Comparison between the contact and effective electron/spin densities at the IOTC quasirelativistic level of theory

Michal Malček[1], Lukáš Bučinský[1], Stanislav Biskupič[1], Dylan Jayatilaka[2]

[1]Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology, Slovakia
[2]Department of Chemistry, University of Western Australia, Australia

michal.malcek@stuba.sk

Effective electron density can be obtained via the derivative of electronic energy by means of the size of nucleus [1, 2]. Alternatively, the electronic energy can be replaced with the matrix representation of the nuclear potential, considering the homogenously charged sphere nucleus model [3]. Another approach, which is able to obtain both the electron and spin densities in the same way, is based on weighting of the density by the normalized Gaussian distribution of the nucleus [3]. All these approaches are considered, hand in hand with the comparison to contact electron/spin densities for two different models of nucleus (point charge nucleus and Gaussian finite model of nucleus).

The calculated values of contact and effective electron/spin densities for the Cu, Ag, Au atoms and the chemical shifts related to their cations are presented. The influence of PCE correction, the use of finite model of nucleus and the sensitivity to the quality of basis set is considered as well. All the calculations have been performed at the IOTC quasirelativistic level of theory, using the TONTO package [4]

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