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Quantum-chemical calculation of the spatial structure of template complexes, forming in systems ion Fe(III) [Co(III)]– ethanedithioamide-1,2 – formaldehyde in gelatin – immobilized matrixes

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Abstract

By means of hybrid of density functional B3LYP with the basic set of 6-31G(d) computation of geometric parameters of macrocyclic complexes Fe(III) and Co(III) with 2,8-dithio-3,7-diaza-5-oxa-nonandithioamide-1,9, forming in the course of template processes between gelatin-immobilized hexacianoferrates (II) of iron(III) or cobalt(III), ethanedithioamide-1,2 and formaldehide have been performed with the program *Gaussian 98*. Coordinates of atoms, bond lengths, angles between bonds and dihedral angles in complexes with metal-chelate node MN_2S_2 .have been presented. It has been noted that both in the case of Fe(III), and Co(III) the indicated metal-chelate node is practically flat. Additional six-membered metallocycle formed as a result of template "cross-linking" in both studied complexes is unwrapped with respect to two five-membered cycles for quite large and practically equal angle (a little more than 75°), in which connection atoms of this cycle are not situated in one plane.