

SOCIETAS SCIENTIARUM VARSAVIENSIS
INSTITUTE OF PHYSICAL CHEMISTRY OF THE POLISH ACADEMY OF SCIENCES
POLISH CRYSTALLOGRAPHIC ASSOCIATION
COMMITTEE OF CRYSTALLOGRAPHY OF THE POLISH ACADEMY OF SCIENCES
ECA SIG 7: MIRSIG MOLECULAR INTERACTION AND RECOGNITION SPECIAL INTEREST
GROUP OF THE EUROPEAN CRYSTALLOGRAPHIC ASSOCIATION

Scientific Programme

Polish School of Crystallography – Chemical Crystallography of the XXIst Century

Gierłoż near Kętrzyn, Mazurian Lake District
Poland

September 5 - 11, 2011



co-financed by the Polish Academy of Sciences



Key Partner of the Polish Academy of Sciences in celebration of the IYC
2011 and MSC-100



Agilent Technologies

Co-sponsor

Monday, 5 September

- 13:00 – 22:00 *Registration*
- 19:00 *Dinner & Get Together Party*

Tuesday, 6 September

- 7:30 – 9:00 *Breakfast*
- 9:00 – 9:15 Opening remarks
- 9:15 – 9:45 **Introductory lecture “History of Polish Crystallography” – Stanisław Hodorowicz (Poland)**
- 9:45 – 10:15 *Coffee break*
- 10:15 – 11:15 **Opening lecture „Crystal Structure Solution – State of the Art.” – Carmelo Giacovazzo (Italy)**
- 11:15 – 11:30 **Discussion**
- 11:30 – 12:30 **“Obtaining chemical information from structural data – analysis of geometrical parameters, weak interactions as Hydrogen bond, CH/ π interactions, π/π interactions” – Fernando Lahoz (Spain)**
- 13:00 – 15:00 *Lunch*
- 15:00 – 18:00 Conference tour
- 19:00 *Dinner*

Wednesday, 7 September

- 7:30 – 9:00 *Breakfast*
- 9:00 – 9:45 **“Direct methods in chemical crystallography of XXIst century – SIR2009” – Carmelo Giacovazzo (Italy)**
- 9:45 – 10:00 **Discussion**
- 10:00 – 10:30 *Coffee break*
- 10:30 – 12:30 **Hands on session with the use of SIR2011**
- 12:30 – 13:00 **“The treatment of chirality in the structural analysis” – Fernando Lahoz (Spain)**
- 13:00 – 15:00 *Lunch*
- 15:00 – 16:00 **Louis Farrugia: Demonstrations and hands - on practical experience of crystallographic software paralel with Fernando Lahoz :The validation of structures and „Practical sessions: procedures for proper integration, and refinement of 'common' complicated structures (disorder etc)**
- 16:00 – 16:30 *Tea break*

16:30 – 19:00 **Poster session**

19:00 *Dinner*

Thursday, 8 September

7:30 – 9:00 *Breakfast*

9:00 – 10:00 **Sponsors time**

10:00 – 10:30 *Coffee break*

10:30 – 12:30 **Louis Farrugia: Demonstrations and hands-on practical experience of crystallographic software parallel with Fernando Lahoz The validation of structures and „Practical sessions: procedures for proper integration, and refinement of 'common' complicated structures (disorder etc)**

13:00 – 15:00 *Lunch*

15:00 – 15:45 **“Detectors in x-ray diffractometry and the results of structure analysis” – Wojciech Wolf (Poland)**

15:45 – 16:00 **Discussion**

16:00 – 16:30 *Tea break*

16:30 – 17:15 **“X-ray analysis of modulated structures” – Adam Pietraszko (Poland)**

17:15 – 17:30 **Discussion**

19:00 *Dinner*

Friday, 9 September

7:30 – 9:00 *Breakfast*

9:00 – 9:45 **“X-Ray structural analysis with twinned crystals” – Maria Gdaniec Poland)**

9:45 – 10:00 **Discussion**

10:00 – 10:30 *Coffee break*

10:30 – 11:15 **“Difficult structures – DIRDIF” – Agnieszka Szumna (Poland)**

11:15 – 11:30 **Discussion**

11:30 – 12:15 **"X-ray structural analysis of soft materials" – Henryk Drozdowski (Poland)**

12:15 – 12:30 **Discussion**

13:00 – 15:00 *Lunch*

15:00 – 15:45 **“Structure of low-dimensional solids” – Radomir Kuzel (Czech Republic)**

15:45 – 16:00 **Discussion**

16:00 – 16:30 *Tea break*

16:00 – 16:45 **“Techniques and methods in high-pressure diffractometry” – Andrzej Katrusiak (Poland)**

16:45 – 17:00 **Discussion**

19:00 *Dinner*

Saturday, 10 September

7:30 – 9:00 *Breakfast*

9:00 – 9:45 **"The Charge Density Approach to Metal-Metal Bonding" – Louis Farrugia (UK)**

9:45 – 10:00 **Discussion**

10:00 – 10:30 *Coffee break*

10:30 – 11:15 **"High-pressure crystal structures" – Andrzej Katrusiak (Poland)**

11:15 – 11:30 **Discussion**

11:30 – 12:30 **"The Future of Macromolecular Crystallography: Rational Structural Genomics – William L. Daux (USA)**

12:30 – 13:00 **Discussion**

13:00 – 15:00 *Lunch*

15:00 – 15:45 **"Crystallography of Supramolecular Inclusion Compounds" – Kinga Suwinska (Poland)**

15:45 – 16:00 **Discussion**

16:00 – 16:30 *Tea break*

16:30 – 18:30 **Poster session**

19:00 *Barbeque*

Sunday, 11 September

7:30 – 9:00 *Breakfast*

9:00 – 10:00 **Closing lecture "Challenges for Supramolecular Crystallography: Metal organic Nanocapsules" – Jerry L. Atwood USA)**

10:00 – 10:30 **General discussion and closing remarks**

10:30 – 11:00 *Coffee break*

11:00 *Departure*