



Synthesis, Structural, Antimicrobial activities and Theoretical Studies of Some New Trivalent Metal Complexes with Thiocarbamide Derivative

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Abstract : The new ligand [N,N'-bis (3-methyl-2-benzothiazilidene) thiocarbamide] [BTC]. [BTC] its complexes with some trivalent metal ions [Cr, Fe, Rh and Ru]. Structures of the new compounds were characterized by elemental and thermal analyses as well as FT-IR and UV-Vis spectra. The magnetic properties and electrical conductivity of metal complexes were also determined. Study of the nature of the complexes formed in ethanol following the mole ratio method. The stability constant of the complexes have been studied with the time, as well as the molar absorptivities have been calculated. The work also include a theoretical treatment of the formed complexes in the gas phase, this was done using the (hyperchem-8) program for the molecular mechanics and semi-empirical calculations. The heat of formation (ΔH_f°), binding energy (ΔE_b) and total energy (ΔE_T) for ligand and their complexes were calculated by (PM3) method at 298 K^o. The electrostatic potential of the ligand [BTC] was calculated to investigate the reactive sites of the molecules. PM3 were used to evaluate the bond length, vibrational and electronic spectra for the ligand [BTC] and their metal complexes then comparing with the experimental values. The antibacterial activity for the [BTC] and its metal complexes were studied against two types of pathogenic bacteria (*Pseudomonas aeruginosa*, as gram negative) and (*Staphylococcus aureus*, as gram positive). The minimal inhibitory concentrations (MIC) have been also studied to determine the low concentration for inhibition. Two antibiotics (Ampicillin and Amoxicillin) have been chosen to compare their activity to those of the new compounds. The results showed higher activity of the new compounds relative to the chosen antibiotics. Furthermore, the antifungal activity against (*Candida albicans*) and (*Aspergillus flavus*) were also studied for [BTC] and their metal complexes.

Keywords : Thiocarbonyldiamine, Benzothiazilidene, Theoretical study, antimicrobial study, Schiff bases Metal complexes.