

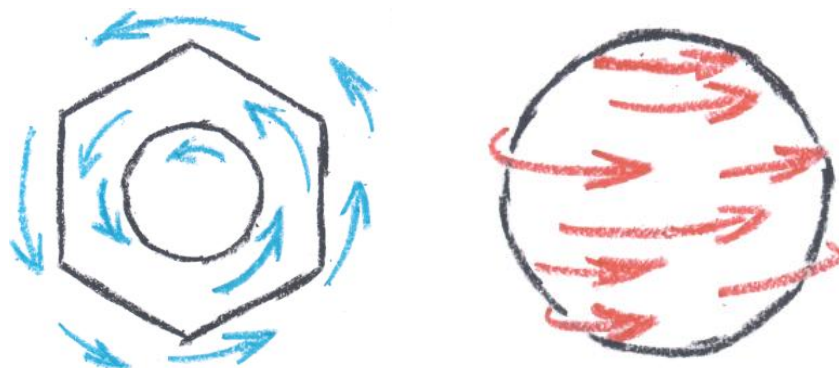
Ring currents and aromaticity

Mikael Johansson

Institut de Química Computacional, Universitat de Girona

mikael.johansson@iki.fi <http://www.iki.fi/~mpjohans>

Several measures of aromaticity have been proposed since the conception of the concept in the 19th century. Today, we will explore the connection between magnetically induced currents in different molecules, and their corresponding degree of aromaticity. The method of choice is GIMIC (Gauge Including Magnetically Induced Currents), which is able to provide not only a pictorial view of the induced currents, but also a quantitative current strength [1]. In this overview, a variety of different systems are considered, ranging from the 2D currents in the arch-aromatic, benzene, *via* the pseudo-2D currents in boron toroids [2], to the full 3D sphere currents of fullerenes [3-5].



- [1] J. Jusélius, D. Sundholm, J. Gauss, "Calculation of current densities using gauge-including atomic orbitals", *J. Chem. Phys.* **121** (2004) 3952.
- [2] M.P. Johansson, "On the Strong Ring Currents in B₂₀ and Neighboring Boron Toroids", *J. Phys. Chem. C* **113** (2009) 524.
- [3] M.P. Johansson, J. Jusélius, D. Sundholm, "Sphere Currents of Buckminsterfullerene", *Angew. Chem. Int. Ed.* **44** (2005) 1843.
- [4] M.P. Johansson, D. Sundholm, J. Vaara, "Au₃₂: A 24-Carat Golden Fullerene", *Angew. Chem. Int. Ed.* **43** (2004) 2678.
- [5] M.P. Johansson, J. Vaara, D. Sundholm, "Exploring the Stability of Golden Fullerenes", *J. Phys. Chem. C* **112** (2008) 19311.