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Physical Organic and Computational Chemistry

Research Interests

Our research program is focused on electronic structures (the distribution of electrons) and molecular structures (the network of bonding interactions) and their interplay in organic and biologically relevant molecules. Both are of fundamental importance in chemistry, and we are particularly interested in how small changes in either can influence reactivities. For the systematic knowledge needed to uncover a link between structure and reactivity, we employ selected experimental (synthetic, spectroscopic) and computational techniques. Our projects usually arise from observations such as a dramatic change in reactivity upon a change in substituent or an unexpected change in geometry between closely related molecules. In terms of electronic structures, we are currently interested in stereoelectronic and resonance effects in compounds as varied as N-sulfinylamines (R–NSO), nitrilimines (R–CNN–R) and phenol radical species, and a wide array of tools from electronic structure theory allows us to explain the experimentally observed data. Our molecular structure studies currently focus on nucleic acid bases and their involvement in hydrogen bonding or stacking interactions as well as the complexation of N-sulfinylamines, and we gain insight into weak bonding interactions from topological analyses of the electron density. And so we can, for example, uncover a cooperativity between an intramolecular weak hydrogen bonding and a complexing interaction for N-sulfinylamines that might have impact on their reactivity.

Selected Publications

L. Zhang, H.M. Muchall, G.H. Peslherbe. Substituent effects in the absorption spectra of phenol radical species: Origin of the red shift caused by 3,5-dimethoxyl substitution. Photochem. Photobiol. 89, 536 (2013)

H. M. Muchall. Computational insight into the carbenic character of nitrilimines from a reactivity perspective. J. Phys. Chem. A 115, 13694 (2011)

P.R.N. Kamya, H.M. Muchall. Revisiting the effects of sequence and structure on the hydrogen bonding and π-stacking interactions in nucleic acids. J. Phys. Chem. A 115, 12800 (2011)

E.V. Ivanova, H.M. Muchall. Hydrolysis of N-sulfinylamines and isocyanates: A computational comparison. J. Phys. Chem. A 111, 10824 (2007)

H.M. Muchall, N.H. Werstiuk. Ionization potentials of nitriles – Photoelectron spectra of succinonitrile and glutaronitrile. Can. J. Chem. 84, 1124 (2006)

R.C. Mawhinney, H.M. Muchall, G.H. Peslherbe. A computational study of the 1,3-dipolar cycloaddition reaction mechanism for nitrilimines. Can. J. Chem. 83, 1615 (2005)

R.C. Mawhinney, H.M. Muchall, J. Lessard. A theoretical analysis of the conformational behaviour of substituted methylenecyclohexanes. Can. J. Chem. 81, 1101 (2003)

H.M. Muchall. The anti-hydrogen bond in aromatic N-sulfinyl amines with ortho H atoms. J. Phys. Chem. A 105, 632 (2001)