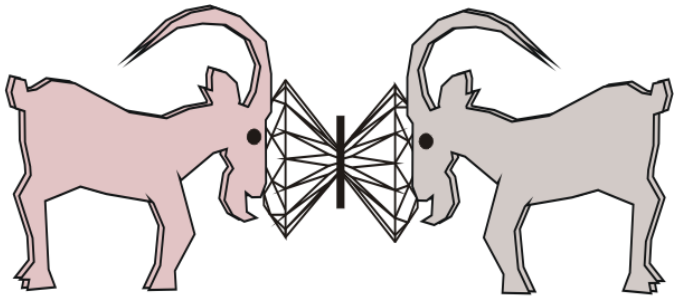
5th Frolic Goats Workshop on High-Pressure Diffraction

15-17 April, 2012

Faculty of Chemistry

Adam Mickiewicz University, Poznań



Local Organizing Committee

Andrzej Katrusiak (chairman), Małgorzata Ratajczak-Sitarz, Armand Budzianowski, Maciej Bujak, Marcin Podsiadło, Anna Olejniczak, Hanna Piotrowicz

The Frolic Goats Workshop on High-Pressure Single-Crystal X-Ray Diffraction using laboratory equipment will consist of a series of general lectures and hands-on laboratory exercises. Its primary goal is to disseminate practical skills allowing one to perform high-pressure experiments in an x-ray lab, and to outline possibilities to continue one's studies at dedicated high-pressure beamlines in synchrotrons, nuclear reactors, and spallation sources.

Modern x-ray diffraction equipment installed in most laboratories can be used for high-pressure experiments straightforwardly, or after few minor modifications – these modifications can be as simple as mounting a shorter collimator and re-positioning the beam-stop to provide space for the diamond-anvil cell (DAC). The DAC is a simple and relatively cheap device, so crystal structures in high pressure can be studied in most x-ray labs.

Registration

Because of the available laboratory space and equipment, the number of participants will have to be limited. The application should be e-mailed to hannap@amu.edu.pl. The candidates will be accepted on the basis of geographical distribution and dates of application. The registration costs will be covered by Organizers and provision will be made for convenient accommodation.

Venue

The workshop will be held at the Faculty of Chemistry, Collegium Chemicum, Adam Mickiewicz University, ul. Grunwaldzka 6, 60-780 Poznań.

The historical building of Collegium Chemicum (PEWUKA, Govermental Palace) is located close to the accommodation, Main Railway Station (1.0 km) and to the Old Market (medieval center of the city, 2.0 km).

Accomodation

Accommodation of various standards is conveniently located close to the Collegium Chemicum:

- Sheraton Hotel ul. Bukowska 3/9 (200 m from Collegium Chemicum) *ca.* 170 Euro/600 złotych (online reservation)
- Jowita ul. Zwierzyniecka 7 (200 m from Collegium Chemicum)
  - – bed & breakfast *ca.* 17 Euro/60 złotych
  - – apartament *ca.* 33 Euro/120 złotych
- Frolic Goats Hostel ul. Wroclawska 16/6 – bed & breakfast; *ca.* 50 Euro/200 złotych (online reservations)

Organizers can assist in booking rooms in Jowita, whereas Sheraton Hotel and Frolic Goats Hostel booking and payments should be arranged by participants themselves.

Travel

Poznań can be easily reached through its airport, railways, and roads. Consult your travel agent or contact us for advice.

Weather

In Poznań we enjoy moderate climate, usually warm and sunny in early Spring, although a jacket and umbrella can prove useful.

Venue: Faculty of Chemistry,
Adam Mickiewicz University (AMU) Poznań
Grunwaldzka 6, Department of Chemistry room. 101

HIGH-PRESSURE DIFFRACTION IN POZNAŃ

Scientific Programme of the 5th Frolic Goats Workshop on High-Pressure Diffraction

Poznań 15-17 April 2012

Sunday 15th:

Arrivals; Kayak trip on the Warta River – participants can either go to Puszczykowo by train, lead by the guides from Poznań, or go there in a cab from the Jowita Dormitory. Please contact the organizers about the details. The trip starts from the marina at Ośrodek Leśny, ul. Wodziczki 3, in Puszczykowo at 15:00.

Monday 16th:

8:30 Registration (Collegium Chemicum, ground floor, room 24)
9:00 *Opening ceremony*
9:10Andrzej Katrusiak (UAM): Introduction to high-pressure techniques in the lab.
9:30 Michał Kaźmierczak (UAM): Absorption and gasket-shadowing corrections for a diamond-anvil cell
10:00 Kamil Dziubek (UAM): Frolic-Goats Spring Project
Coffee break 10:30 - 11:00
11:00 Ewa Patyk (UAM): Interactions in new high-pressure sucrose polymorph
11:30 Armand Budzianowski (U. Warsaw): High-pressure powder-diffraction crystallography
12:00 Damian Paliwoda (UAM): The hidden imidazole polar phase
12:30 Michał Dobrowolski (ESRF): High-pressure experiments at synchrotrons: ID27
Lunch break 13:00
14:30 Laboratory exercises: DAC construction, alignment, loading, diffraction experiment

Tuesday 17th:

9:00 Marcin Podsiadło (UAM): Carney's rule in chloroethanes
9:30 Michał Andrzejewski (UAM):.Remote halogen switch of amine hydrophilicity
10.00 Anna Olejniczak (UAM): Pressure-induced hydration in thiourea
Coffee break 10:30-11:00
11:00 Weizhao Cai (UAM): A new high-pressure polymorph of KH_2PO_4 (KDP)
11:30 Kamil Dziubek (UAM): Computation of interactions energy in molecular crystals I
12:00 Jędrzej Marciniak (UAM): Computation of interactions energy in molecular crystals II
12:30 Andrzej Katrusiak (UAM): Presentation of high-pressure structures - autostereograms
13:00 Round-table-discussion
14:00 Closing Cremony

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY
ADAM MICKIEWICZ UNIVERSITY POZNAŃ
FNP Foundation for Polish Science
EUROPEAN UNION EUROPEAN REGIONAL DEVELOPMENT FUND

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