AB INITIO QUANTUM CHEMICAL CALCULATION OF THE STRUCTURES OF COORDINATION COMPOUNDS ARISING AT TEMPLATE SYNTHESIS IN ION M(II)–HYDROZINOMETHANE THIOHYDRAZIDE–ACETONE (M = Co, Ni, Cu) SYSTEMS

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Using a hybrid B3LYP density functional method with the 6-31G(*d*) basis set and the Gaussian-98 program, the geometrical parameters of macrocyclic complexes of Co(II), Ni(II) and Cu(II) with NNSS-coordination of donor centers of the chelate ligand, formed due to template processes in M(II)-hydrozinomethane thiohydrazide-acetone systems, are calculated. Coordinates of atoms, selected bond lengths and angles, and dihedral angles in complexes with MN_2S_2 metal-chelate site are given. It is noted that for all considered M(II) ions the additional six-membered metal cycle, formed because of template stitching, is turned at a considerable angle to two five-membered cycles, and this cycle itself is not planar either.

Keywords: template synthesis, macrocyclic complex, B3LYP.