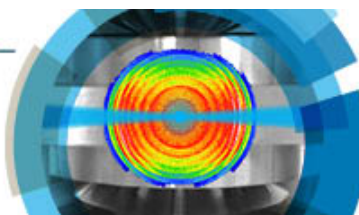


Advances in Ion Spectroscopy – From Astrophysics to Biology

Faraday Discussion



8–10 April 2019
York, UK

Monday 8 April

| | | |
|-------|--|-------------|
| 11:30 | Registration, Tea and Coffee | |
| 12:00 | Lunch | |
| 12:45 | Welcome and Introductions Caroline Dessent and Jan Verlet, <i>Co-Chairs of Scientific Committee</i> | |
| 12:55 | Outline of Discussion Format Amelia Newman and Alexander Whiteside, <i>Royal Society of Chemistry Publishing Editors</i> | |
| 13:00 | Introductory Lecture (Session Chair: Caroline Dessent) Mark Johnson <i>Yale University, USA</i> | |
| | Session 1: Controlling internal degrees (Session Chair: Roland Wester) | |
| 14:00 | Photodetachment and photoreactions of substituted naphthalene anions in a tandem ion mobility spectrometer Evan Bieske, James Bull, Jack Buntine, Michael Scholz, Eduardo Carrascosa, Linda Giacomozzi and Mark Stockett <i>University of Melbourne, Australia</i> | Paper 24878 |
| 14:05 | Hydration motifs of ammonium bisulfate clusters of relevance to atmospheric new particle formation Christopher Johnson and Yi Yang <i>Stony Brook University, USA</i> | Paper 25066 |
| 14:10 | Conformational assignment of gas phase peptides and their H-Bonded complexes using far-IR/THz: IR- UV ion dip experiment, DFT-MD spectroscopy, and Graph Theory for modes assignment Marie-Pierre Gageot, Daria Galimberti, Sana Bougueroua, Jérôme Mahé, Matteo Tommasini and Anouk Rijs, <i>Université Paris-Saclay, France</i> | Paper 25024 |
| 14:15 | Discussion | |
| 15:30 | Afternoon tea | |
| 16:00 | Electronic spectra of ions of astrochemical interest: From fast overview spectra to high resolution Jana Roithová, Juraj Jašík, Dieter Gerlich and Jesus Del Pozo Mellado <i>Charles University, Prague</i> | Paper 24882 |
| 16:05 | Combining ultra-high resolution ion-mobility with cryogenic IR spectroscopy for the study of biomolecular ions Thomas Rizzo, Stephan Warnke, Ahmed Ben Faleh, Robert Pellegrinelli and Natalia Yalovenko <i>École Polytechnique Fédérale de Lausanne, Switzerland</i> | Paper 25028 |
| 16:10 | Storage time dependent photodissociation action spectroscopy of polycyclic aromatic hydrocarbon cations in the cryogenic electrostatic storage ring DESIREE Mark Stockett, Mikael Björkhage, Henrik Cederquist, Henning Schmidt and Henning Zettergren <i>Stockholm University, Sweden</i> | Paper 24986 |
| 16:15 | Discussion | |
| 17:30 | Lightning presentations (by invitation of the scientific committee) | |
| 17:45 | Poster Session and Wine Reception | |
| 19:15 | Close of session | |

Tuesday 9 April

| | | |
|-------|--|-------------|
| | Session 2: Pushing resolution in frequency and time (Session Chair: Knut Asmis) | |
| 09:00 | The FELion cryogenic ion trap beam line at the FELIX free-electron laser laboratory: Infrared signatures of primary alcohol cations <u>Stephan Schlemmer</u> , Pavol Jusko, Sandra Brünken, Oskar Asvany, Sven Thorwirth, Alexander Stoffels, Lex van der Meer, Giel Berden, Britta Redich and Jos Oomens <i>University of Cologne, Germany</i> | Paper 24883 |
| 09:05 | Photoelectron-photofragment coincidence studies of I₃⁻ using an electrospray ionization source and a linear accelerator <u>Jemma Gibbard</u> and Robert Continetti <i>University of California, San Diego, USA</i> | Paper 25105 |
| 09:10 | Towards state selective recombination of H₃⁺ under astrophysically relevant conditions <u>Petr Dohnal</u> , Dmytro Shapko, Ábel Kálosi, Miroslava Kassayová, Štěpán Roučka, Serhiy Rednyka, Radek Plašil, Michal Hejduk and Juraj Glosík <i>Charles University, Prague</i> | Paper 25020 |
| 09:15 | Discussion | |
| 10:30 | Morning Tea | |
| 11:00 | Photoelectron spectra of Al₂O₂⁻ and Al₃O₃⁻ via slow electron velocity-map imaging <u>Daniel M. Neumark</u> , Jessalyn A. DeVine and Mark C. Babin, <i>University of California, Berkeley, USA</i> | Paper 24880 |
| 11:05 | Effect of alkali ions on optical properties of flavins: Vibronic spectra of cryogenic M⁺lumiflavin ionic complexes (M=Li-Cs) <u>Otto Dopfer</u> , David Müller, Pablo Nieto and Mitsuhiro Miyazaki <i>Technische Universität Berlin, Germany</i> | Paper 25037 |
| 11:10 | Spectroscopy of corannulene cations in helium nanodroplets <u>Michael Gatchell</u> , Paul Martini, Felix Laimer, Marcelo Goulart, Florent Calvo and Paul Scheier <i>University of Innsbruck, Austria</i> | Paper 24958 |
| 11:15 | Discussion | |
| 12:30 | Lunch | |
| | Session 3: Going Large(r) (Session Chair: Steen Brøndsted Nielsen) | |
| 13:30 | Interactions of aggregating peptides probed by IR-UV action spectroscopy <u>Anouk Rijs</u> , Sjors Bakels, Mart Greuell, George Rouwhorst, Eline Meijer, Sebastiaan Porskamp, Jerome Mahé, Marie-Pierre Gaigeot <i>Radboud University, The Netherlands</i> | Paper 24881 |
| 13:35 | Ion reactions in atmospherically-relevant clusters: Mechanisms, dynamics and spectroscopic signatures <u>Robert Gerber</u> , Laura McCaslin and Natalia Karimova <i>The Hebrew University of Jerusalem, Israel</i> | Paper 24979 |
| 13:40 | Electronic spectroscopy of isolated DNA polyanions <u>Valérie Gabelica</u> , Steven Daly, Massimiliano Porrini and Frédéric Rosu <i>University of Bordeaux, France</i> | Paper 24914 |
| 13:45 | Electrospray ionization photoelectron spectroscopy of cryogenic [EDTA•M(II)]²⁻ complexes (M = Ca, V–Zn): electronic structures and intrinsic redox properties <u>Xue-Bin Wang</u> , Qinqin Yuan, Xiang-Tao Kong, Gao-Lei Hou, Ling Jiang <i>Pacific Northwest National Laboratory, USA</i> | Paper 24886 |
| 13:50 | Discussion | |
| 15:30 | Afternoon tea | |
| 16:00 | Probing the selectivity of Li⁺ and Na⁺ cations on noradrenaline at | Paper |

| | | |
|-------|--|-------------|
| | the molecular level <u>Sotiris Xantheas</u> , Shun-ichi Ishiuchi, Hiromichi Wako and Masaaki Fujii <i>Pacific Northwest National Laboratory and University of Washington, USA</i> | 24885 |
| 16:05 | Probing solvation and reactivity in ionized polycyclic aromatic hydrocarbon-water clusters with photoionization mass spectrometry and electronic structure calculations <u>Musahid Ahmed</u> , Bo Xu, Tamar Stein, Utuq Ablikim, Ling Jiang, Josie Hendrix, Martin Head-Gordon, <i>Lawrence Berkeley National Laboratory, USA</i> | Paper 24978 |
| 16:10 | Investigation of the position of the radical in z_3-ions resulting from electron transfer dissociation using infrared ion spectroscopy <u>Jos Oomens</u> , Lisanne Kempkes, Jonathan Martens, Giel Berden, Kas Houthuijs <i>Radboud University, The Netherlands</i> | Paper 25017 |
| 16:15 | Selecting and identifying gas-phase protonation isomers of nicotineH⁺ using combined laser, ion mobility and mass spectrometry techniques <u>Adam Trevitt</u> , Samuel Marlton, Benjamin McKinnon, Boris Ucur, Alan Maccarone, William Donald, Stephen Blanksby <i>University of Wollongong, Australia</i> | Paper 25023 |
| 16:20 | Discussion | |
| 18:00 | Close of sessions | |
| 18:30 | Pre-Dinner Drinks, Quarks Restaurant | |
| 19:00 | Conference Dinner, Quarks Restaurant | |

Wednesday 10 April

| | | |
|-------|---|-------------|
| | Session 4: Exotic Systems (Session Chair: Anne McCoy) | |
| 09:00 | EOM-CC guide to Fock space travel: The C₂ edition <u>Anna Krylov</u> , Thomas Jagau and S. Gulania <i>University of Southern California, Los Angeles, USA</i> | Paper 24879 |
| 09:05 | Spectroscopy of temporary anion States: Renner-teller coupling and electronic autodetachment in Copper Difluoride Anion <u>Richard Mabbs</u> , Justin Lyle and Thomas Jagau <i>Washington University in St. Louis, USA</i> | Paper 25013 |
| 09:10 | Model potential study of non-valence correlation-bound anions of (C₆₀)_n clusters: the role of electric field-induced charge transfer <u>Ken Jordan</u> and Tae Hoon Choi <i>University of Pittsburgh, USA</i> | Paper 24964 |
| 09:15 | Discussion | |
| 10:30 | Morning Tea | |
| 11:00 | State-selective coherent motional excitation as a new approach for the manipulation, spectroscopy and state-to-state chemistry of single trapped molecular ions <u>Stefan Willitsch</u> , Ziv Meir, Gregor Hegi, Kaveh Najafian and Mudit Sinhal <i>University of Basel, Switzerland</i> | Paper 24884 |
| 11:05 | Electronic spectroscopy and nanocalorimetry of hydrated magnesium ions [Mg(H₂O)_n]⁺, n = 20–70: Spontaneous formation of a hydrated electron? <u>Martin K. Beyer</u> , Thomas Taxer, Milan Ončák, Erik Barwa, Christian van der Linde <i>Leopold-Franzens-Universität Innsbruck, Austria</i> | Paper 25050 |
| 11:10 | Discussion | |
| 12:00 | Concluding Remarks Lecture (Session Chair: Jan Verlet) Jack Simons | |

| | |
|-------|-----------------------------------|
| | <i>University of Utah, USA</i> |
| 12.45 | Acknowledgements |
| 13:00 | Close of meeting and lunch |

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.