Halogen Bonding: Weak Interactions Result in Strong Opinions

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Halogen Bonding: Weak Interactions Result in Strong Opinions

Seventy international scientists met at the Hospederia Porta Coeli — Doncel's House in Sigüenza, Spain, August 20−21, 2011, to participate in the International Union of Crystallography (IUCr) 2011 Satellite Workshop "Categorizing Halogen Bonding and other Noncovalent Interactions Involving Halogen Atoms" (http://www.iucr2011madrid.es/index.php/program/satellite-meetings). This workshop was the culmination of an International Union of Pure and Applied Chemistry (IUPAC) Physical and Biophysical Chemistry Division project of the same title (http://www.iupac.org/web/ins/2009-032-1-100) chaired by Pierangelo Metrangolo and Giuseppe Resnati. Committee members included Gautam R. Desiraju, P. Shing Ho, Lars Kloo, Anthony C. Legon, Roberto Marquardt, Peter Politzer, and Kari Rissanen. The Committee sought to give a modern definition of halogen bonding that could include all theoretical and experimental evidence available.

Twenty-six technical presentations and 28 posters provided an interesting backdrop for an intense two days of discussion. Clearly the community still has a long way to go in developing consensus; however, this simply seems to be a result of the very different backgrounds and experiences of the scientists present. The breadth of the session topics was representative of the breadth of experiences present. Excellent presentations highlighted key areas such as theoretical modeling, techniques for measuring halogen bonding, classification of donor vs acceptor interactions, and utilizing of halogen bonding in crystal engineering and supramolecular assembly, as well as in the development of functional materials. The complete oral program is reproduced below. The program and abstracts for this meeting are available in PDF format at http://www.iucr2011madrid.es/images/stories/pdf/Book_of_abstracts.pdf.

The Committee and particularly the Chairs, Professors Metrangolo and Resnati, are to be congratulated for their efforts in building and bringing order to this emerging scientific community. The excitement and interest among the practitioners, especially those attending the workshop, were palpable. They are making fundamental contributions to science, while participating in the art of debate. This is good for the field and good for our understanding of intermolecular interactions in general.

Professors Metrangolo and Resnati also agreed to be Guest Editors of a *Crystal Growth & Design* virtual special issue (http://pubs.acs.org/page/cgdefu/vi/index.html) on Halogen Bonding. Many of these excellent contributions are already in production and should appear in the pages of *CGD* soon. The Guest Editors have also agreed to write a Perspective which outlines the state of the field and the outcomes of quite intense discussion and debate at the Sigüenza workshop. I will thus leave it to them to provide a high level overview of the debate and the current working definition of a halogen bond.

I will say, however, that I foresee the same type of ongoing discussion that has characterized attempts at definitions and consistent nomenclature in the past (see, for example, my editorial discussing the debate over nomenclature in the field of polymorphism[1,2]). I believe such debate is actually quite good when kept civil and to the facts. It causes us to carefully evaluate how we think of our science and how we view and evaluate the literature. Often it leads to new insights and new understanding from the individual to the collective scientific community.

My caution here is the same as anywhere such debate goes on. Keep an open mind and do not let definitions and nomenclature restrict your thinking or stop you from trying something new. The voice of experience that says "I tried that 20 years ago and it did not work then and it will not work now" is simply not always correct.

With that in mind, I encourage you to enter the debate, and there are several opportunities for you to do so. A discussion forum specifically for the topic of this workshop has been set up at http://www.halogenbonding.eu/forum/. It is necessary to register before posting a comment, and this can be accomplished directly on the Web site.

I would also encourage broader discussion of this topic via the CGD Network at https://communities.acs.org/community/cgdnetwork. Again, viewing the site is open to everyone, but you must get an ACS ID (registration is free) to post to the discussions.

Finally, I would invite everyone to the 2012 Gordon Research Conference on Crystal Engineering which will be held June 10−15, 2012, in Waterville Valley, New Hampshire (http://www.grc.org/programs.aspx?year=2012&program=crystaleng). Halogen bonding will be a big discussion topic at the meeting.

With all of these opportunities to learn and participate in the ongoing discussion, I hope each of you can find the right venue to become a part of this growing scientific community. Good Luck!

SCIENTIFIC PROGRAM

Categorizing Halogen Bonding and other Noncovalent Interactions Involving Halogen Atoms

Sigüenza, Spain, August 20−21, 2011

Chairs

- Pierangelo Metrangolo — Politecnico di Milano — Italy
- Giuseppe Resnati — Politecnico di Milano — Italy

Session I — Theoretical Modeling

Chair: Pavel Hobza

- **Peter Politzer** — CleveTheo Comp — USA

Perspective on Halogen Bonding

- **Ibon Alkorta** — Instituto de Química Médica — Spain

Traditional, Halogen-Shared, and Ion-Pair Halogen Bonds

- **Catharine Esterhuysen** — University of Stellenbosch — South Africa

Computational Analysis of $I_3^- \cdots I_3^-$ Halogen Bonds

Session II — Experimental Techniques

Chair: Pui Shing Ho

- **Anthony C. Legon** — University of Bristol — United Kingdom

Intermolecular Complexes in the Gas Phase: a Comparison of Halogen Bonds, Hydrogen Bonds and Other Interactions

- **Enrique Espinosa** — Université Henri Poincaré — France

Halogen Bonding From Charge Density Analysis

Published: October 17, 2011

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• **David L. Bryce** — University of Ottawa — Canada
Multinuclear Solid-State Magnetic Resonance Studies of Halogen Bonding Environments

Session III — Crystal Engineering
Chair: Christer Aakeröy

• **Gautam R. Desiraju** — Indian Institute of Science — India
Halogen Bonding in Crystal Engineering
• **Kari Rissanen** — University of Jyväskylä — Finland
Halogen Bonding vs Hydrogen Bonding in Solid State Chemistry
• **Lee Brammer** — University of Sheffield — UK
Halogen Bonds in Inorganic Chemistry

Session IV — Donors & Acceptors
Chair: Marc Fourmigué

• **William T. Pennington** — Clemson University — USA
Expanding the Halogen Bonding Periodic Table: Heavier Congener Acceptors
• **Francesco A. Devillanova** — Università di Cagliari — Italy
C. T. Adducts of S/Se Donors with Di-Halogens as a Source of Information on the Nature of the Halogen Bonding
• **Stefano Libri** — University of Sheffield — UK
Strong Halogen Bond Donors
• **Anna-Carin Carlsson** — University of Gothenburg — Sweden
The Symmetry of N—X^+—N Halonium Ion Complexes in Solution

Session V — Biomolecules
Chair: Kari Rissanen

• **Pavel Hobza** — Academy of Science of the Czech Republic and Center for Biomolecules and Complex Molecular Systems — Czech Republic
Halogen Bonding and In Silico Drug Design
• **P. Shing Ho** — Colorado State University — USA
Anisotropic Models for the Structure —Energy Relationships of Biological Halogen Bonds
• **Maura Malinska** — University of Warsaw — Poland
Experimental Charge Density Analysis of the Nature of C—Br···N≡C Interaction in Biologically Active Compound

Session VI — Materials
Chair: Ibon Alkorta

• **Duncan W. Bruce** — University of York — UK
Halogen Bonding Involving Substituted Pyridines-Liquid Crystallinity and Lability
• **Nikolay Houbenov** — Aalto University School of Science and Technology — Finland
Halogen Bonding Induced Self-Assembly of Extreme Materials
• **Wei Jun Jin** — Beijing Normal University — China
Halogen Bonding toward Assembling Phosphorescent Cocrystals and Probing Specific Solvent Effect

Session VII — Materials
Chair: Duncan W. Bruce

• **Hiroshi Yamamoto** — RIKEN — Japan
Crystalline Halogen-Bonded Network for Nanowire Sheath
• **Marc Fourmigué** — Université Rennes 1 — France
Halogen Bonding in Organic Conductors
• **Gabriella Cavallo** — Politecnico di Milano — Italy
Dynamically Porous Materials Assembled by Halogen Bonding

Session VIII — Supramolecules
Chair: William T. Pennington

• **Christer Aakeröy** — Kansas State University — USA
The Balance Between Hydrogen Bonds and Halogen Bonds
• **Giancarlo Terraneo** — Politecnico di Milano — Italy
Anion Templated Assembly of Halogen Bonded Supramolecular Networks

Session IX — IUPAC Definition of Halogen Bonding
Chair: Roberto Marquardt

• **Elangannan Arunan** — Indian Institute of Science — India
Defining Hydrogen Bonding and Halogen Bonding Through IUPAC
• **Pierangelo Metrangolo** and **Giuseppe Resnati** — Politecnico di Milano — Italy
IUPAC Project No. 2009-032-1-100 "Categorizing Halogen Bonding and other Noncovalent Interactions Involving Halogen Atoms"
• **Robin D. Rogers** — The University of Alabama — USA
Crystallographic Publication in the American Chemical Society Journal Crystal Growth & Design and Contentious Issues Arising During Peer Review: An Editor's Perspective (so pay attention!)

Robin D. Rogers
Editor-in-Chief
The University of Alabama

REFERENCES

(1) Rogers, R. D. Editorial: Introduction: Polymorphism in Crystals. *Cryst. Growth Des.* **2003**, *3*, 867.
(2) Rogers, R. D. Editorial: Polymorphism in Crystals—A Special Issue of *Crystal Growth & Design*. *Cryst. Growth Des.* **2004**, *4*, 1085.