

NBO ANALYSIS OF (E)-5-(2-PHENYLDIAZENYL)-2-HYDROXYBENZALDEHYDE USING DFT METHOD

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ABSTRACT

The NBO analysis of (E)-5-(2-phenyldiazenyl)-2-hydroxy benzaldehyde (PDHB) was calculated using B3LYP/6-311++G(d,p) level of theory. To study the intra-molecular charge transfers within the molecule the Lewis (bonding) and Non-Lewis (anti-bonding) structural calculation was performed.

INTRODUCTION

Azo compounds represent the largest and most important group of synthetic dyes. These compounds have a basic structure of Ar-N=N-Ar' (where Ar and Ar' = aromatic groups). The -N=N- azo group is the chromophore responsible for the color of these compounds [1-7]. The azo compounds are most widely used class of dyes due to their versatile application in various fields such as the dyeing of textile fibers, the coloring of different materials, colored plastics, biological and medical studies, and advanced application in organic synthesis [8-14]. Aromatic and heteroaromatic azo compounds constitute the largest and the most diverse group of synthetic dyes with application not only as textile colorants but in many other industrial fields for coloring different substrates, biological-medical studies, in the field of non-linear optics and optical data storage [15-22].

RESULT AND DISCUSSION

NBO analysis

NBO analysis has been performed to elucidate the intra-molecular interaction, rehybridization and delocalization[23-28]. The second order perturbation analysis of Fock matrix of PDBH is summarized in Table. 1. The strong intra-molecular interactions are formed by the orbital overlap between $\sigma(\text{C-C})$, $\sigma^*(\text{C-C})$ and $\pi(\text{C-C})$, $\pi^*(\text{C-C})$ bond orbitals in the aromatic rings, which leads intra-molecular charge transfer (ICT) causing stabilization of the system[29-31].

Hyper conjugative interaction between electron donating O_{23} atom to $\text{C}_{17}\text{-C}_{21}$ anti-bonding orbitals in the benzaldehyde group are 128.62 KJ/mol. Similarly O_{27} atom ($n\text{-}\pi^*$) transfer energy to $\text{C}_{17}\text{-C}_{25}$ (74.14) and $\text{C}_{25}\text{-H}_{26}$ (99.75 KJ/Mol) orbitals[32-39].

The $\sigma(\text{N12-N13})$ band with ED stabilize the energy of 7.07 and 7.53 KJ/mol to its acceptor anti-bonding orbitals (C2-C3) and C14-C16). More energy transfer takes place during $\pi\text{-}\pi^*$ transition[40-45]. In PDHB, the π bond of N12-N13 transfer 41.88 and 39.2 KJ/Mol energy to the anti-bonding orbitals (C2-C3) and C14-C15), respectively[46-50].

Table 1. The NBO analysis for PDHB

Type	Donor NBO (i)	ED/e	Acceptor NBO (j)	ED/e	$E^{(2)}$ KJ/mol	$E(j)\text{-}E(i)$ a.u.	$F(i,j)$ a.u.
$\sigma\text{-}\sigma^*$	BD (1) N12 -N13	1.98683	BD*(1) C2 - C3	0.02182	7.07	1.54	0.046
			BD*(1) C14 - C16	0.0225	7.53	1.52	0.047

$\pi - \pi^*$	BD (2) N12 - N13	1.91479	BD*(2) C2 - C3	0.37033	41.88	0.4	0.061
			BD*(2) C14 - C15	0.32793	39.2	0.4	0.058
			BD*(1) C16 - C19	0.01133	5.56	1.53	0.04
$n - \sigma^*$	LP (1) N12	1.95425	BD*(1) C3 - C4	0.03352	33.3	0.97	0.079
$n - \sigma^*$	LP (1) N13	1.95432	BD*(1) C14 - C15	0.03162	34.1	0.98	0.08
$n - \sigma^*$	LP (1) O23	1.97726	BD*(1) C17 - C21	0.03424	26.32	1.15	0.076
$n - \pi^*$	LP (2) O23	1.85595	BD*(2) C17 - C21	0.44127	128.62	0.35	0.1
$n - \sigma^*$	LP (1) O27	1.98435	BD*(1) C17 - C25	0.05927	6.19	1.14	0.037
$n - \sigma^*$	LP (2) O27	1.87453	BD*(1) C17 - C25	0.05927	74.14	0.71	0.102
			BD*(1) C25 - H26	0.07093	99.75	0.61	0.109
$\pi^* - \pi^*$	BD*(2) N12 - N13	0.20975	BD*(2) C2 - C3	0.37033	102.01	0.05	0.06
			BD*(2) C14 - C15	0.32793	132.21	0.05	0.067
$\pi^* - \pi^*$	BD*(2) C17 - C21	0.44127	BD*(2) C14 - C15	0.32793	518.82	0.02	0.08
			BD*(2) C16 - C19	0.28584	662.2	0.02	0.082

Conclusion

A NBO analysis has been performed for the first time for PDHB molecule. In this study, the π - π^* interaction can make larger intra-molecular interaction and hence the polarizability of the molecule increases.

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