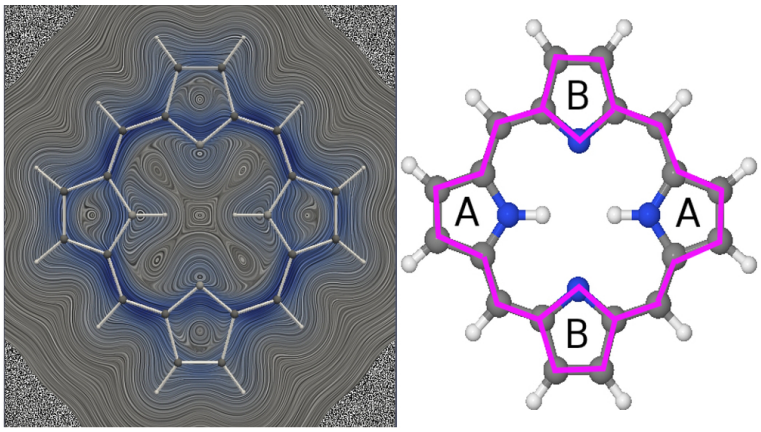
Analysis of magnetically induced current densities in molecules

H. Fliegl[a)] and D. Sundholm[b)]
a) Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, N-0315 Oslo, Norway. b) Department of Chemistry, P.O. Box 55 (A.I. Virtanens plats 1), FIN-00014 University of Helsinki, Finland.

An overview of different ways to systematically analyze the magnetically induced current density in molecules is presented using the gauge including magnetically induced current method (GIMIC).[1, 2] GIMIC is a independent program that is used for the calculation of magnetically induced current densities using London orbitals. Numerical integration of the current flow around molecular rings and along selected chemical bonds can be used for determining current pathways and the degree of aromaticity of various molecules according to the magnetic criterion. A new feature of the GIMIC program is the calculation of the anisotropy of the magnetically induced density using gauge including atomic orbitals.[3] As an example for a multiring system the magnetically induced current density of trans porphyrin is presented and discussed.[4]



[1] J. Jusélius, D. Sundholm and J. Gauss, *J. Chem. Phys.*, **121**, 3952 (2004)
[2] D. Sundholm, H. Fliegl and R. F. Berger, *WIREs*, **6**, 369, (2016)
[3] H. Fliegl, J. Jusélius and D. Sundholm, *J. Phys. Chem. A*, **120**, 5658, (2016)
[4] H. Fliegl and D. Sundholm, *J. Org. Chem.*, **77**, 3408, (2012)