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Department of Chemistry

Moscowitz Memorial Lectureship

4 p.m. Friday, April 19, 2013 • 331 Smith Hall

Professor

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Systematics of Non-Covalent Interactions: The Hydrogen Bond B···HX, the Halogen Bond B···XY, and the Silver Bond B···AgX

Website: http://www.bris.ac.uk/chemistry/people/anthony-c-legon/index.html

Abstract

Various properties of complexes formed by the interaction of pairs of closed-shell molecules can be determined in the gas phase by rotational spectroscopy. These properties (which include the radial and angular geometry, the intermolecular binding strength, and the electric charge redistribution that accompanies complex formation) therefore refer to the isolated species, unperturbed by lattice or solvent effects. As a result of varying the Lewis base B and, then, the halogen X systematically in a series of hydrogen bonded complexes B···HX, some generalisations emerged. Later investigations of complexes B···XY, where XY = ClF, Cl_2, BrCl, Br_2 or ICl, revealed that some of their properties parallel those in the corresponding hydrogen-bonded series, that similar generalisations apply, and that therefore the B···XY non-covalent interaction should be referred to as a halogen bond. Recently, it has been possible to prepare a range of complexes of the type B···MX (M = Ag or Cu) by laser-ablation methods and to characterise them by means of their rotational spectra. Do the properties of B···MX molecules exhibit systematic behaviour as B is varied? Are there parallels with the hydrogen bond and the halogen bond? Should we talk of the B···MX non-covalent interaction as a 'metal' bond analogue of hydrogen and halogen bonds?

The Moscowitz Memorial Lectureship in Chemistry was established by friends and colleagues of Professor Albert Moscowitz (1929-1996) to honor his many contributions to molecular spectroscopy. He was known for his research on the interpretation of optical rotation and circular dichroism spectra in terms of the structures of chiral molecules. In collaboration with colleagues in the medical sciences, he developed important applications of his methods to biomedical systems. Throughout his career, Moscowitz held numerous visiting professorships at other universities, and served on the editorial boards of the leading journals in chemical physics. His work was honored by election as Foreign Member of the Danish Royal Academy of Sciences and Letters, and as a Fellow of the American Physical Society.

Anthony Legon was born in Acton, Suffolk, in 1941, but returned before the end of World War II to the east end of London, where he was educated, first at the Lawrence School (Bethnal Green) and later at the Coopers' Company School (Mile End). He read for a bachelor of science degree in chemistry at University College London (UCL), and conducted doctoral research there with Jim Millen, with whom he subsequently had a long research collaboration. His association with UCL continued as Turner and Newall Fellow (1968-70), lecturer (1970-83), reader (1983-4) and Thomas Graham Professor (1989–90) in its chemistry department. In 1980, he spent a productive and defining sabbatical year working in the laboratory of Willis Flygare at the University of Illinois (Champaign-Urbana). He was later professor of physical chemistry at the universities of Exeter (1984–89 and 1990–2005) and Bristol (2005 -2008). Awards include Tilden Lecture and Medal of the Royal Society of Chemistry (RSC) (1989-90), Engineering & Physical Sciences Research Council Senior Fellow (1997-2002), Hassel Lecturer (University of Oslo, 1997), the Harry Hallam Memorial Lecure (Swansea, 1997), the RSC Spectroscopy Award (1998-9) and Liversidge Award of the RSC (2012). He was elected a Fellow of the Royal Society in 2000, and currently is a senior research fellow and emeritus professor of physical chemistry at Bristol.

The aim of Professor Legon's research is to understand non-covalent interactions of closed-shell molecules. The focus is on factors controlling the properties (especially directionality, interaction strength and electric-charge redistribution) of complexes involving the hydrogen bond B···HX, the halogen bond B···XY and, recently, the 'coinage-metal' bond B···MX (B is a simple Lewis base, HX a hydrogen halide, XY a di-halogen and M is Cu or Ag). Precise values of the properties of such complexes in effective isolation are determined by rotational spectroscopy.

Host: Professor Kenneth Leopold
Refreshments will be served prior to the seminar.