

CHICAGO

ACA

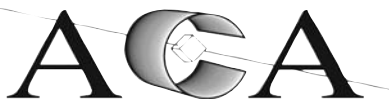
2004

American Crystallographic Association

Call for Papers

Annual Meeting

July 17 - 22



ANNUAL MEETING

JULY 17 - 22, 2004

Hyatt Regency

Chicago, Illinois

www.hwi.buffalo.edu/aca/

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Abstract Submission - March 1, 2004

Advance Registration - June 1, 2004

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ABSTRACT & REGISTRATION OFFICE

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Travel Grant Applications - March 1, 2004

Hotel Reservations - June 15, 2004

IUCr Scientific Freedom Policy Statement

The Organizing Committee of the 2004 Annual Meeting of the ACA shall observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as citizenship, religion, creed, political stance, ethnic origin, race, color, language, age or sex, in accordance with the Statutes of the International Council for Science. At this meeting, no barriers will exist which would prevent the participation of bona fide scientists.

ACA '04

The 2004 Annual Meeting of the American Crystallographic Association, will be held at the Hyatt Regency Hotel and Conference Center in downtown



Chicago, Illinois, from Saturday, July 17 to Thursday, July 22, 2004. All conference activities will take place at the Hyatt, 151 East Wacker Drive. The scientific sessions, poster sessions, and vendor exhibition will take place in a set of rooms on the Gold level of the East Tower. Several workshops and tours will be conducted at Argonne National Labs to exploit the close proximity of the Advanced Photon Source. Transportation will be provided for these scheduled activities. The exhibition will

be directly below in the East Riverside Exhibition Center. The Hyatt Regency has also been designated as the headquarters hotel. A block of sleeping rooms has been secured at a special room rate. Each participant is responsible for making his/her own hotel reservation by contacting the Hyatt at 1-800-233-1234 and identifying themselves as an ACA meeting participant; or by completing and submitting the hotel reservation form on page 19. If you wish to share a room but need a roommate, please go to the meeting web site at www.hwi.buffalo.edu/aca/ for a list of others also looking for roommates. Note: you will need your roommate's name when making your own reservation.

The Sights, Sounds, and Tastes of Chicago

Chicago has some of the finest dining and entertainment options anywhere in the country. From nationally acclaimed theatre (such as Steppenwolf and Goodman), music (Chicago Symphony Orchestra, The Lyric Opera of Chicago, as well as jazz, blues and rock clubs), and museums (Art Institute of Chicago, Field Museum), to sports (White Sox, Cubs) you will find something to suit your tastes. As for food, the city has some of the best restaurants in the country (Charlie Trotter's), as well as many top quality, unique and interesting ones (Frontera Grill, MK, Blackbird, Bin 36, to name a few). Chicago is also a city of neighborhoods, and although many ethnic areas are changing, you can still find neighborhood restaurants serving authentic gnocchi, pirogis or bratwurst from the old world, as well as an expanding menu of choices from the new world and Asia. If the weather permits, a relaxing way to spend time is to take a sightseeing or an architectural boat tour. Boats leave from the Michigan Ave. bridge over the Chicago River. After a boat tour you could get a "Cheezborger" at the Billy Goat Tavern or visit the many shops along Michigan Ave. (Bloomingdales, Nordstrom, Niketown, Apple, FAO Schwartz, Crate and Barrel, Borders, Virgin), or in the loop (Marshall Fields, Carson Pirie Scott, Sears, Tower Records, and the many jewelers along Wabash). Check out Palmer's Walking Guide to Chicago.

Scientific Program Highlights

The 2004 Meeting in Chicago will take full advantage of the close proximity to the Advanced Photon Source (APS) at Argonne National Laboratory and offer opportunities that are unique to this location (see page 4 for details).

The meeting will include four different workshops that will allow participants to gain hands-on experience with diverse topics ranging from data collection at one of the beamlines at APS, to working with the latest software releases from CCP4 and PDB.

Attendees will also be able to sign up for a full-day tour of the APS that will give each participant a rare opportunity to have a close look at many of the outstanding facilities available at the APS (see page 5 for details). Early registration is highly recommended for both the Tour and for any of the Workshops.

An educational outreach initiative, organized by the Protein Database (PDB), the Cambridge Crystallographic Data Center (CCDC), and the ACA will be held on Sunday, July 18th. The program for high school teachers and students in the Chicago area will focus on structure and databases.

The program contains over thirty-five sessions organized by the ACA Special Interest Groups and the AACG, and reflect the broad interest areas of our members. The meeting includes four award symposia to honor the recipients of the Etter, Fankuchen, Supper, and Trueblood Awards. This year's **Transactions Symposium**, entitled **Crystals in Supramolecular Chemistry**, will examine supramolecular chemistry from crystallization to smart materials (see page 6 for details). Several social events are scheduled to provide opportunities to meet and mingle with old and new friends and colleagues, including the Mentor/Mentee Dinner, the Young Scientist Mixer, and several poster sessions/competitions.

Young Scientists Highlights

Travel Grants

Limited funds will be available to help **students and young scientists** in attending the 2004 Meeting by contributing toward travel and related expenses. Preference will be given to those presenting a paper. Interested parties should return the application form on page 15 to ACA Headquarters by March 1, 2004. Applications received after this deadline will be reviewed only if funds remain after the initial review. Applicants who received travel grants in 2003 will NOT be eligible for funding in 2004 and should not apply.

Employment Opportunities

A room in the Hyatt will be set aside to provide an opportunity for those seeking employment to meet with possible employers. A sign-up sheet with 15 minute time slots will be posted on the door for those interested in setting up appointments on site. Those wishing to schedule appointments in advance should contact the Local Chairs.

Young Scientist Mixer

The Young Scientist Mixer provides an opportunity for young scientists (students, postdocs and early career teacher/scientists) to network and socialize with each other in an informal setting. The mixer will be held on Monday, July 19, beginning at 7:30pm in the Crystal Ballroom of the Hyatt. There is no charge for young scientists attending this event with two drink tickets and snacks provided. Tickets for all others are available for \$10. Please indicate on your registration form if you and/or a guest will attend.

Social Events

Opening Reception & 2004 Exhibition

Please join us in renewing old friendships, welcoming new participants and supporting our exhibitors at this year's **Opening Reception and 2004 Exhibition on Saturday, July 17**, in the East Riverside Exhibition Center at the Hyatt. The reception will begin at 8:00p.m. and is free for registered participants. Entry tickets are available for \$30 for accompanying guests.

The Mentor/Mentee Dinner

Since 1995 the ACA has sponsored a Mentor/Mentee Dinner to provide a relaxed opportunity for young scientists to network and seek mentors within the crystallographic community. Unlike previous year's sit-down dinners, this year the evening will be buffet style at the Blue Agave Mexican restaurant on **Sunday, July 18**, with plenty of space for mingling. During the evening, young scientists will have the opportunity to discuss their science and career aspirations with the mentors present. While there is no obligation to maintain contacts made during this event, we hope that both Mentors and Mentees will find it a rewarding experience.

Mentees are usually considered students, post-docs, and early career teachers/scientists (i.e. non-tenured assistant professors) while Mentors are typically more experienced researchers, although assistant professors wishing to mentor are more than welcome to do so.

In previous years, there have been many more Mentees at the dinner than available Mentors. Since the success of this event depends strongly on Mentees being able to interact individually with Mentors, this year we are hoping to have a equal number of Mentors and Mentees. Therefore, if you feel able to offer your time as a Mentor, it would be greatly appreciated by the Young Scientists.

Please indicate on the registration form whether you wish to be considered a Mentee or a Mentor. Participation in the event is \$10 per ticket and is not included in the registration fee.

Annual Banquet and Awards Ceremony

Our annual banquet and awards ceremony will be held in the Hyatt Regency on Wednesday, July 21. Reception with cash bar begins at 6:30 pm with dinner beginning at 7:30p.m. Dinner tickets for registered students are \$25. Tickets for all others are \$55. The menu will include a three course meal with your choice of beef, chicken or vegetarian entree. Please indicate your entree preference on the registration form.

Winners of the 2004 Pauling, Oxford and IUCr Poster Prizes will be announced, along with a presentation by **Madeline Jacobs, 2004 Winner of the ACA Public Service Award**. Ray Davis, currently ACA President, will present his Past President's Address.



Registration

All attendees, including invited speakers, must register. Each registered participant will receive a conference bag and materials, a conference badge securing admission to the Opening Reception, the Exhibition Show and scientific sessions. **Pre-registration for all the Saturday Workshops is mandatory.** No one will be allowed to register for any of the workshops on Saturday morning. Workshop attendees may pick up their registration materials on Friday, July 16, 6:00pm-9:00pm in the Hyatt Hotel. Registration will reopen on Saturday, July 17 at 7:30am. Participants with special needs arising from disabilities are invited to contact the ACA Registration Office to discuss appropriate accommodations.

| Registration Fees | Before June 1 | After June 1 |
|---------------------|---------------|--------------|
| Regular Member | \$330.00 | \$421.00 |
| Retired Member | \$137.00 | \$182.00 |
| Postdoc Member | \$171.00 | \$239.00 |
| Student Member | \$137.00 | \$182.00 |
| AACG Member | \$330.00 | \$421.00 |
| Non-member* | \$444.00 | \$535.00 |
| Postdoc Non-member* | \$228.00 | \$296.00 |
| Student Non-member* | \$182.00 | \$228.00 |
| One-day Member | \$165.00 | \$211.00 |
| One-day Non-member* | \$330.00 | \$421.00 |

*Increment charged to non-member registration may be credited toward **New Member Dues for 2004** by submitting the membership application on page 17 with the registration form. Those registering as non-member postdocs or students, must include documentation with the registration form. **An Advance Registration Form is on page 13.**

There will be no registration fee for Accompanying Guests. However, tickets for the Opening Reception, YSSIG Mixer, Mentor/Mentee Dinner and Annual Banquet are available for Accompanying Guests: Opening Reception-\$30, YSSIG Mixer-\$10, Mentor/Mentee Dinner-\$10, Annual Banquet-\$55. Those wishing to attend the scientific sessions and/or exhibit show must register at the Regular Member rate.

Payment

All prices listed are in U.S. dollars and must be submitted in U.S. dollars. Registration forms must be postmarked or submitted **before June 1, 2004**, to be eligible for the advance registration rate. After June 1, registrations will be accepted at the higher rate. On-site registration will also be available at the higher rate. Fees for workshops, the banquet and the Mentor/Mentee Dinner are separate from the registration fee but should be included in the total payment. Purchase orders will not be accepted. Only U.S. checks, VISA, MasterCard or American Express payments will be accepted. Please make checks payable to ACA and mail to:

ACA Meeting Registration
P.O. Box 96 Ellicott Station
Buffalo, NY 14205-0096 USA
Fax: (716) 852-4846

Forms submitted via fax must include VISA, MasterCard or American Express credit card payment information.

Cancellation Policy

Cancellation and requests for refunds should be made in writing to ACA Headquarters. For cancellations received before June 1, 2004, 100% of the total remittance will be deducted. Requests received between June 1 and June 30, 2004, will be honored minus 50% of the total remittance. Fees will not be refunded after July 1, 2004.

Exhibit Show

An exhibition of the latest instruments and techniques for sample isolation, purifications and preparation; crystal growth and data collection, of computer software for data storage, retrieval analysis, of graphics systems and databases; and books, journals and other materials essential to modern crystallographers **is scheduled to begin on the evening of Saturday, July 17**, in conjunction with the **Opening Reception** in the East Riverside Exhibition Center at the Hyatt Regency Hotel. The **2004 Show** will run through the afternoon of Wednesday, July 21.

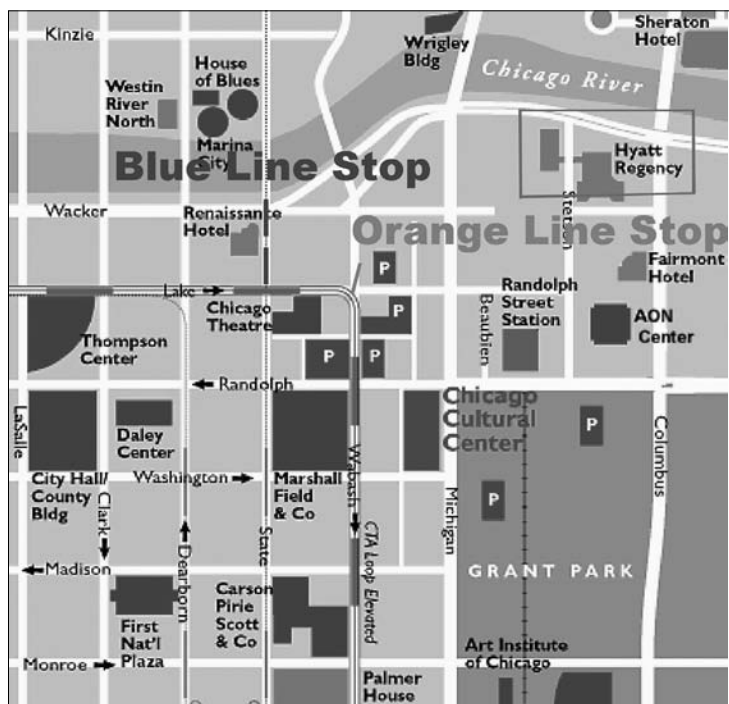
The show is being managed by the Advertising and Exhibits Div. of the American Institute of Physics. For further information contact Bob Finnegan, AIP, 2 Huntington Quadrangle, Suite 1N01, Melville, NY 11747-4502, rgf@aip.org; ph. (516) 576-2433.

Exhibitors from last year included the following:

3D MOLECULAR DESIGNS & MSOE/CENTER FOR
BIOMOLECULAR ENGINEERING
ACCELRYLS
ADVANCED PHOTON SOURCE
AREA DETECTOR SYSTEMS CORP
BLAKE INDUSTRIES, INC.
BRANDEL
BRUKER AXS
CCDC
CCP4
CORNING INC.
CRYO INDUSTRIES OF AMERICA
CYBIO AG
DATACENTRIC AUTOMATION
DECODE GENETICS
DISCOVERY PARTNERS INT'L

DIVERSIFIED SCIENTIFIC
DOUGLAS INSTRUMENTS
FLUIDIGM CORPORATION
FORMULATRIX, INC.
GENOMIC SOLUTIONS
GILSON, INC.
GREINER BIO-ONE
HAMILTON COMPANY
HAMPTON RESEARCH
HEWLETT PACKARD
IUCr
MAR USA, INC.
MICROCAL
MOLECULAR DIMENSIONS
MXI SYSTEMS, INC.
NEXTAL BIOTECHNOLOGIES

OSMIC, INC.
OXFORD CRYOSYSTEMS
OXFORD DIFFRACTION
OXFORD INSTRUMENTS
PRECISION DETECTORS
PROTEINCRYSTALLOGRAPHY.COM
PROTEIN DATA BANK
RIGAKU/MSK
ROBBINS ANALYTICAL
ROBODESIGN INTERNATIONAL
SOUTHEAST REGIONAL
COLLABORATIVE ACCESS TEAM
TECAN
TRITEK CORP.
VEECO INSTRUMENTS
WHITE CARBON
XENOCSSA



Getting to Chicago

Chicago is served by most major airlines. Flights arrive at O'Hare International Airport or Midway Airport. Chicago is also a major hub for Amtrak. From O'Hare Airport to downtown, a taxi will cost about \$40, and take from 30-75 minutes depending on the traffic. A cheaper alternative than the taxi is to take Continental Airport Shuttle which costs about \$19 (check their website for more information, as reservations in advance are sometimes required). Finally you could take the Chicago Transit Authority Blue Line train which costs only \$1.50 to get downtown. The nearest stop to the hotel is Clark and Lake, but you would then still need to get a taxi, so this method is not recommended for the weary traveler.

There are a number of ways to get to the Hyatt from Midway Airport. Located just ten miles southwest of downtown Chicago, Midway is easily reachable by the Chicago Transit Authority's (CTA) Orange line in just 20-30 minutes, as well as by regional buses, downtown shuttles, and taxi.

-- CTA. Follow signs from the airport terminal through the parking garage to the rail station. A CTA transit card can be purchased from a vending machine at the Midway Orange Line Transit Station. The one-way fare is \$1.75. The CTA trains travel frequently from 4am to 1am. You will want to take the Orange line to the State Street exit in the downtown "loop", north on

State Street one block, and then east for two blocks on Wacker past Michigan Avenue to the Hyatt.

-- Shuttles. Continental Airport Express offers daily shuttle service between Midway and downtown Chicago from 6am to 11pm. The fare to the city is about \$16.00. An information counter is located on the Lower Level Arrivals door LL3, and the pickup location is outside door LL3. Continental Airport Express can be contacted at 312-454-7800 or 800-654-7871.

-- Taxi. Taxicabs are available from the Lower Level Arrivals door LL3. You can share cabs to the downtown area, and they all run on meters (no flat rates). The approximate fare will be \$25.00.

For current ground information http://www.ohare.com/midway/ground_transport/ground_transportation_home.shtm

WORKSHOPS – Saturday, July 17

WK.01 Hands On Workshop – MAD/SAD Phasing, Data Collection, Processing, and Structure Solution

Organizer: Jim Fait, SER-CAT (fait@anl.gov).

This all-day workshop will be structured as two half-day sessions, with the workshop participants split in two groups. One session will be at one of several APS beamlines, and will cover all aspects of collection of MAD and SAD data, including collection of diffraction data. The second session will cover the computing aspects of data reduction with various packages, scaling, evaluating quality of data, and structure solution and phase extension. Both practical examples and real data will be emphasized.

Visitor clearance and pass are required. See page 5 for instructions
Lunch will be provided. Sponsored in part by the Advanced Photon Source. The cost for students is \$140, for all other \$160. No Late Registration. Limit 150 people.

WK.02 Small Molecule Crystallography at ChemMatCARS

Organizers: P. James Viccaro, CARS Executive Director, The University of Chicago (viccaro@cars.uchicago.edu) and Victor G. Young, Jr., University of Minnesota (young@chem.umn.edu).

This all-day workshop will take place at the Advanced Photon Source at Argonne National Laboratory. It is intended particularly for small-molecule crystallographers and chemical crystallographers who have not yet conducted experiments at a synchrotron. Transportation will be provided to and from the Hyatt Regency Chicago Hotel.

Pre-registration is mandatory. Visitor clearance and pass are required. See page 5 for instructions. There is no cost for this workshop. Lunch and coffee breaks will be provided. The number of participants is limited so please register early.

| | |
|-------------------------------|---------------------------------|
| Topics to be covered: | 2 hands-on segments include: |
| Microcrystallography | Data collection at Sector 15-ID |
| Charge-density analysis | Beamline operation |
| Time-resolved crystallography | Becoming a user of ChemMatCARS |

WK.03 A Protein Crystallographic Toolbox: CCP4 Software Suite and PDB Deposition Tools

Organizers: Maeri Howard-Eales, CCP4, (m.e.howard_eales@dl.ac.uk), Peter Briggs, CCP4, (p.j.briggs@dl.ac.uk), Judith Flippen-Anderson RSCB, (flippen@rcsb.rutgers.edu), and John Westbrook, RSCB, (jwest@rcsb.rutgers.edu).

The package distributed by CCP4 includes programs for all aspects of protein crystallography up to the model building stage. Version 5 of CCP4 will also include tools that will assist users in preparing files for deposition to the PDB.

This all-day workshop, to be held at the Hyatt Hotel, will provide a brief introduction to the CCP4 suite and general usage of the package, and then focus on the use of key programs from different parts of the structure solution process including the data processing package Mosfilm and the refinement program REFMAC. This will

include detailed analysis of the programs' output and protocols for more demanding problems. As the day progresses we will point out how PDB_Extract works with the various programs in CCP4 to extract information needed for deposition. The PDB team will then demonstrate how ADIT can be used, with the files produced by PDB_Extract, to do preliminary validation and prepare your structure for deposition.

The format of the workshop will be based around presentations by both CCP4 and PDB staff and developers and will include opportunities for informal group discussions. Participants are encouraged to bring their own problem cases in the form of data, to be discussed either during or after the workshop. If you bring your own laptop, and time permits, it may be possible to download and install the standalone version of ADIT (please contact the organizers for more details).

The workshop will be aimed primarily at less experienced users who are familiar with protein crystallography but less familiar with the CCP4 and PDB packages. More experienced users may also benefit from the sessions on individual programs and the opportunity to interrogate the program developers. The cost for students is \$80, for all other \$100.

WK.04 GM/CA - Synchrotrons for the Biologist

Organizers: Janet Smith (smithj@purdue.edu) and Ward Smith (wwsmith@anl.gov).

This one-day workshop will focus on information for non-specialists and scientists interested in learning more about synchrotron structural biology and the new GM/CA facility in particular, including a tour of the GM/CA facilities at the APS.

Visitor clearance and pass are required. See instructions on next page. Fees for the workshop are \$60 for students and \$80 for others. Lunch is included. Attendance is limited to 50 people. More information will be available on the GM/CA website, <http://www.gmca.aps.anl.gov/home.shtml>

Structural biology continues to have a major impact on the advancement of biological science. Synchrotron radiation plays an essential role in modern structural biology, especially in the areas of structure determination of macromolecular complexes, structural genomics, structure determination at ultra high-resolution and structure-based drug design. This workshop is intended as a primer on synchrotron structural biology and will describe a new facility at the Advanced Photon Source (APS) at Argonne National Laboratory, established as a national user resource for biology by the National Institute of General Medical Sciences (GM) and the National Cancer Institute (CA), two of the National Institutes of Health. The GM/CA Collaborative Access Team is currently constructing an experimental facility for macromolecular crystallography at Sector 23 of the APS. The GM/CA user facility will be available to the scientific community, on a peer review basis, for diffraction experiments in structural biology. The GM/CA beamlines will enable structure determinations of proteins and other macromolecules with an emphasis on streamlined, efficient throughput for a variety of crystal types, sizes and qualities, representing the cutting edge of structural biology research. Talks will describe how the special properties of synchrotron radiation are used for macromolecular crystallography, and the design and capabilities of the three GM/CA beamlines.



WK.05 APS/IPNS

Tour

Organizer:

Phillip Fanwick

(pfanwick@purdue.edu).

All-day tour of the synchrotron (APS) and neutron source (IPNS).

The visit will include a tour of the two facilities and lectures illustrating the type of experiments run there. Practical details such as how to obtain beam time will be covered. Visitor clearance and pass are required. See below for instructions. The cost for students is \$40, for all other \$60.



Instructions for Site Access for Visitors to the Advanced Photon Source (APS) for Workshops 1, 2, 4, 5

The APS is located at Argonne National Laboratory (ANL), and U.S. Department of Energy National laboratory. ANL is a controlled-access facility. Participation in workshops or tours will require a temporary or permanent APS badge or a **site-access visitor pass** for the day.

Workshop and tour participants without APS badges must register with the APS User Office for a site-access visitor pass. **Registration for the workshops will not automatically trigger registration with the APS.**

-- **U.S. citizens** should register at least two weeks prior to the visit. Register via email to apsuser@aps.anl.gov. Provide your name, institution, and indicate that you are attending the ACA2004 Annual Meeting.

-- **Non-U.S. citizens** require special access, and may take up to three months for access permission to be granted. Complete the UO-48 registration form on the APS website:

http://www.aps.anl.gov/user/uo48_online.html

Please complete the online form, or fax the completed PDF file to the APS User Office, at least three months in advance of the July 17 visit.

You WILL NOT be allowed entrance to ANL or the APS and IPNS facilities without confirmation from the APS User Office that access for your visit has been granted. For participants with an APS badge, please register with the APS User Office to confirm that your badge is valid, and be sure to carry it with you. Transportation will be provided from the Hyatt to the APS.

Please visit the APS website for any further information:

<http://www.aps.anl.gov>

AWARD SYMPOSIA

AW.01 Etter Award Symposium

Half-day symposium. To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career.

AW.02 Supper Award Symposium in Honor of Prof. Nguyen-Huu Xuong

Half-day symposium organized by K.I. Varughese, Scripps Research Inst. (kiv@scripps.edu) and Andy Howard (ahoward@mca.aps.anl.gov).

AW.03 Fankuchen Award Symposium in Honor of Prof. Alexander McPherson

Half-day symposium organized by Robert Cudney (bob@hrmail.com) and George DeTitta (detitta@hwi.buffalo.edu).

This session in honor of Alexander McPherson will focus on recent development and advances in the field of biological macromolecular crystallization. Breakthrough technologies, novel discoveries, and clever ideas that can be applied immediately to advance the ease, efficiency and successful throughput of crystallization will be emphasized. This broad based session welcomes presentations covering sample preparation, reagents, screening, optimization, production, cryo, automation, hardware as well as methods.

AW.04 Trueblood Award session in Honor of Prof. Richard E. Marsh

Half-day session organized by Larry R. Falvello, University of Zaragoza – C.S.I.C. (falvello@unizar.es) and Alberto Albinati, University of Milan, (alberto.albinati@unimi.it)

This symposium entitled “Important Science from Small Molecule Structures – Chemistry” will honor Richard E. Marsh, Senior Research Associate in Chemistry at Caltech, who is the recipient of the first Kenneth N. Trueblood Award. The award was established in 2001 in memory of Professor Trueblood, and as an honor to his many and multifaceted contributions to the use of computers in crystallography and to the use of crystallography in chemistry, recognizes “exceptional achievement in computational or chemical crystallography.” The first recipient of the Trueblood Award, Dick Marsh, whose impassioned advocacy of exactitude in crystallography is widely known in the crystallography and chemistry research communities, will give the keynote address. The program will reflect the areas of chemistry and crystallography impacted by Dick Marsh’s contributions; and since this is the first Trueblood Award Symposium, the program will also reflect the areas that have been enriched by Ken Trueblood’s enduring scientific legacy.

TRANSACTIONS SYMPOSIUM

TR.01 Crystals in Supramolecular Chemistry

Four half-day sessions organized by Alicia Beatty, Mississippi State University (abeatty@ra.msstate.edu).

Scientists from a broad reach of disciplines, including traditional synthetic, theoretical, analytical, and spectroscopic, come together to further the frontiers of supramolecular chemistry. The symposium represents a time line for the stages of development of crystals, from crystallization to smart materials. The theme of the first session, "Crystal Structure Prediction and Polymorphism," will focus on crystals when they are a mere twinkle in the eye of the supramolecular chemist. "Crystal growth mechanism," an important field for both the small molecule and macromolecular scientist, will focus on the sometimes painful birthing process of a crystal. The painstaking construction of a useful, upstanding, predictable crystal structure will be described in "Crystal Structure Design." Finally, the session on "Applications of Crystal Design" will illuminate some of the success stories, crystalline materials that have achieved a purpose. In conjunction with the symposium, a poster session will highlight recent developments in the field, with a poster prize to be awarded. Presentations for oral and poster sessions are solicited. Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund, for partial support of this symposium.

Confirmed speakers:

Sally Price, University College, London
 Joel Bernstein, Ben-Gurion University, Israel
 Ray Davis, University of Texas, Austin
 Jonathon Steed, University of Durham, U.K.
 Bart Kahr, University of Washington, Seattle
 Tayhas Palmore, Brown University
 Matt Peterson, TransForm Pharmaceuticals
 Jennifer Swift, Georgetown University
 M. W. Hosseini, Université Louis Pasteur
 Christer Aakerøy, Kansas State University
 Lee Brammer, Sheffield University, U.K.
 Jesus Valdez-Martinez, U. N. A. M., Mexico
 Jim Wuest, Université de Montréal, Canada
 Michael D. Ward, University of Minnesota
 Dario Braga, University of Bologna, Italy
 Len MacGillivray, University of Iowa
 Robin Rogers, University of Alabama

CrystEngComm Poster Prize An electronic-only Journal from the Royal Society of Chemistry, CrystEngComm (www.rsc.org/CrystEngComm) has kindly agreed to sponsor a prize to be awarded to the best poster in the Transactions symposium (see special poster session 12.01 on page 10). Please indicate your wish to be considered for this prize with your abstract submission.

**01.01 Structural Insights into Transcription**

Half-day session organized by Cynthia Wolberger (cwolberg@jhmi.edu).

This session will focus on the structures of proteins involved in transcription, transcriptional regulation, and chromatin modification.

Confirmed speakers:

Cynthia Wolberger, John Hopkins Univ. School of Medicine
 Seth Darst, Rockefeller University

01.02 Structural Analysis by Hybrid Methods

Half-day session organized by Karolin Luger (kluger@lamar.colostate.edu) and David M. Belnap (David_Belnap@nih.gov).

This session will focus on the structures and interactions of biomolecules as determined by multidisciplinary approaches in which crystal structures of subunits and domains are integrated with information from other sources (cryo-EM; NMR spectroscopy; fluorescence, computational biology; etc).

01.03 Computational Methods

Half-day session organized by Wayne F. Anderson (wf-anderson@northwestern.edu) and Paul D. Adams (PDA@adams@lbl.gov).

All of the steps in macromolecular crystallography, from bioinformatic selection of a molecule for study through computational analysis of function are benefiting from advances in computational methods. These advances have reduced the amount of time a crystallographer spends working on the average structure, which in turn is increasing the demand for improvements in computational methods. The session will include a combination of invited presentations and presentations selected from submitted abstracts.

01.04 Difficult Structures

Half-day session organized by Todd Yeates (yeates@mbi.ucla.edu) and Zbigniew Dauter (dauter@bnl.gov).

The session on "Difficult Structures" is intended for discussion of problems that require a high degree of "brain engagement" during the process of crystal structure solution. Features such as pseudosymmetry, twinning, disorder, small phasing signal in large structures etc. often present a special challenge, requiring a combination of various approaches. They are usually very rewarding after successful structure solution, and highly instructive for other crystallographers.

01.05 New Structures

Half-day session organized by Lesa Beamer (beamerl@missouri.edu) and P. John Hart (pjhart@biochem.uthscsa.edu).

This session will highlight recent macromolecular crystal structures of particular importance and interest to a wide audience. Presentations will be chosen by invitation and from submitted abstracts.

1.06 Membrane Structures

Half-day session organized by Michael Wiener (mcw2s@virginia.edu) and Declan Doyle (declan@biop.ox.ac.uk).

This session will focus on results and methods in the crystallography of integral membrane proteins. Membrane proteins, 20-30% of the ORFs of an organism's genome and targets of most drugs, are a frontier area of structural biology. The slow trickle of novel

structures has changed to a slightly-less-slow trickle of structures, and technical challenges abound in expression, production and crystallization. Abstracts are solicited for both structural results (new structures especially welcomed!) and methodological efforts directed to any 'bottleneck' areas of the endeavor.

01.07 Macromolecular Assemblies

Half-day session organized by Wei Yang (Wei.Yang@nih.gov) and Stephen Sprang (stephen.sprang@utsouthwestern.edu).

This session will focus on biophysical approaches, including X-ray crystallography and electron microscopy to explore the static and dynamic structures of macromolecular complexes. Asymmetric complexes that mediate signal transduction or mechanical transduction, transport, replication and repair will be of particular interest.

01.08 Structural Bioinformatics

Half-day session organized by Ram Samudrala (ram@compbio.washington.edu) and Daniel Fischer (dfischer@bioinformatics.buffalo.edu).

A variety of experimental and modeling techniques exist to determine the structure of large numbers of biological molecules (proteins and nucleic acids). The exponentially increasing amount of structural data, combined with other kinds of single molecule as well as genomic/proteomic data, has led to the advent of informatics approaches being used to represent, characterize, analyze, and manipulate the data, to infer the biological meaning of these molecules. This half-day session will showcase papers that develop and use such state-of-the-art bioinformatics techniques.

01.09 Fresh Approaches to Express and Purify Biomolecules

Half-day session organized by Song Tan (sxt30@psu.edu) and Aled Edwards (aled.edwards@utoronto.ca).

Isolating sufficient amounts of high quality sample is a critical rate-limiting step of many biomolecular structure determination projects. This half-day session will focus on novel methods to express and purify individual or complexes of proteins and/or nucleic acids. We welcome papers describing cutting edge synthesis or recombinant expression methods as well as novel purification methods. Presentations will be selected by invitation and from submitted abstracts.

SERVICE CRYSTALLOGRAPHY SIG SESSIONS

02.01 Small-molecule Problem Structures

Half-day session organized by Victor G. Young (young@chemsun.chem.umn.edu).

We are soliciting papers for crystal structure determinations (or structure determination attempts) of "Problem Structures". Our definition of Problem Structure is broad, and includes twinned crystals, pseudosymmetry, space group ambiguities, superlattices, disorder, weak diffractors, unstable compounds, or any structure where the data were unusually difficult to collect, solve and/or refine. You may report on a problem structure that you have successfully solved and discuss the technique(s) you used to solve it. We are also very interested in unresolved problems, where the author illustrates a problem structure in which the problem(s) have not been completely mastered, and opens the floor up for discussion and suggestions. These could possibly be shorter talks with more time left for discussion.

02.02 Crystallographic Laboratory Practices

Evening session organized by Alicia Beatty (abeatty@ra.mssta.te.edu).

This session aims to be an informal, hopefully informative and enjoyable, panel discussion concerning issues that come up in the service laboratory. It will cover such subjects as publishing, authorship, charges for services, general laboratory practices. At this time there are no plans for formal or even informal presentations by panel members. New Service SIG members and the curious are especially invited to attend. Refreshments will be served. If you are interested in being a panel member please contact the organizer.

02.03 Teaching Advanced Crystallography

Half-day session organized by Peter Müller (peterm@mbi.ucla.edu).

This session focuses on the teaching of the more advanced aspects of crystallography to people who already have some crystallographic knowledge. How to teach an inexperienced staff-crystallographer about twinning, about how to refine a complicated disorder properly or to avoid overfitting in the refinement of a medium-resolution protein structure? The number of wrong or at least questionable structures published every year reveals the need for further education of people who already work as crystallographers. Offering classes in advanced crystallography at universities is equally important.

While methods to teach basic crystallography have been addressed at earlier ACA meetings, this session calls experienced teachers to share their methods and techniques in teaching advanced crystallography.

Confirmed speaker:

George M. Sheldrick (Universität Göttingen, Germany)

POWDER AND SERVICE SIG SESSIONS

03.01 Interface Between Powder and Single Crystal Diffraction

Full-day session organized by Joseph H. Reibenspies (reibenspies@mail.chem.tamu.edu) and James Britten (xman@xraysg.chemistry.mcmaster.ca).

Single-crystal and powder diffraction have both proven their worth in the arena of materials characterization and structure elucidation. These two fields have often followed their own course, however like many other areas of research, there has always been considerable overlap and areas of common interest. This session will cover topics that are of interest to both disciplines, such as micro diffraction, polymorphism, 2D data collection and structure determination. Investigators are encouraged to participate. Please contact the organizers for more details.

NEUTRON DIFFRACTION SIG SESSIONS

04.01 Frontiers in Single-Crystal Neutron Diffraction

Full-half day session organized by Art Schultz, (ajschultz@anl.gov) and Tom Koetzle (tkoetzle@anl.gov).

The advent of a new generation of neutron sources, including the Spallation Neutron Source (SNS) that is now under construction in Oak Ridge, will make possible many exciting new applications in single-crystal neutron diffraction. With the reduction in crystal size and data collection time that is anticipated at the SNS, the ability to perform systematic studies of a series of crystalline materials will greatly expand the utility of single-crystal neutron diffraction in many areas of interest to chemists and materials scientists. These areas may include organometallic chemistry, hydrogen-bonding, studies of structure as a function of temperature, pressure, applied field, etc. (often called parametric studies), magnetism, and disordered materials. Presentations in this session will discuss a number of frontier areas where 'small molecule' neutron crystallography is of central importance.

SMALL MOLECULE SIG SESSIONS

05.01 Important Bioorganic Science from Small Molecules

Half-day session organized by John Desper (desperj@ksu.edu)

This session will focus on the contribution of "small-molecule" crystallography to bioorganic chemistry. Interactions of organic compounds with biomolecules are intimately determined by molecular geometry. Structural data from small-molecule crystallography, supplemented with the rapidly growing number of published biomolecular crystal structures, can provide guidance for understanding and predicting these interactions. These studies can illuminate such important biochemical phenomena as protein folding, molecular recognition, and enzyme catalysis.

Novel synthetic organic compounds serve both as models for biomolecules and as natural product analogues. Due to advances in synthetic methodology, the size and complexity of these molecules have increased significantly in recent years. Analysis of these "mesomolecules" stretches the traditional definition of small-molecule crystallography, and can require overcoming instrumental and computational problems associated with "large small molecules".

05.02 Combining Spectroscopy, Calculations, and Crystallography for Solving Chemical Problems

Half-day session organized by Alberto Albinati (Univ. of Milan; alberto.albinati@unimi.it) and Larry R. Falvello (Univ. of Zaragoza – C.S.I.C.; falvello@unizar.es).

This session will highlight how the combination of theoretical calculations, spectroscopic techniques, X-ray diffraction and neutron inelastic scattering can give a detailed description not only of the structural features of molecules but of their dynamics and chemical and biological reactivity. We want, once more, to emphasise the importance for crystallographers of using a multidisciplinary approach and stress the importance that crystallographic results have in the study of chemical and biochemical reactivity.



Confirmed speakers:

Prof. A. Deriu, University of Parma, Italy

Dr. J. Eckert, Los Alamos and UCSB

Prof. M. B. Hall Texas A&M,

Prof. P. S. Pregosin, ETHZ, Zuerich, Switzerland

05.03 Non-routine Refinement of Small Molecules

Half-day session organized by Chuck Campana (CCampana@bruker-axs.com):

This session will include presentations on techniques that have been successfully employed to solve and refine problem structures to obtain publication quality results. Examples will include analysis and solution and refinement of various types of twinned structures (e.g. non-merohedral, pseudo-merohedral, merohedral twins), modulated structures, and disordered structures.

GENERAL INTEREST SIG SESSIONS

06.01 General Interest I

Half-day session organized by Alexandre F. T. Yokochi (Alexandre.Yokochi@oregonstate.edu).

Presentations will be selected from submitted abstracts.

06.02 General Interest II: Cool Structures

Half-day session organized by Allen Oliver (alol1@uclink.berkeley.edu).

A "Cool Structure" is anything ranging from, but not limited to, high Z' structures, interesting packing and bonding motifs, alternative and useful crystallization techniques and unusual and interesting structural features. In fact, anything that you may consider to be cool, neat or otherwise interesting crystallographically can be a "Cool Structure".

06.03 General Interest III: Advances in Computing Environments for Crystallography

Half-day session organized by Lachlan Cranswick, Neutron Program for Materials Research (lachlan.cranswick@nrc.gc.ca).

Modern crystallography is undeniably dependent on access to adequate computing resources. New options for inexpensive clustered computing and GRID computing allow for real-time or near-real-time modeling or refinement of complex systems including macromolecules. In addition, the massive amounts of data generated need to be effectively shared creating a need for accessible networks, which in turn create issues with data/network security. This session, and related posters on this topic will be dedicated to exploring these topics.

We welcome abstracts for talks or posters including, but not limited to:

- Real-time visual macromolecular refinement
- Modeling in real-time to match data collection rates
- Crystallographic computation using the GRID
- Cost effective cluster computing using Linux and/or Beowulf
- Super computing power applied to crystallography
- Computer security
- Networking issues
- PC computers optimized for graphics intensive 3D gamers, but applied to crystallography
- Virtual reality hardware systems applied to crystallography
- Crystallographic computing on a chip integrated circuitry optimized for crystallographic number crunching
- Crystallographic collaborative hardware for shared data analysis

AACG SESSIONS

07.01 Biological Macromolecules: Solution Behavior and its Relation to Crystallization

Half-day session organized by Patrick J. Loll (pat.loll@drexel.edu).

The battle to produce high quality crystals is won or lost in solution, before any crystal has the opportunity to form. This half-day session (sponsored by AACG-NASA-ACA) focuses on the role of solution properties in controlling and/or predicting crystallization.

07.02 Macromolecular Crystal Quality and X-ray Diffraction

Half-day session organized by Edward H. Snell (eddie.snell@msfc.nasa.gov).

There are many ways of judging the quality of a crystal. For the structural crystallographer the primary crystal quality requirement is internal order. In this session (sponsored by AACG-NASA-ACA) we are soliciting papers examining the effect of internal order (or the lack of it) on the diffraction properties of macromolecular crystals. Topics include accurate measurement of the order, both long and short-range order, and quantification of the effects of disorder, which may be induced by biochemical, environmental, experimental and other factors. Papers addressing correlations of structural phenomena, such as conformational variations, with disorder, addressing the use of crystal quality measurements to improve structural results, techniques that require high quality crystals, and matching the experimental method to the quality of the crystal are also solicited.

SYNCHROTRON SIG SESSIONS

08.01 Radiation Damage I: Site and Wavelength Specificity; Limits to Dose and Sample Size

Half-day session organized by Gerd Rosenbaum (rosenbaum@anl.gov).

After three international workshops (1999, 2001, 2003) and well attended sessions at the 2002 IUCr-meeting and ACA 2003, radiation damage to macromolecular crystals has re-entered the consciousness of crystallographers like in the days before liquid nitrogen cooling. A number of crystallographic studies have shown the sequence of progressive damage with increasing radiation dose and developed metrics to quantify the damage from the early onset to grossly manifest decay. Also, crystallographers have been alerted to artifacts like change of oxidation state of metal ions. For the first half-day session, we call for papers presenting new results on the mechanism of damage by x-radiation (including model calculations), in particular site specificity, the effects of heavy atoms (including Se) and photon energy. We also call for contributions presenting experimental or calculated data on limits to dose and minimum sample size.

08.02 Radiation Damage II: Extracting Maximum Information from Limited Sample Life

Half-day session organized by Gerd Rosenbaum

For the second of the two half-day sessions on Radiation Damage, we call for papers demonstrating or proposing methods to extract the maximum amount of data within the radiation damage limits of a sample. This includes methods to reduce radiation damage (e.g. scavengers), methods to correct affected data, strategies to maximize redundancy and/or completeness of acquired data for a given radiation dose, and optimal use of detectors.

08.03 Complementary Methods using Synchrotron Radiation

Half-day session organized by Wayne Anderson (wf-anderson@northwestern.edu).

Synchrotron radiation is useful for a wide variety of methods that are complementary to standard crystallographic structure determination experiments. This session will focus on methods that can be applied to non-crystalline samples or that can provide information that can't be obtained from standard crystallographic approaches. Examples might include fiber diffraction, solution scattering, and spectroscopic approaches. The session will include a combination of invited presentations and presentations selected from submitted abstracts.

YOUNG SCIENTISTS SIG SESSIONS

09.01 Topics for the Young Scientist

Half-day session organized Chad Haynes (cah@caltech.edu) and Matthew Clifton (clifto@c@purdue.edu).

This session looks at topics that are of interest to Young Scientists. Following the success of last year's session, this year we will again feature "Interviewing Techniques". In addition, the opportunities and funding available for working/studying outside the US/Canada will be discussed. Any crystallographers who have worked abroad and who would like to share their experiences are invited to contact the organizer about speaking in this session.

MATERIALS SIG SESSIONS

10.01, 10.02 Materials for the 21st Century I & II

Two half-day sessions organized by Brent Heuser (bheuser@uiuc.edu).

Materials development drives technological advancement and structural characterization is a critical step in the development of materials. Two half-day sessions co-sponsored by the Neutron Scattering, Materials Science, and Small Angle Scattering SIGs will focus on the development and/or improvement of materials for 21st century applications. Researchers studying biomaterials, semiconductors, polymers, metals and alloys, and fluids are all invited to submit abstracts. The common theme, of course, is the use of diffraction and/or scattering to study these systems. In addition, materials for 21st energy systems, such as those based on hydrogen or hydrocarbons, are of interest; abstract submission of work in this area is especially encouraged.

SMALL ANGLE SCATTERING SIG SESSIONS

11.01 Ultra Small-angle Scattering Science

Half-day session organized by Peter R. Jemian (jemian@anl.gov).

This session will focus on the scientific progress resulting from ultra-small-angle scattering (USAS, defined loosely as $Q < 10^{-3} \text{ \AA}^{-1}$) experiments, both in the U.S. and abroad. Large things scatter at small angles and even larger things scatter at even smaller angles. USAS is becoming increasingly important in the study of materials. Most, if not all, major neutron and x-ray sources have instruments dedicated to the measurement of the scattering response at ultra small angles. Researchers exploiting the USAS technique with experiments using either X-rays, neutrons, or both, or modeling USAS data are invited to submit abstracts describing their scientific results. This session is co-sponsored by the Small Angle Scattering, Materials Science, and Neutron Scattering SIGs.

11.02 Ultra Small-angle Scattering Techniques

Half-day session organized by Peter R. Jemian (jemian@anl.gov).

This session will focus on emerging demand for development of USAS instruments and techniques, both in the U.S. and abroad. Ultra-small-angle scattering (USAS, defined loosely as $Q < 10^{-3} \text{ \AA}^{-1}$) is becoming increasingly important in the study of materials. Most, if not all, major neutron and x-ray sources have instruments dedicated to the measurement of the scattering response at ultra small angles (defined loosely as $< 10^{-3} \text{ \AA}^{-1}$). Researchers developing USAS instruments or techniques, either with x-rays, neutrons, or both, are invited to submit abstracts. This session is co-sponsored by the Small Angle Scattering, Materials Science, and Neutron Scattering SIGs.

SPECIAL POSTER SESSIONS

12.01 Crystals in Supramolecular Chemistry

Poster presentations that highlight recent developments in supramolecular chemistry or crystal engineering are solicited for this poster session that will complement the Transactions Symposium entitled Crystals in Supramolecular Chemistry. A special poster prize will be awarded. Please contact Alicia Beatty (abeatty@ra.msstate.edu) if you wish to present or if you have any questions.

12.02 Synchrotron and Neutron Research Facilities

The Synchrotron and Neutron SIGs invite members of National Laboratories, Synchrotron Facilities and Neutron Sources to present their unique offerings to the crystallographic community at a special poster session emphasizing these facilities. Posters can highlight or detail their various beamlines and experimental capabilities and laboratory set-ups. Authors and/or beamline representatives manning the posters are strongly encouraged to provide additional literature/hand-outs regarding their facility. If you wish to present, please contact Allen Oliver, University of California, Berkeley (alol1@uclink.berkeley.edu).

Education Outreach

The Protein Database (PDB), the Cambridge Crystallographic Data Centre (CCDC), and the American Crystallographic Association (ACA) are working together to present a workshop on structure and databases. It will be held on **Sunday, July 18th**, and will be targeted towards high school teachers and students in the Chicago area. The morning session will be split into two tracks. Teachers will learn about the classroom version of the CCDC, how to use the PDB as a teaching tool and about tools available to help them in the classroom. They will also receive materials and experiments and demonstrations that they can use in their own classrooms. Students will learn some of the basics of structure from a crystallographic point of view and will have some hands on time to learn about model building and growing crystals. Following lunch we will tour the APS and return to the Hyatt to visit the commercial exhibits and the posters. Attendance will be by invitation. For further information contact Judy Flippen-Anderson (flippen@rcsb.rutgers.edu).

POSTER PRIZES

Pauling Poster Prize

Eligibility: Graduate and undergraduate students only - no post-docs. Awarded to not more than five of the best student (poster) presentations at the Annual Meeting. An additional Pauling Prize sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, will be given to the highest ranked poster from a Canadian laboratory. Each award consists of \$200, a complimentary banquet ticket, and a copy of Linus Pauling's "General Chemistry". Honorable mentions may also be awarded a complimentary banquet ticket. Please indicate your wish to be considered with your abstract submission. Winners will be announced at the banquet on Wednesday, July 21.

Oxford Cryosystems Poster Prize

Eligibility: The Oxford Cryosystems Low Temperature Prize is awarded to any poster describing work in low temperature crystallography. The winner will receive a prize of two hundred and fifty pounds sterling donated by Oxford Cryosystems. Please indicate your wish to be considered with your abstract submission. The winner will be announced at the banquet on Wednesday, July 21.

IUCr Poster Prize

The Executive Committee is pleased to inaugurate a new series of IUCr awards to be 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. Eligibility will be the same as that for the Pauling Poster Prize. Please indicate your wish to be considered with your abstract submission.

Protein Data Bank Poster Prize

Eligibility: The PDB Poster Prize is to recognize a student poster presentation involving macromolecular crystallography. Prize is open to graduate and undergraduate Students only - no postdoctoral posters. Please indicate your wish to be considered with your abstract submission. The winner will be announced at the banquet and an announcement will appear on the PDB Web site and in the PDB Newsletter.

CrystEngComm Poster Prize

An electronic-only Journal from the Royal Society of Chemistry, CrystEngComm (www.rsc.org/CrystEngComm) has kindly agreed to sponsor a prize to be awarded to the best poster in the Transactions symposium (12.01). Please indicate your wish to be considered for this prize with your abstract submission.

Presentation Preparation

Lecture Preparation Each session room will have one projection screen, one slide projector, one overhead projector and one computer projector in each room. The computers will all be IBM PC's (no Macs) loaded with the Windows 2000 operating system, and Microsoft PowerPoint software. Speakers should bring PowerPoint files on Iomega Zip Disks or CD's. **Arrive at the session in which you are speaking well in advance to copy your file onto the computer's hard drive.** It is recommended that you review your presentation in the speaker ready room prior to the beginning of your session. Please indicate your need for this equipment with your abstract submission.

Poster Preparation The allotted size for each poster will be 4' x 4'. Push pins will be available. Poster session chairs will be available to answer questions and provide help during the setup times. The number of poster sessions is dependent upon the number of poster submissions received. Authors will be assigned dates and times to be present at their board. This notification will be sent by postal mail and posted to the meeting web site.

ABSTRACT SUBMISSION

Abstract Submission

Abstracts will be accepted via the web site or by e-mail. Hard copies or disks will not be accepted.

The abstract deadline is March 1, 2004.

Abstracts from members. ACA Members who have paid dues for 2004 should follow the instructions herein; no fee or deposit is required. **Abstracts from non-members.** The Advance Registration Form and payment must accompany abstract submissions from non-members. You may submit the abstract electronically and fax the registration form with payment information to (716) 852-4846 or e-mail your credit card information with your abstract. Acceptable forms of payment: VISA, MasterCard, American Express or checks drawn on U.S. banks in U.S. funds. No purchase orders. Abstracts received without the appropriate fee(s) will be returned to the submitting author and will not be processed until the fee is received.

Preparation of Abstracts

The entire abstract, including title, authors and their affiliations, footnotes, references, tables, equations, etc., should be a maximum of 1500 characters (including spaces) using Times font with 10 point size. Abstracts not conforming to these dimensions will be returned to the author for revision and should be resubmitted before the deadline. Late fees will apply to these revisions. The title should be in upper and lower case letters and should contain no more than 150 characters (including spaces). Titles with more than 150 characters will be truncated. The authors' names and institutions should be in upper and lower case with the **presenting author's name listed first**. A **sample abstract** is available for viewing on the ACA web site under the 2004 Meeting: abstract submission.

Images must be grayscale or black & white line art and be no larger than 1.5" high x 3.5" wide. Size your image in the graphics program before inserting it into your Word file. The image should appear in MicroSoft Word at 100%.

Special characters, symbols, greek characters, mathematical formulae and figures should be confined to the set of fonts that come with the standard distribution of MicroSoft Word.

Authors The author named first in the abstract must present the paper. No one may be first author on more than one abstract.

Invited Abstracts Abstracts for invited papers must be submitted in the same manner as those for contributed papers and are subject to the same applicable abstract fees.

Abstracts on the Web Abstracts will be posted to the ACA web site only if the presenting author's permission is given with the abstract submission. Each abstract will be assigned a temporary abstract number at this time. Presenting authors will be notified by postcard of their final abstract number, session name, date, time, and room assignment approximately 4 weeks prior to the meeting. This information will also be posted on the web site.

Revisions The abstract processing office will not accept revisions. You will have to withdraw the original submission and submit a new one. The same abstract submission fee rules will apply.

Late Abstracts Abstracts received after March 1, 2004, will be considered LATE. There will be a **\$50 late fee** for abstracts postmarked or received electronically after March 1, 2004. This rule will apply to ACA members, non-members, invited and contributed abstracts.

Instructions for Web Site Submission

The recommended method for all abstract submissions is via the web form. Follow the instructions available at:

www.hwi.buffalo.edu/ACA/

For questions send messages to:

aca-inquiries@hwi.buffalo.edu

If an abstract or a question is not acknowledged within 3 working days, please assume that it was not received. Receipt of each file will be acknowledged via a machine generated reply within 24 hours. This means the file has been received but no implication of "readability" is to be assumed. If the file cannot be decoded or has other problems, the sender will be contacted for corrective action.

Instructions for E-mail Submission

Include required information as listed at bottom of this page. The "Subject" line of the e-mail should include presenting author's name & fax number. Example: J. Doe, (555) 555-5555.

E-mail a Microsoft Word file as an attachment to:

aca-abstracts@hwi.buffalo.edu

(please do not send any other messages to this address)

Late fees and/or nonmember registration form and payment must accompany submission.

For questions send messages to:

aca-inquiries@hwi.buffalo.edu

REQUIRED INFORMATION

All Abstract Submissions Must Contain the Following Information in the Order Presented Below:

1. Presenting author's name, address, fax, and e-mail.
2. Session Number (list on page 12). If you are unsure of which number to use, please choose the ".00 " under the appropriate SIG and specify the area of interest.
3. Membership category: Regular, Retired, Postdoc, Student, AACG Member, Non-member, Postdoc non-member, Student non-member
4. Is this an invited paper? yes no
5. Your preferred method of presentation lecture poster
6. May we place your abstract on our web site? yes no
7. May we place your fax and e-mail on web site? yes no
8. List three key words for index, not more than 30 characters each.
9. Is this a poster for consideration for the Oxford Cryosystems Poster Prize? yes no
10. Is this a student poster for consideration for the Pauling Poster Prize? yes no
11. Is this a poster for consideration for the Protein Data Bank Poster Prize? yes no
12. Is this a poster for consideration for the IUCr Poster Prize? yes no
13. Is this a poster for consideration for the CrystEngComm Poster Prize? yes no

SESSION TITLES AND NUMBERS

AWARD SYMPOSIA

- AW.01 Etter Award
- AW.02 Supper Award
- AW.03 Fankuchen Award
- AW.04 Trueblood Award

TRANSACTIONS SYMPOSIUM

- TR.01 Crystals in Supramolecular Chemistry

WORKSHOPS

- WK.01 Hands On Workshop – MAD/SAD Phasing, Data Collection, Processing, and Structure Solution
- WK.02 Small Molecule Crystallography at ChemMatCARS
- WK.03 A Protein Crystallographic Toolbox: CCP4 Software Suite And PDB Deposition Tools
- WK.04 GM/CA - Synchrotrons for the Biologist
- WK.05 APS/IPS Tour

BIOLOGICAL MACROMOLECULES

- 01.00 _____(specify)
- 01.01 Structural Insights into Transcription
- 01.02 Structural Analysis by Hybrid methods
- 01.03 Computational Methods
- 01.04 Difficult Structures
- 01.05 New Structures
- 01.06 Membrane Structures
- 01.07 Macromolecular Assemblies
- 01.08 Structural Bioinformatics
- 01.09 Fresh Approaches to Express and Purify Biomolecules

SERVICE CRYSTALLOGRAPHY

- 02.00 _____(specify)
- 02.01 Small-molecule Problem Structures
- 02.02 Crystallographic Laboratory Practices
- 02.03 Teaching Advanced Crystallography

POWDER DIFFRACTION AND SERVICE CRYSTALLOGRAPHY

- 03.00 _____(specify)
- 03.01 Interface Between Powder and Single Crystal Diffraction

NEUTRON DIFFRACTION

- 04.00 _____(specify)
- 04.01 Frontiers in Single-Crystal Neutron Diffraction

SMALL MOLECULES

- 05.00 _____(specify)
- 05.01 Important Bioorganic Science from Small Molecules
- 05.02 Combining Spectroscopy, Calculations, and Crystallography for Solving Chemical Problems
- 05.03 Non-routine Refinement of Small Molecules

GENERAL INTEREST

- 06.00 _____(specify)
- 06.01 General Interest I
- 06.02 General Interest II: "Cool Structures"
- 06.03 General Interest III: Advances in Computing Environments for Crystallography

AACG SESSIONS

- 07.00 _____(specify)
- 07.01 Biological Macromolecules: Solution Behavior and its Relation to Crystallization
- 07.02 Macromolecular Crystal Quality and X-ray Diffraction

SYNCHROTRON RADIATION

- 08.00 _____(specify)
- 08.01 Radiation Damage I: Site and Wavelength Specificity; Limits to Dose and Sample Size
- 08.02 Radiation Damage II: Extracting Maximum Information from Limited Sample Life
- 08.03 Complementary Methods using Synchrotron Radiation

YOUNG SCIENTISTS

- 09.01 Topics for the Young Scientist

MATERIALS SCIENCE

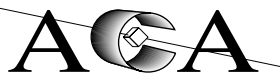
- 10.00 _____(specify)
- 10.01 Materials for the 21st Century I
- 10.02 Materials for the 21st Century II

SMALL ANGLE SCATTERING

- 11.00 _____(specify)
- 11.01 Ultra Small Angle Scattering Science
- 11.02 Ultra Small Angle Scattering Techniques

SPECIAL POSTER SESSIONS

- 12.01 Crystals in Supramolecular Chemistry
- 12.02 Synchrotron and Neutron Research Facilities



ADVANCE REGISTRATION FORM

American Crystallographic Assn. Annual Meeting July 17 - 22, 2004

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City _____

State/Prov. _____

Zip/Postal Code _____

Country _____

Telephone _____

Fax _____

E-mail _____

Registration forms must be postmarked or received on or before June 1, 2004, to qualify for advance registration fee. After June 1, 2004, registration will be accepted at the higher rate. On-site registration will also be available at the higher rate. Cancellations and/or requests for refunds should be made in writing and submitted to ACA Headquarters. For cancellations received before June 1, 2004, 100% of the total remittance will be refunded. Requests received between June 2 and June 30, 2004, will be honored minus 50% of the total remittance. Fees will not be refunded for requests received on or after July 1, 2004.

***Increment charged to non-member registration may be credited toward new member dues for 2004 by submitting a membership application form with the registration form.**

All prices are listed in U.S. dollars and must be submitted in U.S. dollars. Purchase orders will not be accepted. Only U.S. checks, VISA, MasterCard and American Express payments will be accepted. ACA, E.I.N. 22-6075182.

Please make checks payable to ACA and mail to:

ACA Meeting Registration
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Forms submitted via fax
must include credit card payment information.

Fax: (716) 852-4846
E-mail: aca@hwi.buffalo.edu
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REGISTRATION

| | Before June 1 | After June 1 |
|---|------------------|-----------------|
| <input type="checkbox"/> Regular Member | \$330 | \$421 |
| <input type="checkbox"/> Retired Member | \$137 | \$182 |
| <input type="checkbox"/> Postdoc Member | \$171 | \$239 |
| <input type="checkbox"/> Student Member | \$137 | \$182 |
| <input type="checkbox"/> AACG Member | \$330 | \$421 |
| <input type="checkbox"/> Nonmember* | \$444 | \$535 |
| <input type="checkbox"/> Postdoc Nonmember* | \$228 | \$296 |
| <input type="checkbox"/> Student Nonmember* | \$182 | \$228 |
| <input type="checkbox"/> One-day Member | \$165 | \$211 |
| _Sun _Mon _Tues _Wed _Thurs | | |
| <input type="checkbox"/> One-day Nonmember* | \$330 | \$421 |
| _Sun _Mon _Tues _Wed _Thurs | | |

Are you an invited speaker? If yes, list session number _____

REGISTRATION TOTAL \$ _____

WORKSHOPS

| | |
|--|---|
| <input type="checkbox"/> WK01: MAD/SAD Students-\$140 Others-\$160 <input type="checkbox"/> WK02: Small Molecule Cr No charge <input type="checkbox"/> WK03: CCP4/PDB Students-\$80 Others-\$100 | <input type="checkbox"/> WK04: GM/CA- Synchrotrons Students-\$60 Others \$80 <input type="checkbox"/> WK05: APS/IPS Tour Students-\$40 Others-\$60 |
|--|---|

WORKSHOP TOTAL \$ _____

SOCIAL PROGRAM

Opening Reception - Saturday, July 17

No Fee for Registered Participants Will Attend Won't Attend

Guest ticket \$30 ticket # of guest tickets _____

YSSIG Mentor/Mentee Dinner - Sunday, July 18

Mentee \$10 ticket # of tickets _____

Mentor \$10 ticket # of tickets _____

YSSIG Mixer - Monday, July 19

No Fee for Registered Students, Postdocs, Young Scientists

Will Attend Won't Attend

All others \$10 # of tickets _____

Awards Banquet - Wednesday, July 21

\$55 ticket # of tickets _____

\$25 student ticket # of tickets _____

Entree choice: ___ Beef ___ Chicken ___ Vegetarian

SOCIAL TOTAL \$ _____

PAYMENT METHOD

Check (U.S. only) VISA MasterCard American Express

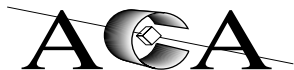
Credit Card Number

____/____/____ - ____/____/____ - ____/____/____ - ____/____/____

Good thru/ Print name of
exp date ____/____ of card holder _____

Authorized Signature
of Card Holder _____

TOTAL REMITTANCE \$ _____



2004 TRAVEL GRANT APPLICATION

Limited funds are available to help students and young scientists attend the **2004 Annual ACA Meeting in Chicago**, July 17-22, 2004. Preference will be given to those presenting a paper or poster. To apply for assistance, send this completed form, a copy of the abstract you plan to submit and a supporting letter from your research advisor. The **deadline for applications is March 1, 2004**; no exceptions. Applicants who received travel grants in 2003 will NOT be eligible for funding in 2004 and should not apply.

Family Name _____

First Name _____

Dept. _____

Inst. _____

Street _____

Box/Apt. # _____

City _____

St/Prov. _____ Zip/Postal Code _____

Country _____

Telephone _____

Fax _____

E-mail _____

Are you an ACA Member?

Yes No

Date of Birth: _____

Have you or will you submit an abstract for presentation at the 2004 meeting? Yes No

If yes, attach a copy to this application but remember that the abstract must also be submitted per the instructions on page 11 to be included in the program.

Estimated cost of transportation: \$ _____

Estimated cost of meals: \$ _____

Estimated cost of lodging: \$ _____

Total amount requested: \$ _____

Are you a:

- Undergraduate Student
- Graduate Student
- Postdoctoral Associate
- Other (explain) _____

Name of Professor or Research Director:

Signature of Professor or Research Director: _____ Date: _____

Signature of Applicant: _____ Date: _____

Submit Application

Mail

Travel Grant Fund
American Crystallographic Association, Inc.
P.O. Box 96, Ellicott Station
Buffalo, NY 14205-0096

Overnight mail

Travel Grant Fund
American Crystallographic Association, Inc.
c/o Hauptman Woodward Medical Research Inst.
73 High St.
Buffalo, NY 14203

E-mail

aca@hwi.buffalo.edu

Fax

(716) 852-4846

Have you:

- Completed this form?
- Attached **copy** of abstract to this application?
- Attached letter of support from Professor or Research Director?



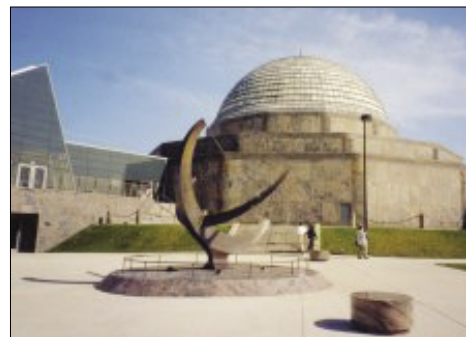
HOTEL RESERVATION FORM

American Crystallographic Association

2004 Annual Meeting

1. YOUR RESERVATION MUST BE GUARANTEED BY USING ONE OF THESE METHODS:
 - A. **GUARANTEED RESERVATION.** USE AMERICAN EXPRESS, CARTE BLANCHE, DINERS CLUB, VISA OR MASTERCARD.
 - B. **ADVANCE DEPOSIT.** ENCLOSE FIRST NIGHT'S DEPOSIT WHEN MAILING YOUR RESERVATION CARD. SHOULD IT BECOME NECESSARY TO CANCEL YOUR RESERVATION, PLEASE REQUEST A CANCELLATION NUMBER.
2. **ALL RATES ARE SUBJECT TO ILLINOIS AND CHICAGO OCCUPANCY OPERATORS AND ACCOMMODATION TAXES, WHICH ARE CURRENTLY 14.9%.**
3. USE THIS FORM ONLY IF YOU ARE UNABLE TO MAKE A RESERVATION VIA THE TELEPHONE OR INTERNET.
4. BE SURE TO MENTION THE ACA CONVENTION CODE "C-GACR" WHEN MAKING A RESERVATION OR YOU MAY NOT BE GIVEN THE CONFERENCE ROOM RATE.
5. **ANY CHANGES MADE TO THIS RESERVATION WITHIN 24 HOURS OF ARRIVAL DATE (INCLUDING EARLY DEPARTURE) ARE SUBJECT TO AN ADMINISTRATIVE FEE.**
6. **CHECK IN TIME IS 3:00 PM CHECK OUT TIME IS 12:00 NOON**
(AFTER 12:00 NOON, ADDITIONAL CHARGES WILL APPLY.)
7. **RESERVATIONS MUST BE RECEIVED NO LATER THAN JUNE 15, 2004**
 - A. VIA FAX: 312-616-6838
 - B. VIA MAIL: ATTN: RESERVATIONS, 151 E WACKER DRIVE, CHICAGO, IL 60601
 - C. VIA TELEPHONE: 1-800-233-1234 OR 312-565-1234.

| | | | | | | |
|--|-----------------------------|--------------------------------|------------------------------------|-----------------------------------|---------------------------|-----------------------------------|
| GROUP NAME: American Crystallographic Association | | DATES: July 15-23, 2004 | | CODE: C-GACR | | |
| GUEST NAME _____ | | | | ARRIVAL DATE: _____ | | |
| COMPANY _____ | | | | Est. time of arrival _____ | | |
| STREET _____ | | | | DEPARTURE DATE: _____ | | |
| CITY, STATE, ZIP, COUNTRY _____ | | | | PHONE: _____ | | |
| ACCOMMODATIONS <small>(please circle rate selection)</small> | SINGLE 1 king bed | DOUBLE 1 king bed | DOUBLE 2 dbl.beds | TRIPLE 2 dbl.beds | QUAD 2 dbl.beds | SUITES 1 bdr. or 2 bdr. |
| GUEST ROOM | \$140 | \$140 | \$140 | \$160 | \$160 | call for rates |
| <small>These group rates are guaranteed if reservation is made prior to June 15, 2004. After that date, prices cannot be guaranteed. Rates do not include 14% taxes.</small> | | | | | | |
| Please indicate preference: Smoking: <input type="checkbox"/> Non-smoking: <input type="checkbox"/> Special requests: _____ | | | | | | |
| TO GUARANTEE RESERVATION: | | | | | | |
| <input type="checkbox"/> CREDIT CARD TYPE: AMERICAN EXPRESS, CARTE BLANCHE, DINERS CLUB, VISA OR MASTERCARD | | | | | | |
| CREDIT CARD NUMBER: _____ | | | EXP. _____ | | | |
| CARDHOLDER NAME: _____ | | | CARDHOLDER SIGNATURE: _____ | | | |
| <input type="checkbox"/> ADVANCE DEPOSIT: Enclosed is a DEPOSIT in the amount of one night's rate. | | | | | | |



CHICAGO

Annual Meeting July 17-22, 2004 Chicago

WORKSHOPS

APS/IPS Tour
MAS/SAD Phasing, Data Collection, Processing, & Structure Solution
Small Molecule Crystallography at ChemMatCARS
CCP4 Software Suite & PDB Deposition Tools
GM/CA - Synchrotrons for the Biologist

AWARD SYMPOSIA

Margaret Etter Award
Supper Instrumentation Award
Isidor Fankuchen Award
Kenneth N. Trueblood Award

TRANSACTIONS SYMPOSIUM

Crystals in Supramolecular Chemistry

MATERIALS SCIENCE

Materials for the 21st Century

SERVICE CRYSTALLOGRAPHY

Small-molecule Protein Structures
Crystallographic Laboratory Practices
Teaching Advanced Crystallography

NEUTRON DIFFRACTION

Frontiers in Single-Crystal Neutron Diffraction



American Crystallographic Association

GENERAL INTEREST

Cool Structures
Advances in Computing Environments

AACG SESSIONS

Biological Macromolecules: Solution Behavior & its Relation to Crystallization
Macromolecular Crystal Quality & X-ray Diffraction

SPECIAL POSTER SESSIONS

Crystals in Supramolecular Chemistry
Synchrotron and Neutron Research Facilities

SMALL ANGLE SCATTERING

Ultra Small Angle Scattering

SYNCHROTRON RADIATION

Radiation Damage: Site and Wavelength Specificity; Limits to Dose and Sample Size
Radiation Damage: Extracting Maximum Information from Limited Sample Life
Complementary Methods using Synchrotron Radiation

SMALL MOLECULES

Important Bioorganic Science from Small Molecules
Combining Spectroscopy, Calculations, and Crystallography for Solving Chemical Problems
Non-routine Refinement of Small Molecules

POWDER DIFFRACTION & SERVICE CRYSTALLOGRAPHY

Interface Between Powder and Single Crystal Diffraction

BIOLOGICAL MACROMOLECULES

Structural Insights into Transcription
Structural Analysis by Hybrid methods
Computational Methods
Difficult Structures
New Structures
Membrane Structures
Macromolecular Assemblies
Structural Bioinformatics
Fresh Approaches to Express and Purify Biomolecules

Abstract Deadline
March 1, 2004

Advance Registration
June 1, 2004

Meeting Information
www.hwi.buffalo.edu/aca