Abstract:

Theoretical study on the intramolecular hydrogen bond in nitro-substituted naphthazarin

R. Farahati, M. Zahedi-Tabrizi*

1Alzahra University, Department of Chemistry, Tehran, Iran

*Email: Zahedi@alzahra.ac.ir

Introduction:

Currently, there is considerable interest in the study on naphthazarin (hereafter NZ) and its derivatives because of biological importance (e.g. antitumor and antiviral activity, wound healing, antimicrobial, antithrombotic properties and their use in the development of cardioprotective&); preparations). This compound has been extensively studied theoretically and experimentally. The aim of the present work is to demonstrate the effect of nitro substitutions of NZ on the intramolecular hydrogen bond strength.

Method:

All calculations were performed using Gaussian03 and NBO 5.0 programs. The full geometry optimization of NZ and its NO2 substitutions were performed with DFT calculations at the B3LYP/6-31G** theoretical level. Wiberg bond orders were calculated using NBO 3.0. The second order interaction energies, orbital population and natural steric analysis were performed at the B3LYP/6-31G** level using NBO 5.0 program. ¹H chemical shift was calculated at this theoretical level by GIAO method.

Results and discussion:

Performed calculations on the 9 derivatives of NZ show that the substitution of nitro increases the O...O and O...H bond length, and decreases OH...O bond angle and ¹H chemical shift. By natural bond orbital (NBO) method, the effect of substitution on the hydrogen bond strength, the charge distributions, steric effects, and electron delocalization in the studied compounds were investigated. NBO analysis are in good agreement with the calculated results the geometrical parameters.

Conclusions:

All performed calculations indicate that the electron-donating effect of NO2 increases the hydrogen bond strength. The geometrical parameters are in good agreement with the NBO analysis and the proton chemical shift results.