

XXI. International Conference „Horizons in Hydrogen Bond Research”
13 – 18 September 2015, Wrocław, Poland
(www.hbond2015.chem.uni.wroc.pl)

Updated Conference Programme

Wrocław, September 3, 2015

Sunday, September 13

15:00 – 21:00 **Registration – Building of the Faculty of Law,
Administration and Economy (Uniwersytecka Street 7-10)**

18:30 **Get-together party**

Monday, September 14

8:00		Registration
8:45 – 9:00		Opening
Chairman:	Henryk Ratajczak	
9:00 – 9:50	OL	Jean-Marie Lehn (Nobel Prize in Chemistry in 1987) From supramolecular chemistry towards adaptive chemistry. Aspects of hydrogen bonding.
9:50 – 10:30	IL-1	Pavel Hobza (Prague, Czech Republic) Hydrogen and sigma-hole bonding: theoretical approach.
10:30 – 11:10	IL-2	Frank Böckler (Tübingen, Germany) Improving the applicability of halogen bonding in drug discovery.
11:10 – 11:40		Coffee break
11:40 – 12:20	IL-3	Célia Fonseca Guerra (Amsterdam, The Netherlands) Covalence, not Resonance-Assistance, behind cooperative hydrogen and halogen bonds.
12:20 – 13:00	IL-4	Andrzej Sokalski (Wrocław, Poland) Towards non-empirical atom-atom potentials for non-bonded interactions.
13:00 – 15:00		Lunch
Chairman:	Martin Suhm	
15:00 – 15:40	IL-5	Angelos Michaelides (London, Great Britain) Quantum nature of the hydrogen bond: Insight from ab initio path integral molecular dynamics.
15:40 – 16:00	OC-1	Judy I-Chia Wu (Houston, Texas, USA) On the nature of low barrier H-bonds in enzyme catalysis/
16:00 – 16:20	OC-2	Ewa Brylska (Wrocław, Poland) Molecular interaction of human serum albumin with meloxicam – molecular modeling studies.
Chairman:	Austin J. Barnes	
16:20 – 16:50		Coffee break
16:50 – 17:10		FQS Poland Presentation of research and development of new software in the field of chemistry, materials and life sciences.
17:10 – 17:30	OC-3	Oleg A. Filippov (Moscow, Russia) Role of hydrogen bonds in hydrogen transfer reaction of metal hydrides.
17:30 – 17:50	OC-4	Igor E. Golub (Moscow, Russia) A study of multifurcate dihydrogen bonded complexes with participation of boron hydrides.
17:50 – 18:10	OC-5	Tomasz Masłowski (Zielona Góra, Poland) What proton conductivity can tell us about H-bond potentials?

Tuesday, September 15

Chairman:	Elangannan Arunan
9:00 – 9:40	IL-6 Sammy El-Shall (Richmond, Virginia, USA) Unconventional hydrogen bonding between organic ions and polar molecules.
9:40 – 10:20	IL-7 Ibon Alkorta (Madrid, Spain) Hydrogen bonded anion-anion aggregates.
10:20 – 11:00	IL-8 Lars Pettersson (Stockholm, Sweden) Water – a tale of two liquids.
11:00 – 11:30	Coffee break
Chairman:	Poul Erik Hansen
11:30 – 12:10	IL-9 Markus Gerhards (Kaiserslautern, Germany) Combined IR/UV spectroscopy on hydrogen-bonded systems: from peptides to photophysical reactions.
12:10 – 12:30	OC-25 Vlasta Mohaček Grošev (Zagreb, Croatia) Evidence of polaron excitations in Raman spectra of oxalic acid dihydrate at low temperatures.
12:30 – 12:50	OC-6 Barbara Golec (Warsaw, Poland) Hydrogen bond-induced changes in photophysics and photostability of indolenaphthyridines.
12:50	Conference photo – Leopoldian Assembly Hall, the main building of the University
13:10 – 15:00	Lunch
Chairman:	Hans-Heinrich Limbach
15:00 – 15:20	OC-7 Erik T. J. Nibbering (Berlin, Germany) Correlating photoacidity to hydrogen-bond structure by use of the local O-H stretching probe in hydrogen-bonded complexes of aromatic alcohols.
15:20 – 15:40	OC-8 Mark Sigalov (Negev, Israel) Structure, intermolecular and photoinduced intramolecular hydrogen bonding in 2-pyrrolylmethylidene cycloalkanones.
15:40 – 16:00	OC-9 Pierre Asselin (Paris, France) Jet-cooled high resolution infrared spectroscopy of hydrated hetero clusters.
16:00 – 16:20	OC-10 Jose A. Fernandez (Leioa, Spain) Exploring the conformational preferences of aniline aggregates in jets.
16:20 – 16:40	OC-11 Michał Gil (Warsaw, Poland) Structural distortion and fluorescence enhancement in diazatriphenylenes and their hydrogen-bonded complexes in supersonic jets.
16:40 – 17:10	Coffee break
17:10 – 18:40	Poster session I (Posters: 1 – 36)

Wednesday, September 16

- Chairman:** Wouter Herrebout
- 9:00 – 9:40** IL-11 **Walther Caminati** (Bologna, Italy)
Tunneling dynamics, proton transfer, conformational equilibria and Ubbelohde effect in adducts of carboxylic acids.
- 9:40 – 10:20** IL-12 **Ehud Pines** (Beer-Sheva, Israel)
Understanding factors affecting red-shifts for the proton stretch vibration frequency of O-H...B hydrogen bonding complexes.
- 10:20 – 10:40** OC-12 **Matthias Heger** (Göttingen, Germany)
Anharmonicity and the hydrogen bond.
- 10:40 – 11:00** OC-13 **Ruslan E. Asfin** (St. Petersburg, Russia)
Structure of the absorption bands of complexes in the gas phase with different hydrogen bond strengths. Fourier spectra and *ab initio* anharmonic calculations.
- 11:00 – 11:30** **Coffee break**
- Chairman:** Janez Mavri
- 11:30 – 11:50** OC-14 **Stéphane Coussan** (Marseille, France)
From water aggregates trapped in cryogenic matrices to amorphous solid water.
- 11:50 – 12:10** OC-15 **Igor Reva** (Coimbra, Portugal)
Near-infrared-induced conformational cis-trans switching in carboxylic acids isolated in cryogenic inert matrices.
- 12:10 – 12:30** OC-16 **Ragupathy Gopi** (Kalpakkam, India)
Study of blue shifting hydrogen bond in fluoroform with Lewis bases (HCl, H₂O, and C₆H₆): A matrix isolation infrared and *ab initio* studies.
- 12:30 – 12:50** OC-17 **Aude Bouchet** (Berlin, Germany)
Binding motifs of a microhydrated neurotransmitter: IR spectroscopy of rare gas-tagged protonated phenylethylamine and its water clusters.
- 12:50 – 15:00** **Lunch**
- Chairman:** Jan Lundell
- 15:00 – 15:20** OC-18 **Michel Mons** (Gif-sur-Yvette, France)
NH – OC amide-amide H-bonds in peptides revisited in light of gas phase spectroscopy of beta-peptides.
- 15:20 – 15:40** OC-19 **Sylwia Olsztyńska-Janus** (Wrocław, Poland)
Weakening of hydrogen bonds of biological structures by near infrared radiation.
- 15:40 – 16:00** OC-20 **Kasper Mackeprang** (Copenhagen, Denmark)
The effect of large amplitude motions on the vibrational spectra of hydrogen bonded complexes.
- 16:00 – 16:30** **Coffee break**

Special session to honour prof. Lucjan Sobczyk

Chairman:	Kazimierz Orzechowski
16:30 – 17:10	IL-13 Aleksander Koll (Wrocław, Poland) Polarity of hydrogen bond.
17:10 – 17:50	IL-14 Hans-Heinrich Limbach (Berlin, Germany) Acid-base hydrogen bonds in different environments: From organic solvents to enzymes.
17:50 – 18:30	IL-15 Poul Erik Hansen (Roskilde, Denmark) Isotope effects in hydrogen bond research.

Thursday, September 17

Chairman:	Konstatin G. Tokhadze
9:00 – 9:40	IL-16 Christoph A. Schalley (Berlin, Germany) Multistimuli-responsive supramolecular gels.
9:40 – 10:20	IL-17 Ilya Shenderovich (Regensburg, Germany) Hydrogen bond reveals the morphology of non-crystalline solids.
10:20 – 10:40	OC-21 Vytautas Balevicius (Vilnius, Lithuania) Solid state NMR study of materials for innovative medicine: sub-nano structure and dynamics of spin clusters containing hydroxyl groups.
10:40 – 11:00	OC-22 Elena Bogdan (Nantes, France) Experimental and theoretical evidences of intramolecular OH...F hydrogen bonding in saturated acyclic fluoroalcohols.
11:00 – 11:30	Coffee break
Chairman:	Zofia Mielke
11:30 – 12:10	IL-18 Sanjay Wategaonkar (Mumbai, India) NH...S interaction perspective.
12:10 – 12:30	OC-23 Anne Schou Hansen (Copenhagen, Denmark) Comparing second and third row elements, N, O, P and S, as hydrogen bond acceptor atoms.
12:30 – 12:50	Patrycja Radek (Wrocław, Poland) Wrocław Research Centre EIT+
12:50 – 14:30	Lunch
14:30 – 16:00	Poster session II (Posters: 37 – 73)
16:00 – 18:00	Excursion
19:30 – 23:00	Conference dinner – HP Park Plaza Hotel restaurant (11-13 Bolesław Drobner street, Wrocław)

Friday, September 18

Chairman:	Jacek Waluk
9:00 – 9:40	IL-19 Andrzej Katrusiak (Poznań, Poland) Pressure-induced anomalous transformations of hydrogen-bonds and their consequences for material sciences.
9:40 – 10:20	IL-20 Barbara Wyslouzil (Columbus, Ohio, USA) The role of hydrogen bonding in phase transition.
10:20 – 10:50	IL-21 Grażyna Bator (Wrocław, Poland) The unconventional C-H...X hydrogen bonds. An application of the neutron scattering.
11:00 – 11:30	Coffee break
11:30 – 12:10	IL-22 Jože Grdadolnik (Ljubljana, Slovenia) Hydrogen bonding in, and structure of blocked dipeptides.
12:10 – 12:30	OC-24 Agnieszka Rybarczyk-Pirek (Łódź, Poland) N-oxide group as a proton acceptor in p-nitropyridine-N-oxide cocrystals.
12:30 – 12:50	Closing the HBond2015
	Invitation to HBond2017
12:50 – 14:30	Lunch