

Fundamentals Interest Group Workshop and Business Meeting
Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy
ASMS 2015, St. Louis, MO

Presiding Officers: Alessandra Ferzoco and Jonathan Martens as proxy for Jos Oomens

Attendance: ~85 peak

Business Meeting Notes

Michael Van Stipdonk was selected as the new co-chair for the upcoming year and Alessandra will rotate in as chair. The group would like to thank Jos for two years of service to the group and his efforts in organizing this year's workshop! We would also like to thank Jonathan for his assistance during the workshop.

The group was solicited for suggestions for oral session and workshop topics at future conferences. It was noted that the number of dedicated fundamental sessions has decreased from ~6-7 in the prior several years to ~5 this year. The current trajectory seems to be away from named and dedicated fundamentals sessions and toward topic-based sessions that could include both fundamental and applied presentations. The audience was of mixed opinion about this strategy.

Workshop Notes

The scientific portion of the workshop was comprised of six short presentations spanning the purview of mass spectrometry fundamentals with each talk followed by discussion.

- Valérie Gabelica of Inserm and the University of Bordeaux spoke of the trade offs when trying to study the details of systems of biological size. Questions she raised with the audience were about whether it was feasible or useful to do full ab initio molecular dynamics for only critical protons, whether or not cooling helps for large systems, whether force field parameters specifically for the gas phase should be developed, and whether all atomic details need to be known. Discussion of these questions alone could have comprised an entire workshop!
- Alex Nickel of Kent Ervin's group at the University of Nevada, Reno, presented his measurements on the gas phase acidities of linear hexanols. It is a good thing his presentation was this year instead of 2014 as his measurements disagree with John Bartmess', the honoree of the 2014 workshop! Alex used branched hexanols as a control to see if the linear anions are most stable as a cyclic structure as previously thought. The cyclic anion was not found to be the most stable, and the discussion focused on the caveats of the kinetic method.
- David Marshall from Steven Blanksby's group at the Queensland University of Technology in Brisbane, Australia, posed the question "as the charge is moved away from the radical in a distonic ion does the bond dissociation energy (BDE) or proton affinity approach the value of the neutral?" In fact they saw the opposite trend in BDE. They went on to question what other scaffolds and charge carriers, in particular biochemically relevant structures, can stabilize radicals.
- Kaveh Jorabchi of Georgetown University presented his new method for measuring the time of ionization in an electrospray droplet, and wonders what chemical information the

measurement can convey. His experiment is based on a synchronized pulsed droplet source and ion mobility cell in front of the vacuum orifice of his mass spectrometer. His results are interpreted based on the statistics of small versus large droplets and the expected surface activity of the ion.

- Ken Lazlo from Matt Bush's group at the University of Washington showed results from gas phase proton transfer reactions where folding of the protein occurs upon conversion from an anion to a cation. Intriguingly the final cross-section is consistent and independent of the initial charge state and cross-section.
- Richard Cox of Peter Armentrout's group at the University of Utah presented bond dissociation energies for a series of lanthanide and actinide oxides and showed the two groups to have statistically equivalent values. Due the radioactive and pyrophoric nature of the actinides the results could be of practical usefulness. Theory failed to predict the trend, and it was unexpected as the lanthanides have buried 4f electrons and exhibit mostly size-dependent properties whereas the actinides exhibit a greater variety of hybridization of the 5f orbitals.