BEST: International Journal of Humanities, Arts, Medicine and Sciences (BEST: IJHAMS)
ISSN (P): 2348-0521, ISSN (E): 2454-4728
Vol. 4, Issue 10, Oct 2016, 21-32

THEORETICAL STUDY OF SOME MIXED-LIGAND COMPLEXES OF SODIUM [5-(P-NITRO PHENYL)-4-PHENYL-1, 2, 4-TRAIZOLE-3-DITHIOCARBAMATO HYDRAZIDE] AND 1, 10 PHENANTHROLINE WITH FE (III) AND MN (II) IONS

MAHASIN ALIAS[1], SAHAR ISMAEL[2], MAHA FAISAL[3] & FARAH SAADOON[4]

[1, 2] Department of Chemistry/ College of Science for Woman/ University of Baghdad, Iraq

[3] Colleges of Dentistry/ University of Baghdad, Iraq

[4] University of Ibn Sina of Medical and Pharmaceutical Sciences, Iraq

ABSTRACT

A new mixed ligand complexes have been prepared by reaction of Sodium [5-(p-nitro phenyl)-4/-phenyl-1, 2, 4-traizole-3-dithiocarbamato hydrazide] L1, and 1, 10 phenanthrolineL2with Fe (III) and Mn (II) ions. The newly prepared complexes were isolated and characterized by (FT-IR) and (UV-Vis) spectroscopy, elemental analysis, flame atomic absorption technique, in addition to magnetic susceptibility and conductivity measurements. The ligands and the newly prepared complexes were studied theoretically in the gas phase using two programs hyper chem.8 and Gaussian program (Gauss View Currently Available Versions (5.0.9) along with Gaussian 09 which is the latest in the Gaussian series of programs).

KEYWORDS: Hyper chem.8, Gaussian program, Sodium [5-(p-Nitro Phenyl)-4/-Phenyl-1, 2, 4-Traizole-3-Dithiocarbamato Hydrazide], Transition Metals