International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.15, pp 146-162, 2017

Spectro-thermal characterization and molecular modeling of bioactive metal complexes of 4 -diethylaminosalicyldeoxime

Bibhesh K Singh[1]*, Jagdish Chandra[1], Hament K. Rajor[2], Pinkee[1]

[1]Department of Chemistry, Govt. Postgraduate College, Ranikhet, Uttarakhand-263645, India
[2]Department of Chemistry, Ramjas College, University of Delhi, Delhi-110007, India

Abstract : Newly synthesized ligand 4-diethylaminosalicyldeoxime (4-DEASDOX) and their Co(II), Ni(ii), Cu (II), and Zn(II) complexes have been prepared and characterized by different physicochemical techniques. The ligand 4-diethylaminosalicyldeoxime behaves as a bidentate ligand forming neutral metal chelates through the phenolic oxygen and the oxime nitrogen. The M-O stretching frequencies for the transition metals show good agreement with the Irving-William's stability order. Similar trend is seen for the M-N stretching frequencies in vibrational spectra and the shift in transitions from electronic spectral data for the metal complexes. Mass spectrum explains the successive degradation of the molecular species in solution and justifies ML_2 complexes. Electronic spectra and magnetic susceptibility measurements suggest square planer geometry of the metal complexes. Thermodynamic activation parameters were computed from the thermal data using Coats and Redfern method, which confirm first order kinetics. The geometry of the complexes has been optimized with the help of molecular modeling. The bio-efficacy of free ligand and its metal complexes have been examined against the growth of bacteria and pathogenic fungi *in vitro* to evaluate their anti-microbial potential.

Keywords : Bioactivity, Metal complexes, Molecular modeling, Salicyldeoxime, Spectra, Thermal studies.

Bibhesh K Singh *et al* /International Journal of ChemTech Research**,** 2017,10(15): 146-162.

*****