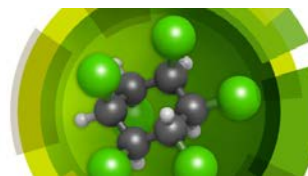


Halogen Bonding in Supramolecular and Solid State Chemistry

Faraday Discussion



Monday 10 July

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 Kevin E. Riley 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	

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

Tuesday 11 July

	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 Alcalá</i>	Paper 13741
13:25	Discussion of Paper 13741	
13:40	Exploring the construction of multicompartamental micelles by	Paper

	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)	
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.