

Sunday, September 11th 2011

- 12.40 – 13.40 Registration
- 13.45 – 13.50 Opening, *Chair: M. A. Suhm*
- 13.50 – 14.30 **WI1: D. M. Benoit**
Weak hydrogen bonds – an anharmonic perspective
- 14.30 – 14.50 **T01: Y. Cornaton**
Toward a new, global potential energy surface for the H₂O-HF complex
- 14.50 – 15.10 **T02: F. Kollipost**
Far infrared spectroscopy of hydrogen bonded clusters in supersonic jet expansions
- 15.10 – 15.30 **T03: V. A. Levina**
On the role of group 10 transition metals in dihydrogen bonding
- 15.30 – 15.50 **T04: N. Lüttchwager**
Spontaneous Raman spectroscopy of low-volatility molecules in a supersonic jet
- 15.50 – 16.20 Coffee break
- 16.20 – 16.25 *Chair: P. M. Tolstoy*
- 16.25 – 17.05 **WI2: E. V. Boldyreva**
Variable-temperature and variable-pressure studies of hydrogen bonds in molecular crystals
- 17.05 – 19.05 **P01–31: Poster advertisements** (3 minutes each)
- 19.05 – 22.00 Buffet dinner and poster session

Monday, September 12th 2011

- 09.15 – 09.20 *Chair: H.-H. Limbach*
- 09.20 – 10.00 **WI3: D. Sebastiani**
Hydrogen bonding and proton mobility – wife and husband – characterized by *ab-initio* molecular dynamics simulations and spectroscopy
- 10.00 – 10.20 **T05: M. A. Vovk**
Investigation of microstructure of hydration shells of HCOO⁻, CH₃COO⁻ and SO₄²⁻ ions by NMR-relaxation and quantum-chemical methods
- 10.20 – 10.30 Short coffee break

- 10.30 – 10.50 T06: **R. Misra**
Deciphering contrasting hydrogen bonding pattern of PACO with solvents in the ground and excited states
- 10.50 – 11.10 T07: **R. M. Forck**
Size resolved infrared spectroscopy of $\text{Na}(\text{CH}_3\text{OH})_n$ ($n=4-7$) clusters in the OH stretching region
- 11.10 – 11.30 T08: **B. A. Zakharov**
Monitoring selected hydrogen bonds in crystal hydrates of amino acid salts: Combining variable-temperature single-crystal x-ray diffraction and polarized Raman spectroscopy
- 11.30 – 11.50 T09: **M. Nedić**
Polarization FTIR microspectroscopy of sublimated methyl mandelate, mandelic acid and phenylethylamine crystals
- 11.50 – 13.45 Lunch break
- 13.45 – 13.50 *Chair: I. G. Shenderovich*
- 13.50 – 14.30 WI4: **A. V. Nemukhin**
Modeling hydrogen-bonded biomolecular systems by the quantum-mechanics-molecular mechanics (QM/MM) methods
- 14.30 – 14.50 T10: **M. G. Khrenova**
Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1
- 14.50 – 15.10 T11: **L. I. De Beuckeleer**
Pyrrole in liquid xenon, an $\text{N}-\text{H}\cdots\pi$ bonding experience
- 15.10 – 15.30 T12: **G. A. Silant'ev**
Hydrogen bonding dichotomy in ruthenium hydride complex $\text{CpRuH}(\text{dppe})$
- 16.00 – 17.00 Coffee break (physics building)