

Synthesis, spectral studies and quantum-chemical investigation of Cd and Zn complexes of S-benzyl β -N-((E)-2-nitrophenylallyl)dithiocarbazate

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A Schiff base is a nitrogen analog of an aldehyde or ketone in which the C=O group is replaced by C=N-R group. It is usually formed by condensation of an aldehyde or ketone with a primary amine. The Metal complexes of Schiff bases have played an important role in the development of coordination chemistry and have variety of applications in biology and industry due to their role in catalysis and organic synthesis [1-4]. A novel Schiff base of S-benzyl dithiocarbazate (Figure 1) has been synthesized by 1:1 condensation of trans-o-nitro cinnamaldehyde and S-benzyl dithiocarbazate. Also their metal complexes with Zn (II) and Cd(II) were synthesized in 2:1 Molar ratio and were characterized by UV, FT-IR, ^1H NMR (Figure 2). The synthesized Schiff base and metal complexes has been subjected to theoretical studies by DFT approach. The molecular geometry, vibrational frequencies, HOMO-LUMO energy gaps, molecular hardness (η), ionization energy (IE), electron affinity (EA), total energy and dipole moment were analyzed. The experimental results obtained from quantum chemical calculations at the DFT (minimal STO-3G basis-set) level corroborate our experimental findings from FTIR, UV and ^1H NMR.

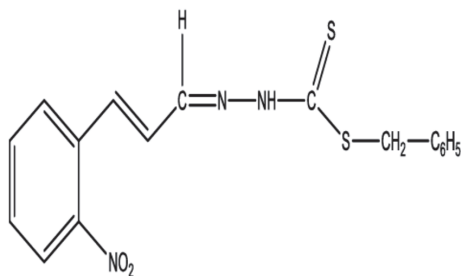


Figure 1: S-benzyl β -N-((E)-2-nitrophenylallyl)dithiocarbazate

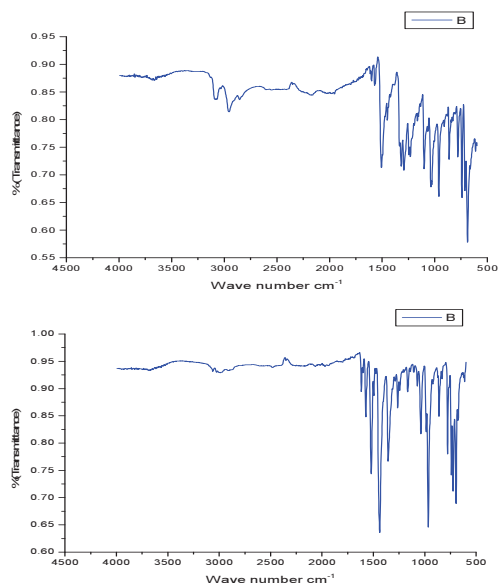


Figure 2: FT- IR OF Schiff base (mentioned in abstract)

References

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