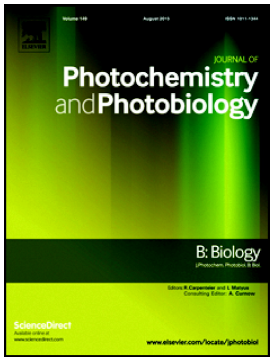

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Synthesis, Single-Crystal, DNA interaction, spectrophotometric and spectroscopic characterization of the hydrogen-bonded charge transfer complex of 2-aminopyrimidine with π-acceptor chloranilic acid at different temperature in acetonitrile

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Abstract

The charge transfer (CT) interaction of 2-aminopyrimidine (AP) with chloranilic acid (CLA) as π-acceptor was investigated spectrophotometrically in acetonitrile at different temperatures in the range of 25−50 ^{o}C. The 1:1 stoichiometry of the synthesized CT complex was detected using straight line method. Benesi–Hildebrand equation was used to determine the association constant (K_{CT}), molar extinction coefficient (ε) and other physical parameters. Various thermodynamics parameters such as enthalpy (ΔH), entropy (ΔS) and free energy (ΔG) were determined using UV–visible spectrophotometry in acetonitrile at different temperatures. ^{1}HNMR, FTIR, ESI−MS, elemental analyses, and UV–visible techniques were used to characterize the hydrogen-bonded CT complex. ^{1}H NMR spectroscopy was also used for the analysis of the CT complex where both hydrogen bond and charge transfer were present in its molecular composition. The interaction of the selected organic compound with Ct−DNA was well investigated using fluorescence spectroscopic method. Stern–Volmer constant (Ksv) was used to estimate the fluorescence quenching efficiency. Circular dichroism (CD) spectroscopy was employed to measure the conformational change of DNA in the presence of CT complex. Furthermore, the drug CT complex detected changes in its viscosity. The charge transfer complex was formed as a result of the transfer of the lone pair of electrons from donor to the acceptor and exhibits well resolved charge transfer bands in the regions where absorption by both donor and acceptor were absent. The thermal composition and stability of the CT complex were analyzed using thermogravimetric and differential thermal analysis (TGA and DTA) studies. The X-ray crystal structure was used for the interpretation of the structure of the [$(AP)^{+}$ $(CLA)^{-}$] CT complex. The crystal structure indicated that cation and anion are linked through strong N^{+}—H----O^{-} type of hydrogen bond.