

## The 2011 ACA Summer Course in Small Molecule Crystallography.

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### (1) Announcement

The 10-day intensive course will be offered tentatively July 18<sup>th</sup> through July 27<sup>th</sup>, 2011 at the Indiana University of Pennsylvania. IUP is located in the town of Indiana about 80 miles east of Pittsburgh, PA. The course will cover both single crystal and powder diffraction. Each day will consist of lectures in the morning, hands-on workshops in the afternoon and computer tutorials at night. While some advanced topics will be introduced (Structure solution from powder data, advanced probability methods, solving difficult structures), the curriculum will mostly emphasize fundamental crystallography and no prior crystallographic experience will be assumed. Attendees are encouraged to bring their own single crystal or powder samples for X-ray data collection and are expected to have completed at least undergraduate courses in chemistry, physics and mathematics. Students are advised to read in advance “*Crystal Structure Analysis: A Primer*”, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 24 attendees, who in past years have come from the U.S. and abroad from academia (students and faculty), government and corporate institutions. There will be at least 12 experienced teaching faculty present. Tuition will be \$300 (or \$800 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for an additional \$450 (housing and tuition would cost \$750 or \$1,250 for corporate labs). Approximately 12 student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a tuition waiver, housing costs (double occupancy), breakfast and lunch. The scholarships will be awarded based on the student’s (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments at IUP will include two Bruker-Nonius CAD4 single crystal diffractometers, a Bruker D8 Advance and a Rigaku Miniflex powder diffractometer. Both Rigaku-Americas Inc. and Bruker AXS Inc. have strongly supported the course at IUP and have brought their state-of-the-art bench top diffractometers (SCXmini X-ray Crystallographic System and Smart X2S Benchtop Diffractometer) to the IUP laboratory for student use. This is a very valuable addition to the course. Students will also have access to the Duquesne University X-ray Facility which has a Bruker APEX II single crystal diffractometer and a PANalytical X’Pert Pro powder diffractometer. The IUP computer facilities are excellent and each student will have access to an individual computer during the nightly tutorials. Access will also be available to the Cambridge

structural data base and the ICDD powder diffraction data base. The software used in the course will be Bruker-Nonius SHELXTL, GSAS/EXPGUI, FullProf and and CRYSTMOL.

The Course registration form can be obtained from the ACA web site at <http://www.hwi.buffalo.edu/ACA/>. Completed forms must be received before May 27<sup>st</sup>, 2011 by Prof. Charles H. Lake, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically [lake@iup.edu](mailto:lake@iup.edu) for full consideration. Further information will be updated on the web site or can be obtained from [lake@iup.edu](mailto:lake@iup.edu) or [craven@icubed.com](mailto:craven@icubed.com). International students may receive an early acceptance for VISA purposes.

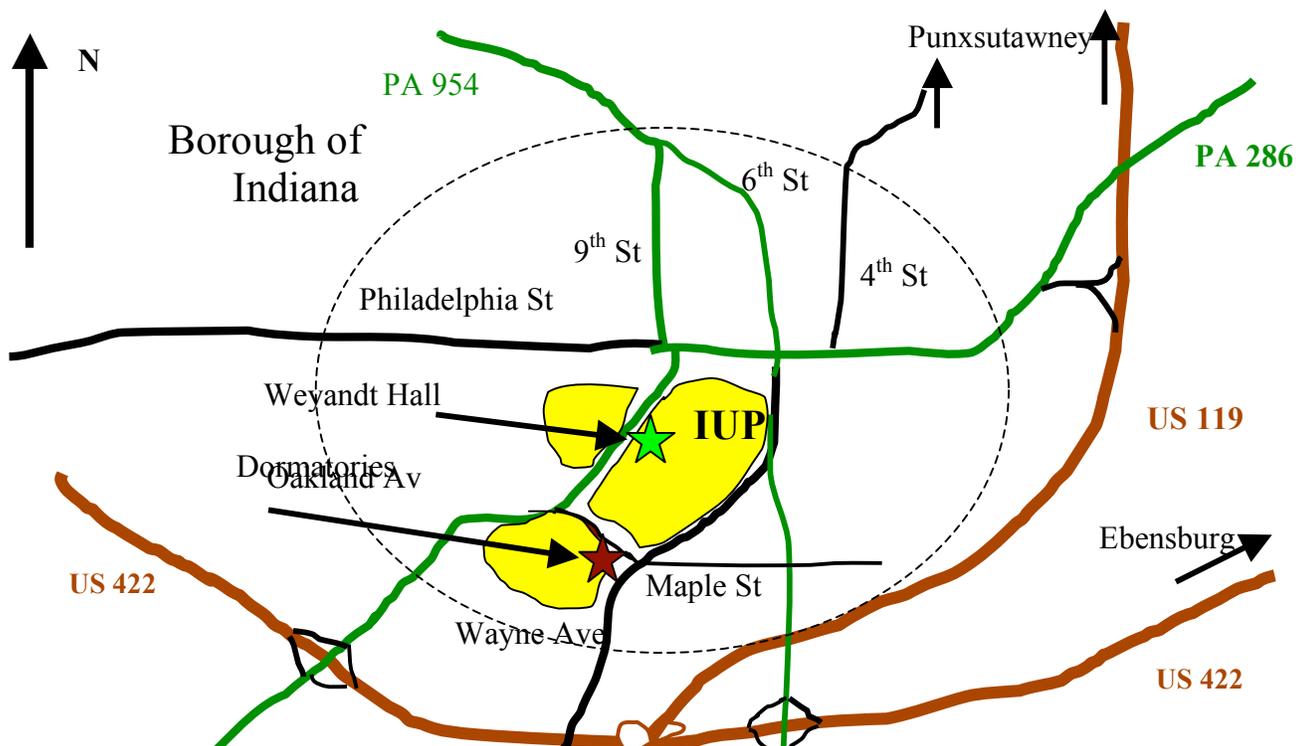
We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of bona fide scientists. Foreign students may be accepted early to provide extra time to process VISA's.

### (2) Scholarships.

Up to twelve student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a waiver of tuition and campus housing costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We aim to provide at least two scholarships specifically for Latin American students. Modest travel support may be requested and will be awarded based upon need.

### (3) Housing.

Campus housing will be available at IUP. Attendees who are awarded scholarships will be lodged in double-occupancy, that is, in an apartment with a bedroom having twin beds.





All apartments have a living room, one bedroom, a bathroom and are air-conditioned. They have a refrigerator and stove and the usual furniture. Attendees who plan to use the kitchen facilities will need to bring utensils, plates, etc. The beds will have linen (sheets, pillow cases, pillows and towels) but it is recommended that attendees should bring an extra towel, blanket and an alarm clock. Attendees who are awarded scholarships will not be charged for housing. For others, the cost will be a total of \$450 including a cafeteria breakfast and lunch. Parking will be available. More information will be provided once, the actual dormitory has been assigned by IUP. A supermarket and the restaurants of downtown Indiana are within walking distance.

#### **(4) Travel to Indiana, PA.**

Indiana, PA is located in South Western Pennsylvania about 80 miles east of Pittsburgh. The nearest major airport is Pittsburgh International. Organizers for the Course plan to run a van service from the airport to IUP on Sunday, June 21<sup>st</sup> 2009 and on Wednesday, July 1<sup>st</sup> upon completion of the course. The ride to the airport takes roughly two hours.

For those traveling by car, Indiana is located about halfway between the interstate highway I 80 and the Pennsylvania turnpike (I 76) which both run east-west (see the map below).

(1) Those coming from the west are advised to take the Turnpike or interstate I 70 and exit at New Stanton, then take the Turnpike extension (route PA 66 north). After the Turnpike ends continue on PA 66 north beyond Delmont about 5 miles. Watch for a sharp turnoff on the right for PA 286 east. Follow this through Saltsburg and eventually to the IUP campus (scenic route). Avoid the alternate route via US 22 and US 119 (see note below).

(2) Those coming from the east on interstate I 80 should exit at Milesburg and follow US 220 south, skirting Penn State University. US 220 becomes interstate I

99 south. Follow this to Holidaysburg then take US 22 west to Ebensburg. From Ebensburg take US 422 west to the South Sixth Street exit in Indiana.

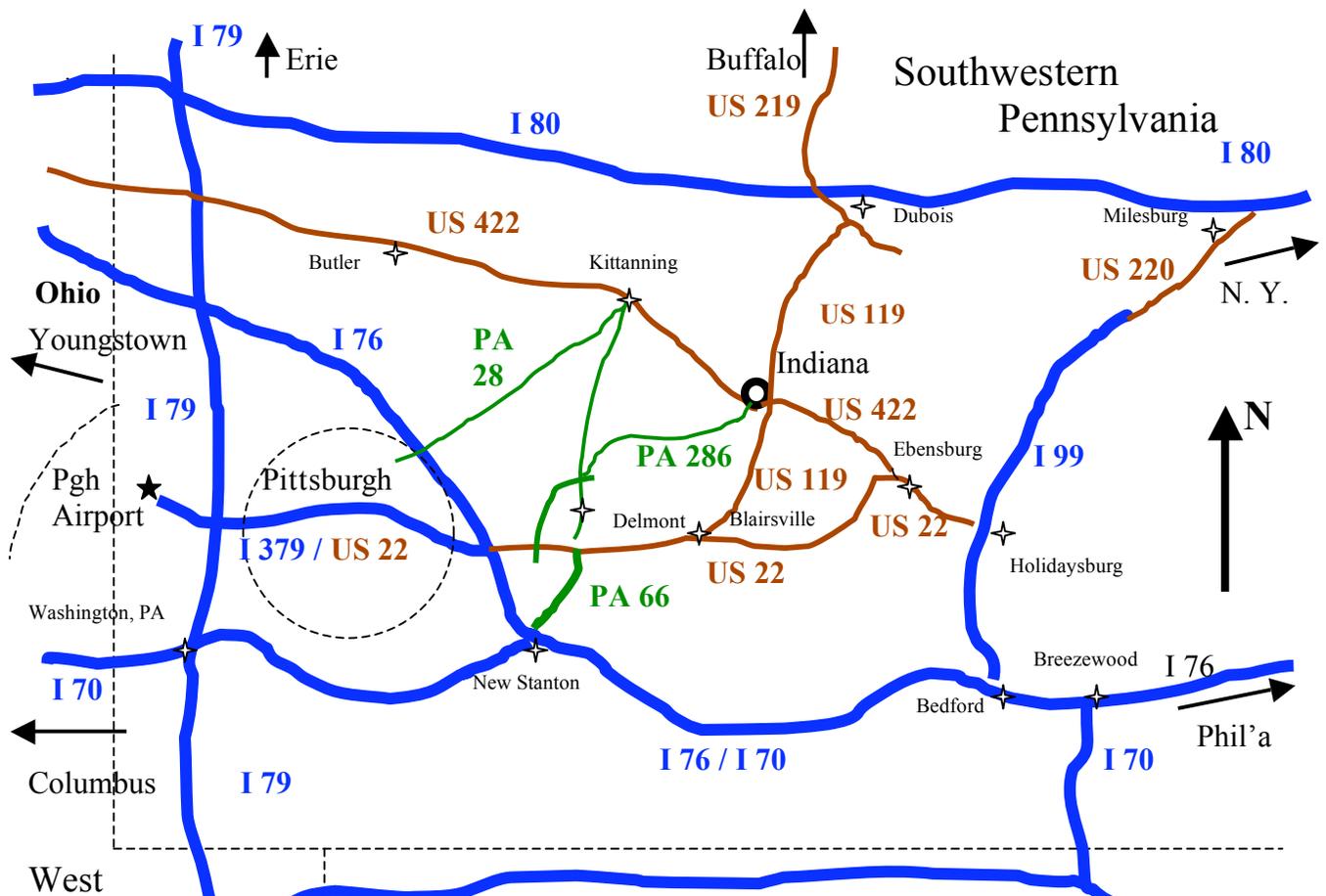
(3) Those coming east on the Turnpike should exit at Bedford then follow US220 north (which is also interstate I 99) and exit on US 22 west. At Ebensburg, take US 422 west to the S. 6<sup>th</sup> Street exit.

(4) Those coming from the north or south on interstate I 79 should exit to interstate I 70 west at Washington, PA. Take I 70 west to New Stanton and then follow directions under (1) above.

(5) Those coming south on US 219 (from Buffalo, NY), should switch to US 119 south a few miles south of Dubois. Take US 119 to the Wayne Ave exit.

(6) Those coming from the southeast on interstate I 70 should exit at Breezewood, go one exit west on the PA Turnpike to Bedford and then follow directions under (3). Note that there is no easy connection from interstate I 68 via Somerset and Johnstown to Indiana. The better approach is along I 70.

(7) Those coming from the city of Pittsburgh on I 379 / US 22 east should exit from US 22 at the Golden Mile Highway (PA 286) then follow (1) above. This will avoid construction around Murrysville.



Attendees will find that, once they are established on campus, there will be little need for a car. The dormitories, lecture halls, computer facility and X-ray lab and workshops are within walking distance of the main street in town (Philadelphia Street) where, between 9<sup>th</sup> and 5<sup>th</sup> Streets, there are restaurants, bars and shops that are popular with IUP students.

**(5) Additional information:**

Indiana County, named after the original inhabitants, was formed in 1803. The land for the borough of Indiana, the County seat, was given by George Clymer, a co-signer of the Declaration of Independence. The County grew into a center for the coal and gas industry. Coal powers the huge generating stations at Shelocta and Homer City that are important resources for the US Northeast. Most of the coal mines have now been shut down so that the County shows little sign of its mining history except for the gaswells. It is said that Indiana County has over 700 miles of gas underground pipeline. Much of the land is presently farmed or covered with hardwood forest. The Fall is a spectacular season in Indiana. On US 422 entering Indiana County there is a sign proclaiming that this is the Christmas tree capital of the world. Certainly there are many nurseries and market gardens in Indiana.

The most famous of Indiana's sons was the movie actor and Air Force General James M. Stewart whose father ran a hardware business on Philadelphia Street. The Jimmy Stewart Museum is on the corner of Philadelphia Street and 9<sup>th</sup> Street. His statue is in front of the County Court House almost across the street from the plaque commemorating the family hardware business.

Indiana has some fine buildings, including the Old County Court House with its gold cupola, located on 6<sup>th</sup> Street and Philadelphia Street. At the back of what is now a bank can be seen the bars of the former jail and the Bridge of Sighs for bringing prisoners into court. Sutton Hall with its tower is a century-old foundation building of IUP from the time when it was a teachers' college. Among other national heritage buildings in town is the Historical Society on South 6th Street. (See also <http://www.indiana-co-pa-tourism.org>)

The Indiana University of Pennsylvania (IUP) has about 13,000 students and faculty, mostly involved in undergraduate studies. IUP is now the County's largest employer. It is the largest of a system of 14 universities that is funded by the Commonwealth of Pennsylvania.

An interdisciplinary X-ray Laboratory was formed at IUP in 1997 when Prof Craven moved from the University of Pittsburgh bringing with him most of the facilities of the former Crystallography Department. For the summer course, the X-ray Lab at IUP will be linked electronically to the Bruker-Nonius diffractometer at Duquesne University (Prof. Aitken). This instrument, which has a CCD detector, will enable students to collect single crystal data rapidly by remote control. An all-day excursion to Pittsburgh will enable students to see this diffractometer at first hand.

In 1999, a consortium of faculty at IUP from Chemistry, Physics and Geology were successful in an application to NSF for a Bruker-Nonius D8 powder diffractometer which is equipped with a heating stage. This will be available for powder data collection during the summer course. The X-ray Lab will have a new acquisition of a Rigaku-Americas Miniflex powder diffractometer. There will be adequate computing facilities, including access to the Cambridge structural data base and the ICDD powder diffraction data base.

Charles H. Lake and Bryan M. Craven,  
Organizers,  
ACA Summer Course, 2011.

**(6) Proposed course curriculum and schedule:**

| Day                              | Morning lectures   | Afternoon/evening  |
|----------------------------------|--|--|
| Sunday, July 17 <sup>th</sup>    | None   | Campus Towers check-in   |
| Monday, July 18 <sup>th</sup>    | Point, Translational and Space Symmetry  | (a) Sample preparation; (b) International Tables, (c) Symmetry practice, Radiation Safety, Databases |
| Tuesday, July 19 <sup>th</sup>   | Principles of X-rays and neutrons, Basic Diffraction Theory, Reciprocal Space  | Repeat (a), (b), (c)<br>Diffraction Instrumentation, Crystmol Tutorial                               |
| Wednesday, July 20 <sup>th</sup> | Atomic Scattering Factors, Systematic Absences, Fourier Methods.               | Repeat (a), (b), (c)<br>Introduction to SHELX  |
| Thursday, July 21 <sup>st</sup>  | Atomic Thermal Vibrations, Single Crystal Data Processing, Probability Methods | Synchrotron Sources, SHELX tutorials, Basic Crystallography Workshops                                |
| Friday, July 22 <sup>nd</sup>    | Intro To Powder Diffraction, Least Squares Analysis, Indexing Powder Patterns  | Basic Crystallography Workshop, Powder Indexing Tutorials. Intro to Fullprof.                        |

|                                  |   |   |
|----------------------------------|---|---|
| Saturday, July 23 <sup>rd</sup>  | Patterson Methods, Rietveld Analysis, Structure Solution from Powder Data | Basic Crystallography Workshop, Intro to GSAS/EXPGUI. Course Picnic       |
| Sunday, July 24 <sup>th</sup>    | Pittsburgh excursion (all day)  | Visit X-ray lab, Chem. Dept, Duquesne University                          |
| Monday, July 25 <sup>th</sup>    | Error Analysis, Shake and Bake, Neutron Diffraction                       | Basic Crystallography Workshop, Difficult Structure Refinement Tutorial.. |
| Tuesday, July 26 <sup>th</sup>   | Problem Structures Twinning Modulated Structures                          | Basic Crystallography Workshop, Prepare Student Presentations             |
| Wednesday, July 27 <sup>th</sup> | Student Presentations   | Course concludes 11:00am  |

The first one-hour lecture each day begins at 8:45 am, the next at 9:45 am and the last at 11:00 am with a lunch break at 12:30pm. The afternoon/evening workshop sessions begin at 2:00pm. Some special one-hour lectures will also be given in the afternoon. Attendees will be in groups of three for purposes of diffractometer data collection and problem solving. Data collection will begin on Tuesday, July 19<sup>th</sup> after the Monday night X-ray safety lecture and will continue throughout the course. Hard copy of the lecture notes and a CD-ROM containing all notes, presentations, photographs and non-proprietary software will be provided as part of the tuition cost for the course.

#### (7) The invited faculty.

The following is a list of invited faculty with research interests:

Jennifer **Aitken**, Duquesne University. *Powder diffraction and Solid-state chemistry*

Sue **Byram**, Bruker-AXS Inc., *Single crystal diffraction.*

Bryan **Craven**, Indiana Univ of Penna. (Course co-organizer). *Crystallography, charge density, neutron diffraction.*

Lee **Daniels**, Rigaku-Americas Inc., *Single crystal diffraction.*

David **Duchamp**, formerly Pharmacia Inc., Kalamazoo. *Structures of small biomolecules, crystallographic software.*

Jenny **Glusker**, Fox Chase Cancer Center. *Structural Biol., Crystallographic education*

Curt **Haltiwanger**, Cephalon Inc. *Single crystal and powder diffraction.*

James **Kaduk**, formerly Innovene., Naperville, IL. *Crystal structure determination from powder diffraction.*

Charles **Lake**, Indiana Univ of Penna. (Course co-organizer). *Solid-state chemistry, crystallographic education, single crystal and powder diffraction.*

Cora **Lind**, University of Toledo *Powder Diffraction and Solid-State Chemistry.*

Aina **Cohen**, Stanford, *Synchrotron Sources, Single Crystal Diffraction.*

Peter **Mueller**, MIT, *Single crystal diffraction, SHELX*

Bruce **Noll**, Bruker AXS Inc., *Single crystal diffraction*

Thomas **Proffen**, Los Alamos National Laboratory. *Neutron Diffraction, Powder Crystallography.*

Brian **Toby**, Argonne National Laboratory. *Neutron Diffraction, Synchrotron Sources, Powder Structure Determination.*

John **Woolcock**, Indiana Univ of Penna. *Inorganic structures, crystallographic databases.*

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**(8) Registration form**

**ACA Summer Course in Small Molecule Crystallography, July 18<sup>th</sup> - July 27<sup>th</sup>, 2011.**

*Chemistry Dept., Indiana University of Pennsylvania, Indiana PA 15705, USA.*

**Registration form.**

This completed form must be received by Prof. Charles H. Lake by May 27<sup>th</sup>, 2011 at the above address, or electronically at [lake@iup.edu](mailto:lake@iup.edu) to be fully considered.

Title                      First name                      Last name

.....  
Name, department, street address, town, state or province and country.

E-mail address:  
.....

Will you need campus parking?                      Will you be traveling by air?  
.....

Will you require campus housing?    If "yes", are you male or female?  
.....

Does your research concern single crystal methods? Powder methods?  
.....

Will you be bringing a sample for X-ray data collection?  
If so state briefly the type of chemical compound; powder or single crystal?

(Preference will be given to samples that are stable and for which data collection under ambient conditions will be satisfactory.)  
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Note that the registration fee for the Course is \$US300 (\$800 for students from Corporate Labs). Campus housing is available for 10 days for an additional cost of \$US450 (registration plus housing totals \$US750 / \$US1250 for Corporate Labs). A check for the total amount (which must be drawn on a U.S. bank) must be received by Profs Craven or Lake at Indiana University of Pennsylvania by July 4<sup>th</sup>, 2011. The check should be made out to “*ACA Summer Course*”.

Up to twelve graduate student scholarships will be awarded, each consisting of a waiver of tuition costs and campus housing costs with two meals a day. Applications will be judged on the basis of (1) scientific ability, (2) expected benefit from the course and (3) skills in the English language. Student applicants must enclose with this form a personal statement addressing the above three criteria. Also, the student’s mentor is asked to send a letter of recommendation to Prof. Lake.

Scholarship awards will be announced by June 3<sup>rd</sup>, 2011. Qualified international students, may be accepted early to help with the VISA process.

Are you applying for a scholarship? Will you attend if this is not awarded?

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