Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 204 (2018) 403–408

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.elsevier.com/locate/saa

Determination of vertical ionization potential of nitroso-benzoimidazothiazole using charge transfer interaction with a series of acceptors

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ARTICLE INFO

Article history:
Received 1 March 2018
Received in revised form 16 June 2018
Accepted 21 June 2018
Available online 22 June 2018

Keywords:
CT band
Benzoimidazothiazole compound
Vertical ionization potential
Binding constant
^{1}H NMR
DFT

ABSTRACT

This is the first report of UV–Vis spectral investigations of electron donor-acceptor complexes of bio active 3-Nitroso-2-phenylbenzo[*d*]imidazo[2,1-b]thiazole (**BIT1**) with chloranils, nitrobenzenes and fullerenes in DMSO medium. Well defined charge transfer (CT) absorption bands in the visible region have been sited. Oscillator strengths, transition dipole and resonance energies of the CT complexes have been estimated. Utilizing Mulliken's equation vertical ionization potential of **BIT1** has been determined. A possible mechanism for the interaction between electronic subsystems of chloranils, nitrobenzenes, [60]- and [70] fullerenes with this benzoimidazothiazole compound (**BIT1**) have been discussed in comparing the parameters like degree of charge transfer and binding constant in polar DMSO. ^{1}H NMR study helps to explain the mechanism well. Comparison of complexes is done with DFT/PW1PW91/6-31G* optimized gas phase geometries and FMO features of adducts.

1. Introduction

Among organic compounds, natural or synthetic, heterocyclic rings are important components that can influence solubility, molecular conformation, chemical and biological activity [1, 2]. Actually heteroatoms are the centre of versatility. The hetero centers can act as hydrogen bond donors or acceptors, general acids or bases, and confer different electrostatic properties that tune chemical or biological reactivity [3]. Imidazothiazoles are such biologically active well known compounds [4–6]. This biologically important compound was mainly studied for its biological activity [7, 8]. But till date the physical characteristics of Imidazothiazole compound is not studied vividly.

We have taken this panorama to judge whether 3-Nitroso-2-phenylbenzo[*d*]imidazo[2,1-b]thiazole (**BIT1**) can form stable ground state charge transfer complex with electron deficient fullerene or chloranil like acceptors in DMSO medium. Seven different acceptors (**A1** – **A7**) are used viz. DDQ, p-chloranil, o-chloranil, 2,4-di nitro toluene, 2-Chloro-5-Nitro-benzoic acid, [60]- and [70]-Fullerenes respectively. All the EDA complexes (**BIT1**/**A**), have shown charge transfer transition in the visible region. Charge-transfer (CT) absorption bands have been precise in each case from which some important molecular parameters like Ionization potential of the benzoimidazothizole (**BIT1**), degree of charge transfer, ground state stability of complexes, etc. have been estimated.

2. Experimental

2-Chloro-5-Nitro-benzoic acid (**A5**), [60]- and [70]-Fullerenes (**A6** and **A7** respectively) have been purchased from Merck, Germany and Aldrich, USA respectively. *o*-chloranil (**A3**) is collected from Aldrich, USA. *p*-chloranil (**A2**) has been obtained from Fluka, Lausanne, Switzerland, and 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ, **A1**) and 2,4-di nitro toluene (**A4**) from Sigma. 3-Nitroso-2-phenylbenzo[*d*] imidazo[2,1-b]thiazole (**BIT1** in Fig. 1) has been synthesized by our reported method [9]. The solvent, DMSO, is of HPLC grade (Merck) and is used without further purification. Shimadzu UV 1800 spectrophotometer is used to record UV–Vis absorption spectra. ^{1}H NMR spectra using $CDCl_3$ solvent are recorded on 400 MHz spectrometer. Theoretical calculations have been performed in DFT/mPW1PW91 (modified Perdew-Wang exchange and Perdew-Wang 91 correlation [10]) level in 6-31G* basis set (Gaussian'09).

3. Results and Discussion

3.1. Photophysical Study

The visible CT bands is obtained taking spectra of mixtures containing (**1** + **A6**) and/or (**1** + A5) solution (in DMSO medium) recorded

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https://doi.org/10.1016/j.saa.2018.06.083
1386-1425/