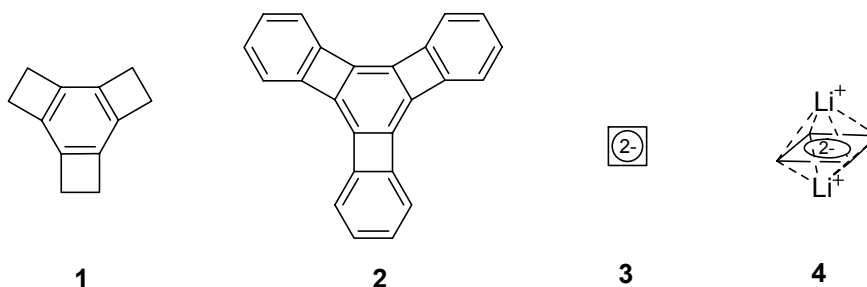


Spatial Magnetic Properties of Trisannelated Benzenes and Cyclobutadiene Dianion Derivatives Subjected to Aromaticity

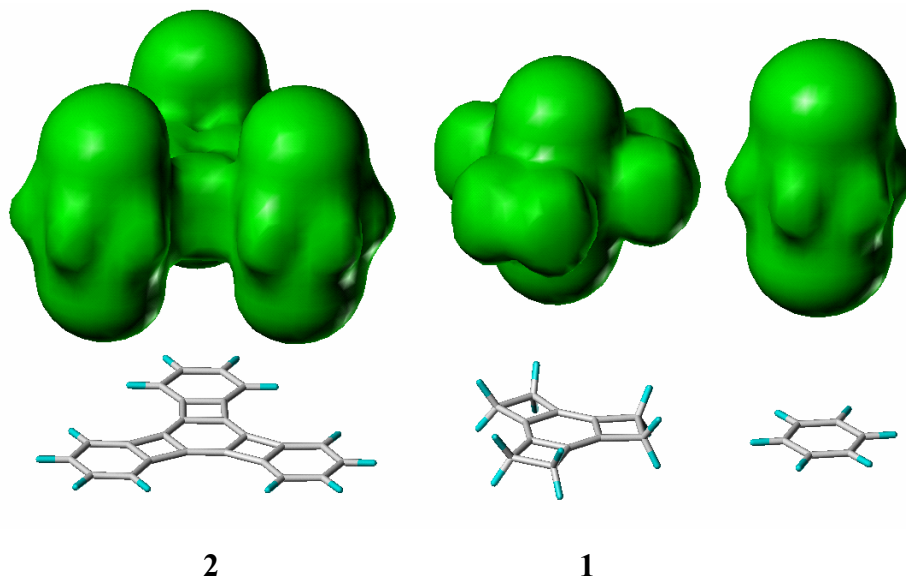
Erich Kleinpeter and Andreas Koch

*Universität Potsdam, Chemisches Institut, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam (Golm), FR Germany
e-mail: kp@chem.uni-potsdam.de*

The spatial magnetic properties (Through Space NMR Shieldings - *TSNMRS*) of tricyclobutabenzene (*TCBB*) **1**, of $[4n]$ annuleno $[4n+2]$ annulene **2**, of the cyclobutadiene dianion **3** and of the corresponding 2Li^+ complex **4** have been *ab initio* calculated by the GIAO perturbation method employing the Nucleus Independent Chemical Shift (*NICS*) concept of Paul von Ragué Schleyer [1], and visualized as Iso-Chemical Shielding Surfaces (*ICSS*) of various size and direction.



TSNMRS values can be successfully employed to quantify and visualize the (anti)aromaticity of the compounds studied and to discuss the influence of Li^+ complexation to cyclobutadiene dianion **4** on *planar 4c,6e* or *three-dimensional 6c-6e* aromaticity.



[1] P. von R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N.J.R. von E. Hommes, *J. Am. Chem. Soc.* 118 (1996) 6317.