from *Salmonella typhimurium* Complexed with 5,6-Dimethylbenzimidazole, Its Reaction Products and Several Other Aromatic Bases Determined to 1.9 Å Resolution. Cheom-Gil Cheong, Jorge Escalante-Semerena, Ivan Rayment.
- P037** Poster Session I
How Do Aromatic Rings in Drug Molecular Alter the Conformation of Receptors. Connie Chidester.
- P038** Poster Session II
Structural Evidence for the Competition Between Amp and Catalytic Metals in Fructose-1,6-Bisphosphatase. Jun-Yong Choe, Cristina Iancu, Richard Honzatko.
- P039** Poster Session III
Snapshots of Molecular Recognition in Cyclodextrin Complexes with Derivatized Amino Acids - Perturbing the System with Changes in Functionality and Kinetic Energy. Joanna Clark, Jennifer Alexander, Tom Brett, Charles Ross II., Gerard Harbison, John Stezowski.
- P040** Poster Session I
Structure-Based Enzyme Inhibitor Design: Modeling and Analysis of pCDHFR-NADPH Ternary Complex with PT653 and its Analogues. Nikolai Galitsky, V. Cody, J.R. Luft, W. Pangborn, A. Rosowsky, S.F. Queener.
- P041** Poster Session II
The Role of Water in the Antigen-Antibody Interface of the Lysozyme-HyHEL-5 Complex. Gerson H. Cohen, Enid W. (Deceased) Silverton, Eduardo A. Padlan, David R. Davies.
- P042** Poster Session III
Krypton-Edge MAD on a Frozen Crystal of Myoglobin at SSRL Beamline 9-2. Aina Cohen, Paul Ellis, Michael Soltis.
- P043** Poster Session I
Probing Axial Water Bonding in Copper Proteins Using 170 ESEEM Spectroscopy. Michael J. Colaneri, Adewuyi O. Asimolowo, Jacqueline Vitali, Jack Piesach.
- P044** Poster Session II
Using an N-terminal Fragment from Moloney Murine Leukemia Virus Reverse Transcriptase to Facilitate Crystallization and Analysis of DNA. Marie Cote', Millie Georgiadis.
- P045** Poster Session III
Structural Comparison of a Glyoxysomal Precursor Protein with its Proteolytically Cleaved Mature Form. Bryan Cox, Leonard Banaszak.
- P046** Poster Session I
The Crystal Structure of an Ettringite Mineral. B.M. Craven, R.E. Newnham.
- P047** Poster Session II
The Crystal and Molecular Structure of a Novel Thallium(I) Porphyrin. David Cullen, Sharam Khademi, Edgar Meyer.
- P048** Poster Session III
How Does the Cytochrome Influence Catalytic Activity and Covalent Flavinylation in *p*-Cresol Methylhydroxylase? Louise Cunane, Zhi-wei Chen, Maria-Luisa Veisaga, F. Scott Mathews, William McIntire.
- P049*** Poster Session I
Crystal Structure of a Novel Disulfide Oxidoreductase: Ferredoxin:Thioredoxin Reductase. Shaodong Dai, Hans Eklund.
- P050** Poster Session II
Seeking the Unknown Cofactor: The Quinohemoprotein Amine Dehydrogenase from *Paracoccus denitrificans*. Saumen Datta, F. Scott Mathews, Kazuyoshi Takagi, Kenji Kano, Tokuji Ikeda, Youichi Mori, Katsuyuki Tanizawa.
- P051** Poster Session III
1.9 Å Crystal Structure of an Octamer RNA with Tandem GG/UU Mispairs. Junpeng Deng, Muttaiya Sundaralingam.
- P052** Poster Session I
Is Ion Channel Chemistry Solid, Surface, Solution or Gas Like? W.L. Duax, B. Burkhart, V. Pletnev, N. Li, W. Pangborn.
- P053** Poster Session II
SBC Beamline Standard: Optimizing Crystallization of Lysozyme in the Presence of Cryoprotectant. Norma E. C. Duke, Andrzej Joachimiak.
- P054** Poster Session III
Novel, Very Large Area Detectors for Macromolecular Crystallography. R. D. Durst, A. Brown, S. F. Foundling, J. C. Phillips, A. Pitas.
- P055** Poster Session I
Crystal Structure of D-Lactate Dehydrogenase; A Membrane-Associated Respiratory Enzyme. Orly Dym, Ann Pratt, Chien Ho, David Eisenberg.
- P056** Poster Session II
New Approaches to Analyzing Multiple Conformers in Protein Crystals. Zeljko Dzakula, Daniel Berard, Sandor Szalma, John Badger.
- P057** Poster Session III
Structure of Streptococcal Pyrogenic Exotoxin a Reveals a Novel Metal Cluster. Cathleen A. Earhart, Gregory M. Vath, Manuela Roggiani, Patrick M. Schlievert, Douglas H. Ohlendorf.

- P058** Poster Session I
Efficient Searches for Multiple Crystal Forms Using Designed Experiments. Lisa A. Edberg, Lawrence J. DeLucas, Ming Luo.
- P059** Poster Session II
Chalcogen-Rich Lanthanide Clusters. Thomas Emge, John Brennan, Deborah Freedman, Jonathan Melman, Anna Kornienko.
- P060** Poster Session III
Structure of EVH1: A Novel Proline-Rich Ligand Binding Module Involved in Cytoskeletal Dynamics and Neural Function. Alexander Fedorov, Elena Fedorov, Frank Gertler, Steve Almo.
- P061** Poster Session I
A Detailed Stereochemical Mechanism for Thymidylate Synthase. Janet Finer-Moore, David Birdsall, Richard Morse, Tom Lee, Tim Fritz, Daniel Santi, Robert Stroud.
- P062** Poster Session II
Structure of an Aminoglycoside Phosphotransferase Non-Productive Complex. Desiree Fong, Albert Berghuis.
- P063** Poster Session III
ab initio Phasing of Macromolecular Crystals Through an Alternative Orthogonal Representation. Jonathan M. Friedman.
- P064** Poster Session I
Structure of Novel Polynucleating Strand Ligands Incorporating Pyridine and Pyrimidine Rings. Igor Fritsky, Roland Krämer, Larisa Mokhir.
- P065** Poster Session II
Crystallization of Rat Mevalonate Kinase. Zhuji Fu, Ming Wang, David Potter, Henry Mizioro, Jung-Ja P. Kim.
- P066** Poster Session III
Scaling Bio-Macromolecular Crystal Diffraction Data Using 3-Dimensional Models with Free-R Test. Zheng-Qing Fu, Mark Pressprich, Robert Sparks, Stephen Foundling, James Phillips.
- P067** Poster Session I
Towards Automated Macromolecular Structure Determination: The SnB-Phases Interface. William Furey, Charles M. Weeks, Russ Miller.
- P068** Poster Session II
Structure-Based Design of Potent Inhibitors of EGF-Receptor Tyrosine Kinase as Anti-Cancer Agents. Sutapa Ghosh, Rama Krishna Narla, Yaguo Zheng, Xing-Ping Liu, Chen Mao, Elise A. Sudbeck, Fatih M. Uckun.
- P069** Poster Session III
The Structure of Glutamine Synthetase from *Mycobacterium tuberculosis*: Illumination of Enzymatic Inhibition and Mechanism. Harindarpal S. Gill, Gaston M. U. Pfluegl, David Eisenberg.
- P070** Poster Session I
The Structural Biology Center User Program at the Advanced Photon Source, Argonne National Laboratory. Stephan L. Ginell, Randy Alkire, Norma E. C. Duke, Sergey Korolev, Krzysztof Lazarski, Frank Rotella, Ruslan Sanishvil, Rongguang Zhang, Andrzej Joachimiak.
- P071** Poster Session II
Radiation Damage Leads to Limitations on Crystal Size and X-Ray Flux Density that are Practical for Protein Crystallography. Robert Glaeser, Marc Facciotti, Shahab Rouhani, Alastair MacDowell, Howard Padmore.
- P072** Poster Session III
Crystal Structure Analysis of 1-Oxa-2-Hydroxy-2-(4-Chlorophenyl)-3,3-Dimethoxy Cyclopenta[F]Phenanthrene. Laksmanan Govindasamy, V. Rajakannan, Devadasan Velmurugan, S.Narasinga Rao, Suh Il-Hwan, Jose Binoy.
- P073*** Poster Session I
Platinum MAD Phasing and Crystal Structure of Shikimate Kinase from *Mycobacterium tuberculosis* Complex with ADP at 1.9 Å. Yijun Gu, Ludmila Reshetnikova, Yue Li, Honggao Yan, Shivendra Singh, Xinhua Ji.
- P074** Poster Session II
Structures of Enolase Superfamily Members: Glucarate Dehydratase and Alanine Glutamate Racemase. Andrew M. Gulick, Brian K. Hubbard, Dawn M. Schmidt, John A. Gerlt, Ivan Rayment.
- P075** Poster Session III
Direct Methods and Protein Structures. D.Y. Guo, R.H. Blessing, D.A. Langs.
- P076** Poster Session I
The Structure of Rubisco from *Chlamydomonas reinhardtii*. Eric Haas, Jennifer Alexander, Tzanko Doukov, John Stezowski.
- P077** Poster Session II
Dynamic Light Scattering Analysis of Full-Length, Human RPA14/32 Dimer: Purification, Crystallization and Self-Association. Jeff E. Habel, Gloria E. O. Borgstahl.
- P078** Poster Session III
Structural Analysis of Eukaryotic and Prokaryotic Ornithine Decarboxylases. Marvin Hackert, Andrew Kern, Jeff Almrud, Dan Keller, Don Carroll, Steve Ernst.
- P079*** Poster Session I
Crystal Structure of the Blood-Type Converting Enzyme Alpha-N-Acetylgalactosaminidase. Linda I. Hannick, Alex Zhu, David N. Garboczi.
- P080** Poster Session II
Structural Similarities Between Influenza Matrix Protein M1 and HIV Matrix and Capsid Proteins: An Evolutionary Link Between Negative-Stranded RNA Viruses and Retroviruses. Audray Harris, Ming Luo.
- P081** Poster Session III
A Protein Involved in Bacterial Quorum Sensing is a Zinc Metalloenzyme: The 1.6 Å Crystal Structure of LuxS. Mark Hilgers, Martha Ludwig.
- P082*** Poster Session I
New Model Building and Scaling Procedures in a Multi Structure Comparison of Concanavalin A. Peter Hoecht, Brent Segelke, Sabine Ringhofer, Bernhard Rupp.
- P083** Poster Session II
Control of Transport in Crystal Growth Using Restrictive Geometry Crystallization. Anna Holmes, Liqing Chen, Joseph Ng, Edward Meehan, Robert Naumann.
- P084** Poster Session III
Enzyme and Enzyme-DNA Structures of Endo IV Reveal Specificity for Damage Recognition and Catalysis. David J. Hosfield, John A. Tainer.
- P085** Poster Session I
Structure of Yeast and Human ER Class I α 1,2-mannosidases Involved in N-glycan Processing and ER Quality Control. P. Lynne Howell, Francois Vallee, Francois Yip, Francesco Lipari, Barry Sleno, Pedro Romero, Annette Herscovics, Khanita Karaveg, Kelley Moremen.
- P086*** Poster Session II
Mechanisms for Auto-Inhibition and Forced Product Release in Glycine N-Methyltransferase. Yafei Huang, Junichi Komoto, Fusao Takusagawa.
- P087** Poster Session III
Crystal Structure and Magnetic Properties of the Molecule-Based Magnet $M[N(CN)_2]_2$, $M=Co, Ni, Mn, Fe$. Qingzhen Huang, J. W. Lynn, R. W. Erwin, C. R. Kmetz, A. J. Epstein, J. S. Manson, J. S. Miller.

- P088*** Poster Session I
Crystal Structure Determination of the Small GTPase Sar1, a Regulator for Endoplasmic Reticulum (ER) Budding. Mingdong Huang, Cheng-Qian Wang, Weissman Jacques, Balch William E., Wilson Ian A.
- P089** Poster Session II
Perturbations of NADPH-Cytochrome P450 Oxidoreductase: Implications for Pi-Pi Orbital Overlap. Paul Hubbard, Rosemary Paschke, Anna Shen, Charles Kasper, Jung-Ja Kim.
- P090** Poster Session III
Structure-Based Design of a Purine Repressor with Extended Specificity for Corepressor. J. L. Huffman, D. N. Arvidson, M. A. Schumacher, F. Lu, H. Zalkin, R. G. Brennan.
- P091** Poster Session I
X-Ray Diffraction Studies of Human Articular Cartilage. Tom Irving, Matthias Aurich, Giorgi Khelashvili, Juergen Mollenhauer.
- P092** Poster Session II
The Crystal Structure of Redox-Sensitive Chaperone, Hsp33. Vijayalakshmi Janakiraman, Mathew K. Mukherjee, Bart L. Staker, Ursula Jacob, James C. A. Bardwell, Mark A. Saper.
- P093** Poster Session III
Atomic Model of Protein 4.1R Core Domain: Insights into Calmodulin Regulated Activities of Protein 4.1R on Cytoskeletal Structure. Bing K. Jap, Bong-Gyoon Han, Wataru Nunomura, Yuichi Takakuwa, Narla Mohandas.
- P094** Poster Session I
Mechanically Induced Disorder in Inverse Spinel Ferrites. Peter Jencik, Vladimir Sepelak.
- P095** Poster Session II
Configuration Study of Confocal Max-Flux Optical Systems by Using Ray-Tracing Method. Licai Jiang, Boris Verman, Karsten Dan Joensen.
- P096** Poster Session III
Synthesis and Structure of Transition Metal Complexes of 2-Thienyl-2-Pyridyl Ketone. Alan J. Jircitano, Ian K. Moon.
- P097** Poster Session I
Arginine: Structurally Unappreciated. Andrea Jorjorian, Virginia Pett.
- P098** Poster Session II
Crystal Structure of an Engineered Monomeric Form of IL-10 Complexed to an anti-IL10 Fab. Kristopher Josephson, Brandi Curry, Walter Leigh, Walter Mark.
- P099** Poster Session III
Macromolecule Crystal Quality Improvement in Microgravity: The Role of Impurities. Russell Judge, Edward Snell, Marc Pusey, Michael Sportiello, Paul Todd, Henry Bellamy, Gloria Borgstahl, Matthew Pokros, John Cassanto.
- P100** Poster Session I
Aromatic Carboxylates. Crystal Structures of Ni(II) and Co(II) 2,6-Naphthalenedicarboxylate Tetrahydrate. James Kaduk, Jason Hanko.
- P101** Poster Session II
TWIN3.0 - A Program for Testing on Twinning by Merohedry. Volker Kahlenberg, Thomas Messner.
- P102** Poster Session III
Aquabis(Nitrioltriacetato)Gadolate(III): If Hard Work Does Not Work, Try the Easy Way. Margaret Kastner, Steven Baldwin.
- P103** Poster Session I
The Structure of Low-Potential Cytochrome C-549. Cheryl Kerfeld, David Krogmann, Todd Yeates.
- P104** Poster Session II
Structural Study of Cephalosporin Acylase. Youngsoo Kim, Ki-Hong Yoon, Wim Hol.
- P105** Poster Session III
Human Topoisomerase I: Mechanistic Insights from Novel Covalent Complexes. Hidong Kim, Alex Burgin, Kathryn Hjerrild, Gregory Ireton, Lance Stewart.
- P106*** Poster Session I
Beta-Carbonic Anhydrase Active Site Architecture is a Mirror Image of that of Alpha-Carbonic Anhydrases. Mathew S. Kimber, Emil F. Pai.
- P107** Poster Session II
Spiros Kioulanis Home Page: Discussion About Education. Spiros Kioulanis.
- P108** Poster Session III
Important Inter- and Intra- Molecular Contacts in Canavalin Protein Crystal Growth. Natalie Kirkland, M. Elizabeth Green, Edward Snell, Marc Pusey, Joseph D. Ng.
- P109** Poster Session I
1.8Å Structure of Recombinantly Expressed Botulinum Neurotoxin Type A Light Chain. Mark Knapp, Brent Segelke, Sally Kadkhodayan, Bernhard Rupp.
- P110** Poster Session II
Phasing of Protein Structures by Using Anomalous Signal from Rubidium Ions. Sergey Korolev, Irina Dementieva, Ruslan Sanishvili, Wladek Minor, Zbyszek Otwinowski, Andrzej Joachimiak.
- P111** Poster Session III
Local Simulated Annealing Refinement with a Real Space Target. Andrew Korostelev, Richard Bertram, Zhi Chen, Eric Blanc, Michael Chapman.
- P112** Poster Session I
Fast Alignment of Arbitrary High and Low-Resolution 3D Models Providing a Measure for Their Similarity. Mikhail Kozin, Dmitri Svergun.
- P113** Poster Session II
Two Concomitant Polymorphs of bis(trifluoromethyl) Derivative of bis-o-diynylarene and Related bis-o-diynylarenes (BODAs). Mariusz Krawiec, Prasanna U. Perera, Dennis W. Smith, Khalil A. Abboud.
- P114** Poster Session III
Crystal Structure of RbsR, a Member of the LacI-GalR Family, in Complex with a *rho*O Operator Fragment. Cheryl Kreinbring, Huide Zhang, Mark Hermodson, Cynthia Stauffacher.
- P115** Poster Session I
1,2,3,4,4A,12A-Hexahydro-5,5-Dimethyl-1-H-[2] Benzopyrano[3,2-C]Coumarin. Ramodasan Krishna, Devadasan Velmurugan, Shanmuga Sundara Raj, Hoog Kun Fun, Shanmuga Sundaram, Nathan Raghu, S.Narasinga Rao.
- P116** Poster Session II
Crystal Structure of Yeast Hypothetical Protein YLR351C: Report from a Structural Genomics Pilot Project. D. Kumaran, S. Eswaramoorthy, H. Kycia, S. Gerchman, W. Studier, S. Swaminathan.
- P117** Poster Session III
New Directions in NASA's Biological Crystal Growth Program on the International Space Station. Craig E. Kundrot.
- P118** Poster Session I
X-Ray Crystallographic Analysis of the Interactions of Pokeweed Antiviral Protein with Ribosomal RNA Substrate Analogs. Igor Kurinov, Fatih M. Uckun.

P119 Poster Session II

Crystal Structures of *Toxoplasma gondii* HGPRT Complexed with Substrate Analogues. Alexandre P. Kuzin, Annie Heroux, Larry Ross, E. Lucile White, David W. Borhani.

P120 Poster Session III

Structural Studies of the Copper Chaperones for Superoxide Dismutase. Audrey Lamb, Amy Wernimont, Robert Pufahl, Thomas O'Halloran, Amy Rosenzweig.

P121* Poster Session I

Peculiarities of Anomalous Behavior of PMN Crystal Atoms in the Temperature Region of 183-203 K. Alla R. Lebedinskaya, Mikhail F. Kupriyanov.

P122* Poster Session II

Temperature- and Humidity-Dependent Cation Relocation in Zeolites: Pb-RHO. Yongjae Lee, Glover A. Jones, Jonathan Hanson, Andrea Freitag, John B. Parise, John Z. Larese, David R. Corbin, Volker Kahlenberg.

P123 Poster Session III

Structural Comparison of *Mycobacterium avium* and Human Dihydrofolate Reductase - Different Binding Modes of the Lipophilic Antifolates Trimethoprim and SRI-8686. Adelaine Leung, Laine Seitz, Vibha Pathak, James R. Piper, Larry Ross, E. Lucile White, David W. Borhani.

P124 Poster Session I

An Unprecedented Mode of Enzyme Inhibition: The Aspartic Proteinase from *S. cerevisiae* Folds its Own Inhibitor into a Helix. Mi Li, Lowri Phylip, Wendy Lees, Jacob Winther, Ben Dunn, Alexander Wlodawer, John Kay, Alla Gustchina.

P125 Poster Session II

Crystal Structure of a Novel Red Copper Protein from *Nitrosomonas europaea*. Raquel L. Lieberman, David, M. Arciero, Alan, B. Hooper, Amy C. Rosenzweig.

P126* Poster Session III

Sulfur SAS Phasing at 3Å Resolution for the Direct Determination of the Photo-Protein Obelin Structure. Zhi-Jie Liu, Eugene S. Vysotski, John P. Rose, Gerold Rosenbaum, John Lee, Bi-Cheng Wang.

P127 Poster Session I

Crystal Structure of an RNase A Dimer Displaying a new Type of 3D Domain Swapping. Yanshun Liu, Giovanni Gotte, Duilio Cascio, Massimo Libonati, David Eisenberg.

P128 Poster Session II

High Resolution Views of Protein Farnesyltransferase Substrate and Product Complexes. Steve Long, Kimberly Terry, Lorena Beese.

P129 Poster Session III

Beam-Ish: A Graphical User Interface for the Physical Characterization of Macromolecular Crystals. Jeff Lovelace, Edward Snell, Matthew Pokross, Andrew Arvai, Chris Nielsen, Nguyen-Huu Xuong, Henry Bellamy, Gloria Borgstahl.

P130 Poster Session I

Syntheses and Structural Study of Two Osmium (II) Complexes of Azoimidazoles. Tian-Huey Lu, K. Panneerselvam, Fen-Ling Liao, Prithwiraj Byabartta, Sanjib Pal, Chittaranjan Sinha.

P131 Poster Session II

Structural Analysis of Hydrogen Bonding Mutants of *Staphylococcal nuclease*. Zhiqiang Lu, Wesley Stites, Joshua Sakon.

P132* Poster Session III

Atomic Resolution Structures of Bacteriorhodopsin Photocycle Intermediates: The Role of Discrete Water Molecules in the Function of this Light-driven Ion Pump. Hartmut Luecke.

P133 Poster Session I

The Prediction of the Crystal Structures of Perovskites Using the Software Program SPuDS. Michael Lufaso, Patrick Woodward.

P134 Poster Session II

The Structure of Arachidonate Bound in the Cyclooxygenase Channel of Prostaglandin H2 Synthase-1. Michael Malkowski, Stephan Ginell, William Smith, R. Michael Garavito.

P135 Poster Session III

Arsenate Reductase: A Unique Heavy Atom, an Unexpected Product, and an Unprecedented Hydration Sphere, at 1.65 Å. Philip D. Martin, Srinidevi DeMel, Andrew Howard, Jin Shi, Barry Rosen, Brian Edwards.

P136 Poster Session I

Monomeric Sarcosine Oxidase: Inhibitor Binding by a Covalent Flavoprotein. F. Scott Mathews, Zhi-Wei Chem, Peter Trickey, Mary Ann Wagner, Marilyn Schuman Jorns.

P137 Poster Session II

Assessment of Radiation Damage in Lysozyme Crystals by High Resolution Triple Axis X-Ray Diffraction. Heather Völz, Richard Matyi.

P138 Poster Session III

Purification and Crystallization of the Nucleotide-Binding Domains of Mammalian P-Glycoprotein. Brigitte Maurer, David Rose.

P139 Poster Session I

Structural Studies of a Transcriptional Inhibitory Antibody Fragment Fab4.1. Johanna Mazlo, Tzanko I. Doukov, John J. Stezowski, Steven H. Hinrichs.

P140 Poster Session II

SnB V2.0: An Example of Crystallographic Multiprocessing. Russ Miller, Martins Innus, Jason Rappleye, Charles M. Weeks.

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