

Pyridine-Based Organic Radicals as Prospective Ligands in Hybrid-Spin Cu(II) Complexes

Silviya Ninova¹, T. Miteva¹, J. Romanova¹, A. Ivanova¹, A. Tadjer¹, M. Baumgarten²

¹ University of Sofia, Faculty of Chemistry, 1 James Bourchier Ave., 1164 Sofia, Bulgaria.

E-mail: sylvia.ninova@gmail.com

² Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany.

A possible classification of the magnetic systems is: entirely inorganic, purely organic and organic-inorganic (hybrid-spin). The latter are the most promising candidates for novel magnetic materials, the organic component allowing fine tuning of the desired properties.

The present study is focused on investigation of different stable organic radicals, testing their suitability for ligands in Cu(II) hybrid-spin complexes. The radicals have as common feature a pyridine ring and they differ in the unpaired-electron-bearing substituents used and in the type and length of the π -conjugated system. Two of the positional isomers of the radicals are examined – meta- and para-substituted with respect to the N-atom of the pyridine ring. All stable conformers with respect to the dihedral angle between the radical moiety and the adjacent aromatic ring [1] are subject to full UB3LYP/6-31G* geometry optimization. The Mulliken atomic spin density distribution is assessed in order to monitor spin polarization and to quantify the atomic spin density at the N-atom of the pyridine ring – a key factor [2] for the efficiency of the exchange interaction with the copper ion: a high value being indication of a successful candidate. Several radicals are outlined as appropriate components of Cu(II) hybrid-spin complexes. Based on molecular orbital analysis, a prediction about the magnetic properties of model complexes is made derived from the pattern of coupling between the radicals and the metal ion. The sign and value of the energy difference between the high-spin and the low-spin states is used as measure of the type and amount of spin coupling in several designed complexes.

References

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 2. J. Romanova, T. Miteva, A. Ivanova, A. Tadjer, M. Baumgarten, *Phys. Chem. Chem. Phys.* 11 (2009) 9545.