



Initial studies of the effects of halogenated dispersions on the amount of NICS of rings for $C_8H_{12}XNO_2$

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Abstract

In this research at the first complex and its halogenated derivatives were optimized. NBO calculations and NMR for the complexes were carried out at the B3LYP/6-31G* quantum chemistry level. In the 1-(4-fluorophenyl)-2,3-dihydro-1H-naphtho-[1,2-e][1,3]oxazine-3-n, there are 4 rings, respectively, rings from the side attached to the halogen. They are named C, B, A, and D. Calculations and studies show that the amount of aromatics in the halogen-ring A in all cases has the highest number. In the B loop, the predicted aromatization level is zero, and in the ring C and D, relative to the A loop, the aromaticity increase is as follows: $A > D > C$. In the next stage of the study, with the replacement of the halogen ring A from F to I, this process was researched. In ring A, when halogens were changed, the increase in aromaticity in halogenated compounds was as follows: $F > Cl > Br > I$. The data in tables and graphs and shapes were compared and discussed.

Keywords: halogenated derivatives, NICS, 4-fluorophenyl

1. Introduction

In the naphthalene-compressed molecule, 1 and 3-oxazine is not flat with the $C_8H_{12}FNO_2$ closed formulation, and has a boat configuration that has a two-edged angle between flat naphthalene, 6/4 quaternary loops (4/4), and 41/4 benzene ring (5) 81 and (3) make up 40.77 with 6-membered naphthalene rings. (Fig. 1) exists in the crystalline structure of the N-H hydrogen intermolecular bonds. The high composition is reported as an antibacterial reagent. This class of compounds is used as (precursor) in the preparation of phosphonics ligands for asymmetric catalysts [1-5].

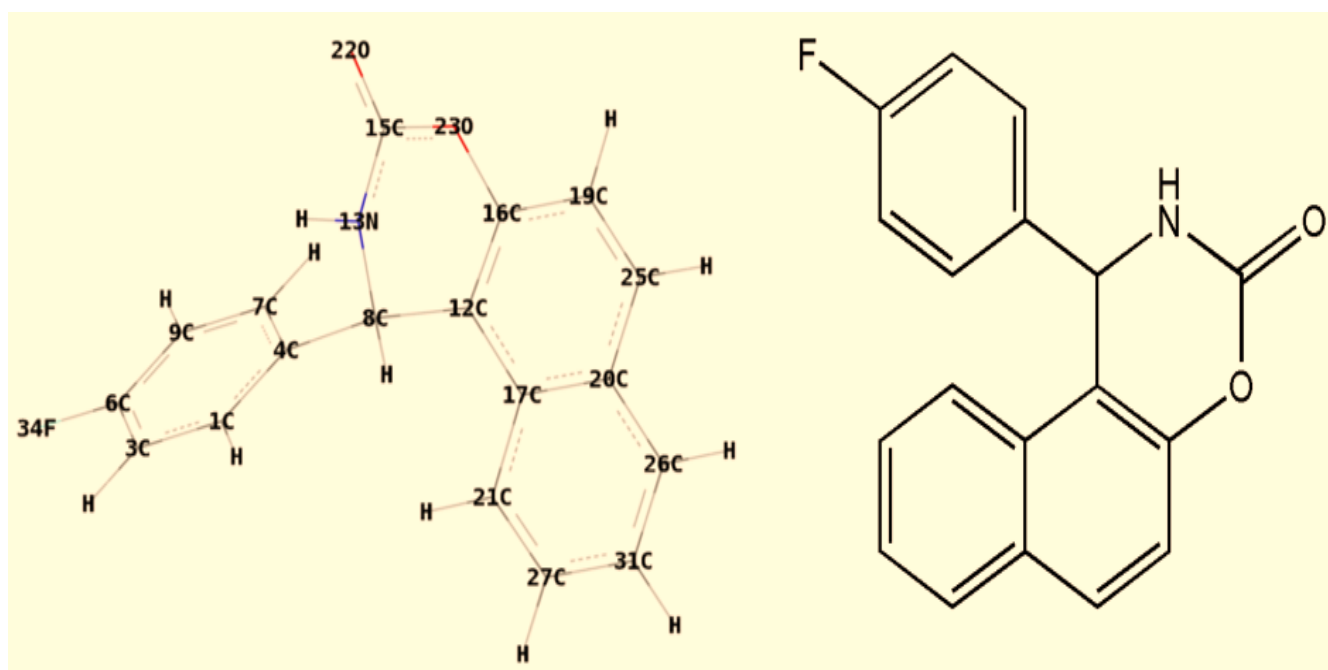


Fig 1. View of The image of the $C_8H_{12}XNO_2$ combination in the case of $X = F$

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [6-8]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of Complexes on Fullerene were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Complexes on Fullerene were investigated [9-12]. Through attachment to three different base positions. All these calculations are

done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor [12-16].

Results

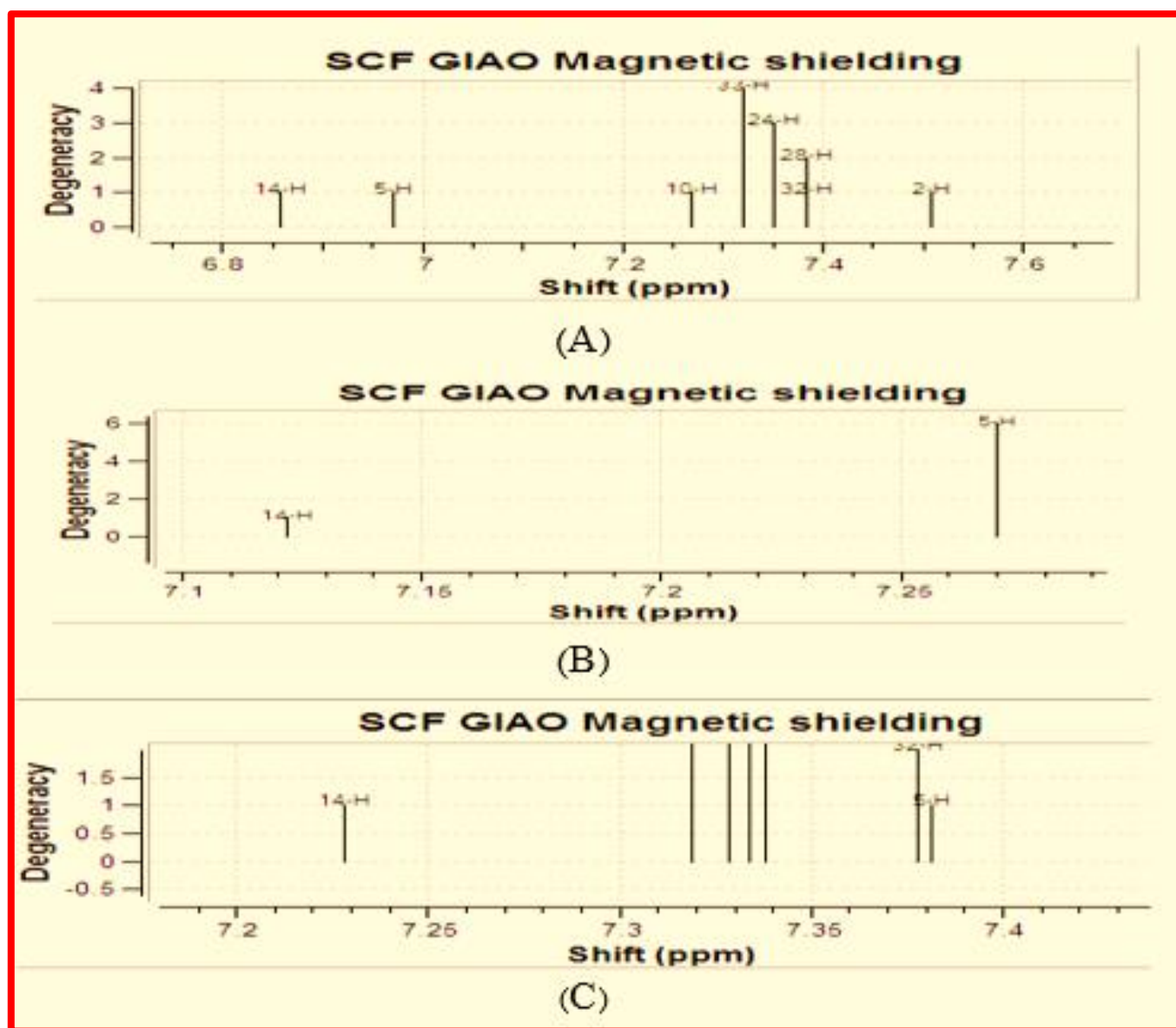
In this paper, computational calculations on C₈H₁₂FNO₂ were performed using Gaussian 2003 and Gossive software. The compounds were initially optimized by two hacker-type and density functional theory methods in a 6-31G* -nature series. Then, NICS studies related to the aromatic characterization of the loops in this composition were performed, and by changing the only existing halogen on one of the rings of this compound, the trend of variation The aromatism in the ring has been evaluated, which indicates that the level of aromatics of the ring A is greater than that of the F halogen. In addition, in each of the halogenated ring constituents, it is more aromatic than the other rings, regardless of the type of halogen. (Table 1).

Table 1: Computation of NICS (0) and NICS (1) Combination of C₈H₁₂XNO₂ with halogen type change at HF / 6-31G* and B3LYP / 6-31G*

HF/6-31G* ^a, B3LYP/6-31G* ^b								
	A		B		C		D	
	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(0)
F	-12.9238	-12.6479	0.391	1.0781	-10.8945	-11.4657	-11.2296	-13.0001
	-10.841	-10.9265	0.8625	1.4597	-9.5646	-10.3097	-9.7033	-11.6041
Cl	-12.0315	-12.5081	0.3352	0.9934	-10.9255	-11.5037	-11.2639	-13.0381
	-10.0159	-10.7531	0.814	1.384	-9.5895	-10.3417	-9.7317	-11.6359
Br	-11.7214	-12.3845	0.3456	0.9962	-10.9179	-11.495	-11.2551	-13.0274
	-9.7497	-10.6375	0.8172	1.374	-9.5873	-10.3393	-9.7268	-11.6292
I	-10.9875	-12.2475	0.3456	0.9296	-10.7203	-11.3622	-11.0409	-12.8695
	-9.0598	-10.5692	0.7845	1.2328	-9.3282	-10.2708	-9.4855	-11.5681

conclusion

The NMR spectrum of these compounds showed that by changing the amount of halogen present on the ring A, the amount of lamination varies on the A-hydrogens, in particular the adjacent halogens (5 and 14). The comparison of the displacement of the peaks in Fig. 2 is presented



* Fig. 2. shows the NMR spectra of halogen A) F B) Cl C) Br calculated in HF / 6-31G

The presence of halogen changes the anisotropic effects of the aromatic ring flow. The amount of these streams in the loop contains more halogen than halogen-like loops. Meanwhile, by increasing the electronegativity of halogens from iodine to fluorine, the flow rate of the rings increases. This table is shown in Table 1 using calculations at HF / 6-31G * and B3LYP / 6-31G * levels

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