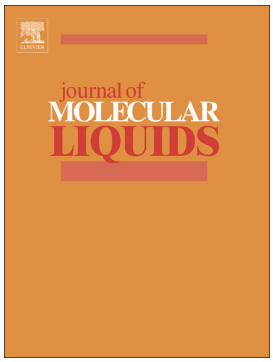

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Spectroscopic and spectrophotometric studies on hydrogen bonded charge transfer complex of 2-amino-4-methylthiazole with chloranilic acid at different temperatures

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Abstract

The synthesized hydrogen bonded charge transfer (CT) complex between 2-amino-4-methylthiazole (AMT) and chloranilic acid (CLA) was characterized using various spectral techniques such as UV-visible, FTIR, ^{1}H NMR, ESI-MS, P-XRD and TG/DTA analysis. The CT complexes act as an intermediate in a variety of reactions involving electron rich and electron deficient molecules. The spectral analysis of the CT complex suggests that N and NH_2 groups play a major role in determining the orientation in the reaction mechanism. The fluorescence studies show that Ct-DNA interacted with CT complex and quenched its intrinsic fluorescence in a static quenching process. Stern-Volmer equation was used to determine the binding ability of the CT complex with in vitro calf thymus DNA. The different physical parameters such as the association constant (K_{CT}), molar extinction coefficient (ε) energy of interaction (E_{CT}), ionization potential (I_D), resonance energy (R_N), free energy (ΔG), oscillator strength (*f*) and transition dipole moment (μ_{EN}) were determined using Benesi-Hildebrand equation. The Van't Hoff equation was used to calculate the various thermodynamic parameters such as enthalpy (ΔH), entropy (ΔS) and free energy (ΔG). The nature of interaction between donor and acceptor moieties can also be visualized by calculating thermodynamic parameters. The molecular interaction between AMT and CLA has been established through N^+—H·····O^- hydrogen bonding. The straight line method was established by the 1:1 stoichiometry of the CT complex. TG/DTA analysis provided information about changes in material properties as a function of temperature. The various fragmentation of the CT complex was evaluated using ESI-mass spectroscopy.

Keywords*:* 2-amino-4-methylthiazole; CT complex; Benesi-Hildebrand equation; DNA-binding; and FTIR analysis

1. Introduction

In the last few decades, numerous studies were devoted to the synthesis and characterization of new complex molecular assemblies containing electron donor and π-acceptor organic molecules have been reported either in liquid or in solid states [1-9]. Enormous amount of