

Advancing the chemistry of the f-elements

Dalton Discussion 14



28-30 July 2014
Edinburgh, UK

Programme

Monday 28 July

12:00	Registration
12.30	Lunch
13:45	Welcome and Introductions Jason Love
	Session 1: Structure and bonding in f-element compounds Session Chair: Michael Buehl
14:00 K1	Selective C-H bond reorganisation mediated by the (Me_5C_5) ligand in f-element chemistry: a new mechanism revealed by calculations and named Carambole. Christos E. Kefalidis, Lionel Perrinb, Carol J. Burnsc David J. Berg, Laurent Maron* and Richard A. Andersen <i>Universite Paul Sabatier, Toulouse</i>
14:40 C1	Uranyl Extraction by N,N-Dialkylamide Ligands Studied by Static and Dynamic DFT Simulations Nicolas Sieffert* and Georges Wipff <i>Université Joseph Fourier Grenoble I</i>
14:45	Discussion
15:10	Afternoon Tea
15:40 I1	The Strength of Actinide–Element Bonds from the Quantum Theory of Atoms-in-Molecules Qian-Rui Huang, Jennifer R. Kingham and Nikolas Kaltsoyannis* <i>University College London, UK</i>
15:50 C2	On the selectivity of poly-N-dentate and poly-O-dentate ligands in solvent extraction processes of actinide/lanthanide separation – a theoretical approach Jerzy Narbutt*, Artur Wodynski, and Magdalena Pecul <i>Institute of Nuclear Chemistry and Technology</i>
15:55 C3	Ab Initio Investigation of the Layered Uranium Oxides U_3O_8 and U_2O_5 Nick Brincat* Steve Parker, Marco Molinari, Geoff Allen and Mark Storr <i>University of Bath</i>
16:00	Discussion
17:10	Poster Session and Wine Reception
18:30	Close of Sessions

Tuesday 29 July

	Session 2: Properties and materials applications Session Chair: Euan Brechin
09:00 K2	Actinide-Based Single-Molecule Magnets Katie R. Meihaus and Jeffrey R. Long* <i>University of California, Berkeley, USA</i>
09:40 I2	CS₂ activation at uranium(III) siloxide ate complexes: the effect of a Lewis acidic site Clément Camp, Oliver Cooper, Jacques Pécaut, and Marinella Mazzanti* <i>CEA, Grenoble</i>
09:50	Discussion
10:20	Morning Coffee
10:50 C4	Ultimate miniaturization with the design of discrete polynuclear molecular complexes displaying near-infrared to visible upconversion Davood Zare, Yan Suffren, Laure Guéneé, Svetlana V. Eliseeva, Homayoun Nozary, Lilit Aboshyan-Sorgho, Stéphane Petoud, Andreas Hauser, and Claude Piguet* <i>Dept of Inorganic Chemistry/University of Geneva</i>
10:55 C5	A self-assembling lanthanide molecular nanoparticle for optical imaging Katherine A Brown*, Xiaoping Yang, Desmond Schipper, Justin W. Hall, Lauren J DePue, Annie J Gnanam, Jonathan F Arambula, Jessica N Jones, Jagannath Swaminathan, Yakhya Dieye, Jamuna Vadivelu, Don J Chandler, Edward M Marcotted, Jonathan L Sessler, Lauren I R Ehrlichd, and Richard A Jones <i>University of Cambridge</i>
11:00	Discussion
12:00	Poster Session and Lunch
	Session 3: Advances in reactivity and catalysis Session Chair: Polly Arnold
13:30 K3	Mixed Sandwich Thorium Complexes Incorporating Bis(tri-isopropylsilyl)cyclooctatetraenyl and Pentamethylcyclopentadienyl Ligands: Synthesis, Structure and Reactivity Zoë E. Button, Jessica A. Higgins, Marketa Suvova, F. Geoffrey N. Cloke*, and S. Mark Roe <i>University of Sussex, UK</i>
14:10 I3	Radical Anionic versus Neutral 2,2'-Bipyridyl Coordination in Uranium Complexes Supported by Amide and Ketimide Ligands Paula L. Diaconescu* and Christopher C. Cummins <i>University of California, Los Angeles, USA</i>
14:20	Discussion
14:50	Afternoon Tea
15:20 C6	Thermodynamics of self-assembly of dicarboxylate ions with binuclear lanthanide complexes Thomas Just Sørensen*, Leila R. Hill and Stephen Faulkner <i>Nano-Science Center & Department of Chemistry, University of Copenhagen</i>
15:25 C7	Synthesis and characterisation of lanthanide-hyporphyrin dyads Ruisheng Xiong, Julien Andres, Kira Scheffler and K. Eszter Borbas* <i>Uppsala University</i>

15:30 C8	Coordination polymers of uranium (IV) terephthalates Clément Falaise, Ayalew Assen, Ionut Mihalcea, Christophe Volkringer*, Adel Mesbah, Nicolas Dacheux, and Thierry Loiseau <i>University of Lille</i>
15:35	Discussion
16:50	Close of Session
19:00	Pre-dinner drinks
19:30	Conference dinner

Wednesday 30 July

	Session 4: f-elements in the environment Session Chair: Louise Natrajan
09:00 K4	Synchrotron applications to f-element research in the nuclear fuel cycle Melissa A. Denecke* <i>Karlsruhe Institute of Technology, Germany</i>
09:40 C9	Utilizing Block Copolymers with CMPO Derivatized Side Chains for the Selective Binding of Actinides over Lanthanides Lauren A. Mitchell, Julie M. Stanley and Bradley J. Holliday* <i>The University of Texas at Austin</i>
09:45 C10	Sonochemical Redox Reactions of Pu(III) and Pu(IV) in Aqueous Nitric Solutions Matthieu Virot*, Laurent Venault, Philippe Moisy and Sergey I. Nikitenko <i>ICSM Marcoule - UMR 5257</i>
09:50	Discussion
10:40	Morning Coffee
11:10 I4	Influence of riboflavin on the reduction of radionuclides by <i>Shewanella oneidensis</i> MR-1 Andrea Cherkouk, Gareth T. W. Law, Athanasios Rizoulis, Katie Law, Joanna C. Renshaw, Katherine Morris, Francis R. Lives and Jonathan R. Lloyd* <i>University of Manchester, UK</i>
11:20 C11	Spectroscopic study on uranyl carboxylate complexes formed at the surface layer of <i>Sulfolobus acidocaldarius</i> Thomas Reitza, Andre Rossberg, Astrid Barkleit, Robin Steudtner, Sonja Selenska-Pobell and Mohamed L. Merroun* <i>Department of Microbiology, University of Granada</i>
11:25 C12	Structural characterization of environmentally relevant ternary uranyl citrate complexes present in aqueous solutions and solid state materials Madeline Basile, Daniel K. Unruh, Adam Johns, Erin Flores and Tori Z. Forbes* <i>University of Iowa</i>
11:30	Discussion
12:20	Acknowledgements Jason Love
12:30	Close of meeting