HBOND2019
Amsterdam

24-27 SEPTEMBER 2019

Conference Book

23rd International Conference on

"Horizons in Hydrogen Bond Research"

Welcome to HBOND2019

On behalf of the Organizing Committee, it is a pleasure to welcome you at the 23rd International Conference on "Horizons in Hydrogen Bond Research" (HBOND2019), which takes place on September 24-27, 2019 at the Ol2 Building on the campus of the Vrije Universiteit Amsterdam.

The International Conference on "Horizons in Hydrogen Bond Research" is a biennial conference series and has a long tradition with meetings being held across Europe.

1977	L. Sobczyk, Karpacz, Poland	1997	P. Schuster, Niederöblarn, Austria
1978	G. Zundel, Munich, Germany	1999	L. Sobczyk, Świeradów Zdrój, Poland
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1980	I. Olovsson, Sångy-Såby, Sweden	2003	H. H. Limbach, Berlin, Germany
1981	A. Potier, Montpellier, France	2005	P. E. Hansen, Roskilde, Denmark
1982	P. Huyskens, Leuven, Belgium	2007	K. G. Tokhadze, St. Petersburg, Russia
1985	W. A. P. Luck, Marburg, Germany	2009	M. C. Bellissent-Funel, Paris, France
1987	L. Sobczyk, Polanica Zdrój, Poland	2011	M. Suhm, Göttingen, Germany
1989	J. Kroon, Zeist, The Netherlands	2013	W. Herrebout, Antwerpen, Belgium
1993	Y. Maréchal, Autrans, France	2015	Z. Latajka, Wrocław, Poland
1995	L. Kimtys, Birstona, Lithuania	2017	J. Lundell, Jyvaskyla, Finland

The series gathers scientists working in the field of hydrogen bonding research and other weak interactions, who study virtually all states of matter by a multitude of experimental and theoretical methods.

We wish you a wonderful stay in the beautiful city of Amsterdam and a pleasant and inspiring conference, with many interesting discussions, at Vrije Universiteit Amsterdam.

Célia Fonseca Guerra and F. Matthias Bickelhaupt

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Poster 44

Outer electronic shell visualization by the Laplacian of helium chemical shift

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In the toolbox of a modern quantum chemist there are a few methods of outer electronic shells visualization, among them are constructing and analysis of maps of molecular electrostatic potential (MESP),[1] and electron localization function (ELF).[2] We propose a different visualization method which can be briefly described as follows: the space around a studied species is probed by ^{3}He atom, and in each point helium chemical shift is calculated. It has previously been shown, that for fluorine-containing molecules[3,4] Laplacian of ^{3}He chemical shift is sensitive to such features of electronic shells as lone pairs. Proposed approach has significant advances compared with standard quantum mechanical approaches – Laplacian of helium chemical shift preserves its sensitivity to lone pair regions at significantly larger distances (>1.5–2 Å), and its maximal values could be used to quantitatively estimate the electron-rich character of lone pairs. In this work, we extend a set of studied objects to the "classical" molecules with localized lone pairs – NH_3, $H_2C{=}NH$, HCN, H_2O, $H_2C{=}O$, H_3P, H_2S etc.

3D isosurface of Laplacian of ^{3}He chemical shift $\nabla^2\delta_{He}$ near fluoroacetylene ($\nabla^2\delta_{He}$ = 8 ppm/Å^2). Dashed line indicates maximum values of $\nabla^2\delta_{He}$.

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