CONFORMATIONAL ANALYSIS OF ORGANO-SILICON DERIVATES ATTACHED ON SUPERPARAMAGNETIC IRON OXIDE (Fe_3O_4)

Horatiu Moldovan[1], Marius Chirita[2], Liviu Mocanu[2*]

[1]Politehnica University, P-ta Victoriei No. 2, RO-300006, Timisoara, Romania
2National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, PlautiusAndronescu Str. No. 1, RO-300224, Timisoara, Romania
Corresponding author:mocanuliv@gmail.com

Continuing our previous works [1,2] the present study is a conformational analysis of the structure of the 3-(trimethoxysiyl propan)-1-amine, attached on the Fe_3O_4 superparamagnetic microparticles. The reason of this conformational study it is due to the fact that some physico-chemical properties of any compound depend in a determinant manner of its conformers. For instance (and especially) the steric properties or the electronic ones can be of major importance in the elementary processes of chemical mechanisms and are crucial in the ligand-substrate interactions. The latter ones constitute the main reason of our concerning related to the superparamagnetic properties of the Fe_3O_4 microparticles.

Keywords: superparamagnetic, magnetite, conformers

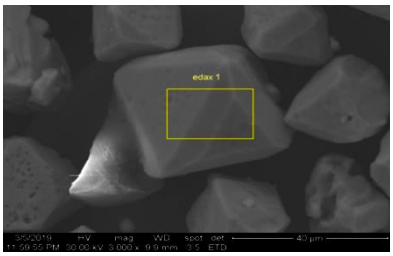

Fig.1 : SEM image of the MPTM's functionalized microcristals

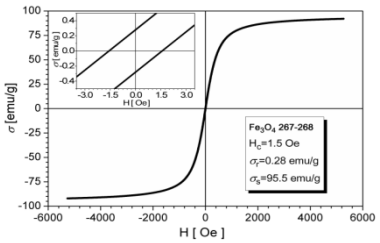

Fig.2 : Hysteresis loop of the sample

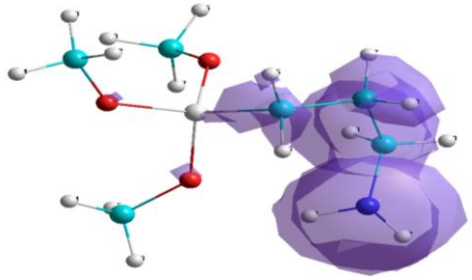

Fig 3 : One of the conformers and electronic distribution on the HOMO

References:

[1] Horatiu Moldovan, Liviu Mocanu, Francisc Peter, Marius Chirita, *Surface Modification of Singlecrystalline Superparamagnetic Iron Oxide (Fe_3O_4) Microparticles with Various Functional Organo-Silicon Derivatives.* Titlu conferinta: "Physics Conference TIM 19", Timisoara, 29-31'st May 2019.

[2] M. Chirita, M.L.Kiss, A. Ieta, I. Grozescu, NSTI-Nanotech 2013, Washington DC, USA, www.nsti.org, ISBN 978-1-4822-0581-7 Vol. 1, 20.