

Halogen Bonding in Supramolecular and Solid State Chemistry

Faraday Discussion



Monday 10 July

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| 11:00 | Registration, Tea and Coffee | |
| 12:00 | Lunch | |
| 12:45 | Welcome and Introductions David Bryce, <i>Chair of Scientific Committee</i> | |
| 12:55 | Outline of Discussion Format Jeremy Allen and Debora Giovanelli, <i>Royal Society of Chemistry Publishing Editors</i> | |
| 13:00 | Introductory Lecture (Session Chair: David Bryce) <u>Tim Clark</u> <i>University of Erlangen, Germany</i> | |
| | Session 1 Computational approaches and sigma-hole interactions (Session Chair: Catharine Esterhuysen) | |
| 14:00 | Using one halogen bond to change the nature of a second bond in ternary complexes with P...Cl and F...Cl halogen bonds <u>Janet E. Del Bene</u> , Ibon Alkorta and José Elguero <i>Youngstown State University</i> | Paper 13664 |
| 14:05 | Discussion of Paper 13664 | |
| 14:20 | Strength, character, and directionality of halogen bonds involving cationic halogen bond donors <u>Kevin E. Riley</u> and Khanh-An Tran <i>Xavier University of Louisiana</i> | Paper 13772 |
| 14:25 | Discussion of Paper 13772 | |
| 14:40 | The anomalous halogen bonding interactions between chlorine and bromine with water in clathrate hydrates Hana Dureckova, Tom K. Woo, Konstantin A. Udachin, John A. Ripmeester and <u>Saman Alavi</u> <i>University of Ottawa</i> | Paper 13743 |
| 14:45 | Discussion of Paper 13743 | |
| 15:00 | General Discussion | |
| 15:30 | Afternoon tea | |
| 16:00 | Probing covalency in halogen bonds through donor K-edge X-ray absorption spectroscopy: polyhalides as coordination complexes Chantal L. Mustoe, Mathusan Gunabalasingam, Darren Yu, Brian O. Patrick and <u>Pierre Kennepohl</u> <i>University of British Columbia</i> | Paper 13960 |
| 16:05 | Discussion of Paper 13960 | |
| 16:20 | Intermolecular interactions in molecular crystals: what's in a name? <u>Alison J. Edwards</u> , Campbell F. Mackenzie, Peter R. Spackman, Dylan Jayatilaka and Mark A. Spackman <i>Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization</i> | Paper 13945 |
| 16:25 | Discussion of Paper 13945 | |
| 16:40 | Close contacts and noncovalent interactions in crystals Jane S. Murray, Giuseppe Resnati and <u>Peter Politzer</u> <i>University of New Orleans</i> | Paper 13667 |
| 16:45 | Discussion of Paper 13667 | |
| 17:00 | General Discussion | |

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| 17:30 | Lightning presentations (by invitation of the scientific committee) |
| 17:40 | Poster Session and Wine Reception |
| 19:30 | Free evening |

Tuesday 11 July

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| Session 2 Beyond the halogen bond (Session Chair: David Bryce) | | |
| 09:30 | Prospects for ²⁰⁷Pb solid-state NMR studies of lead tetrel bonds <u>Scott A. Southern</u> , Dylan Errulat, Jamie M. Frost, Bulat Gabidullin and David L. Bryce <i>University of Ottawa</i> | Paper 13729 |
| 09:35 | Discussion of Paper 13729 | |
| 09:50 | Building new discrete supramolecular assemblies through the interaction of isotellurazole N-oxides with Lewis acids and bases Peter C. Ho, Hilary A. Jenkins, James F. Britten and Ignacio Vargas-Baca <i>McMaster University</i> | Paper 13704 |
| 09:55 | Discussion of Paper 13704 | |
| 10:10 | General Discussion | |
| 10:30 | Morning Tea | |
| 11:00 | Do halogen bonds dictate the packing preferences in solid solutions? Titus Pramanik, Mysore S. Pavan and <u>Tayur N. Guru Row</u> <i>Indian Institute of Science</i> | Paper 13666 |
| 11:05 | Discussion of Paper 13666 | |
| 11:20 | Comparison of halide receptors based on H, halogen, chalcogen, pnictogen, and tetrel bonds <u>Steve Scheiner</u> <i>Utah State University</i> | Paper 13668 |
| 11:25 | Discussion of Paper 13668 | |
| 11:40 | General Discussion | |
| 12:00 | Lunch | |
| Session 3 The halogen bond in solution (Session Chair: Kevin Riley) | | |
| 13:00 | Cationic all-halogen bonding rotaxanes for halide anion recognition Xiaoxiong Li, Jason Y. C. Lim and <u>Paul D. Beer</u> <i>University of Oxford</i> | Paper 13663 |
| 13:05 | Discussion of Paper 13663 | |
| 13:20 | Comparison of halogen bonding networks with Ru(II) complexes and analysis of the influence of the XB interactions on their reactivity <u>Marta E. G. Mosquera</u> , Irene Egido, Carlos Hortelano, María López-López and Pilar Gómez-Sal <i>Universidad de Alcala</i> | Paper 13741 |
| 13:25 | Discussion of Paper 13741 | |
| 13:40 | Exploring the construction of multicompartamental micelles by | Paper |

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| | halogen bonding of complementary macromolecules Alan Vanderkooy and <u>Mark S. Taylor</u> <i>University of Toronto</i> | 13669 |
| 13:45 | Discussion of Paper 13669 | |
| 14:00 | General Discussion | |
| 14:30 | Afternoon Tea | |
| 15:00 | Comparative study of non-covalent interactions between cationic <i>N</i>-phenylviologens and halides by electrochemistry and NMR: the halogen bonding effect G. Creste, S. Groni, C. Fave, <u>M. Branca</u> and B. Schöllhorn <i>Université Paris Diderot</i> | Paper 13739 |
| 15:05 | Discussion of Paper 13739 | |
| 15:20 | Electron-transfer reactions of halogenated electrophiles: a different look into the nature of halogen bonding <u>Sergiy V. Rosokha</u> <i>Ball State University</i> | Paper 13693 |
| 15:25 | Discussion of Paper 13693 | |
| 15:40 | The ¹⁵N NMR chemical shift in the characterization of weak halogen bonding in solution Sebastiaan B. Hakkert, Jürgen Gräfenstein and <u>Mate Erdelyi</u> <i>University of Gothenburg</i> | Paper 13991 |
| 15:45 | Discussion of Paper 13991 | |
| 16:00 | General Discussion | |
| 16:30 | Close of sessions | |
| 18:30 | Pre-Dinner Drinks | |
| 19:00 | Conference Dinner | |

Wednesday 12 July

| Session 4 Solid-state chemistry and applications (Session Chair: William Pennington) | | |
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| 09:00 | Competition and selectivity in supramolecular synthesis: structural landscape around 1-(pyridylmethyl)-2,20-biimidazoles C. A. Gunawardana, J. Desper, A. S. Sinha, M. Đaković and <u>C. B. Aakeröy</u> <i>Kansas State University</i> | Paper 13662 |
| 09:05 | Discussion of Paper 13662 | |
| 09:20 | Toward a reverse hierarchy of halogen bonding between bromine and iodine Emmanuel Aubert, Enrique Espinosa, Irène Nicolas, Olivier Jeannin and Marc Fourmigué <i>Université de Rennes 1 & CNRS</i> | Paper 13671 |
| 09:25 | Discussion of Paper 13671 | |
| 09:40 | General Discussion | |
| 10:00 | Morning Tea | |
| 10:30 | Photoresponsive ionic liquid crystals assembled via halogen bond: en route towards light-controllable ion transporters Marco Saccone, Francisco Fernandez Palacio, Gabriella Cavallo, <u>Valentina Dichiarante</u> , Matti Virkki, Giancarlo Terraneo, Arri Priimagi and Pierangelo Metrangolo <i>Politecnico di Milano</i> | Paper 13949 |
| 10:35 | Discussion of Paper 13949 | |
| 10:50 | Halogen effects on the solid-state packing of phenylalanine derivatives and the resultant gelation properties Susana M. Ramalheite, Jamie S. Foster, Hayley R. Green, Karol P. Nartowski, Margaux Heinrich, Peter C. Martin, Yaroslav Z. Khimyak and <u>Gareth O. Lloyd</u> <i>Heriot-Watt University</i> | Paper 13804 |
| 10:55 | Discussion of Paper 13804 | |
| 11:10 | Assembly and dichroism of a four-component halogen-bonded metal-organic cocrystal salt solvate involving dicyanoaurate(I) acceptors Jan-Constantin Christopherson, Karlie P. Potts, Oleksandr S. Bushuyev, Filip Topić, Igor Huskić, Kari Rissanen, Christopher J. Barrett and <u>Tomislav Friščić</u> <i>McGill University</i> | Paper 13665 |
| 11:15 | Discussion of Paper 13665 | |
| 11:30 | General Discussion | |
| 12:00 | Concluding Remarks Lecture (Session Chair: Anthony Legon) <u>Lee Brammer</u> <i>University of Sheffield, United Kingdom</i> | |
| 12:40 | Acknowledgements | |
| 12:45 | 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.