Investigating the Effect of Changes of Halogenated Compounds on the Aromaticity Flow (NICS) of Rings 5-fluorophenyl-1, 3, 7, 9-tetra methylpyrido [2,3] [d-5,6 dipyrimidine -2, 4, 6 and 8 tetron

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Abstract

In the combination of 5-fluorophenyl-1, 3, 7, 9-tetra methyl pyrido [2, 3, d, d, 5, 6 di pyrimidine -2, 4, 6, and 8 tetron, there are 4 rings, respectively, ring that is attached to the halogen ring A and, respectively, a ring The lower and the right to the left of the ring A are called C, B, and D. Calculations and studies show that the amount of aromatics in halogen-ring A in all cases has the highest amount. In the B and D loop, the predicted aromaticity level is low and close to zero, and there is a reduction in aromatics in the C loop than the A ring. In another stage of the study, with the replacement of the halogen ring A from F to I, the following trend was observed. In ring A, when halogens were changed, the increase in aromaticity in halogenated compounds was as follows: F> Cl> Br> I.

Keywords: NICS, aromaticity, halogenated compounds.

1. Introduction

In combination with the closed formula C19H16F1N5O4, the fluorophenyl ring is not flat. The two-tailed angle between the C, B, and D rings is flat with a fluorophenyl ring of 83.24 (5) ° and 71.76 (4) °. (Fig. 1) in the crystalline structure of the interaction between aromatic rings is effective in the stability of the composition. Pharmaceutical properties Pyridopyrimidines are well known as anticancer and anti-viral drug [1-5].
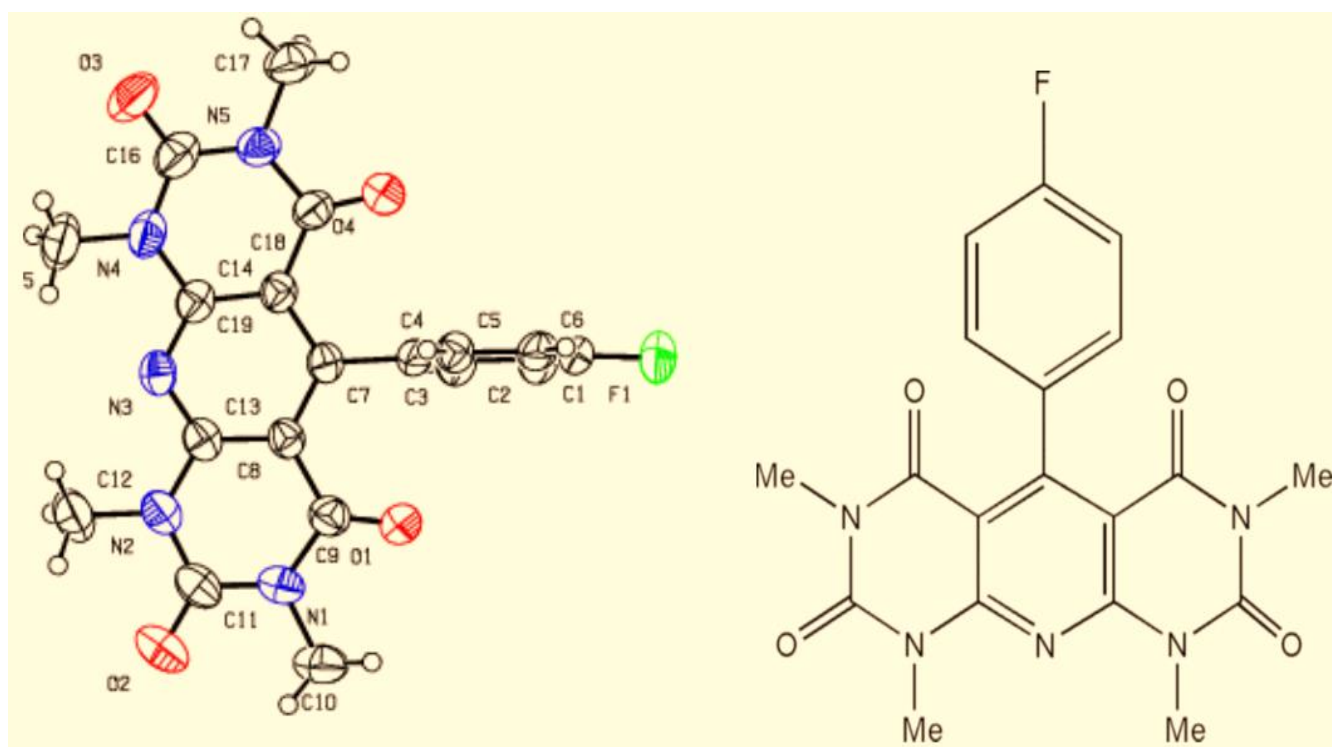

Fig 1. View of Combine image of C19H16X1N5O4 with X = F

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. 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 [9-10].

3. Results

In this paper computer simulations on C19H16X1N5O4 were performed using Gaussian 2003 and Gauss view 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 aromatics in the ring has been evaluated[11-15]. The results indicate that the aromaticity of the ring A is greater than that of the F-halogen. In addition, halogen-containing ring contains no more aromatics than any other loop, regardless of the type of halogen. (Table 1)

Table 1: Computation of NICS (0) and NICS (1) Compound C19H16X1N5O4 by changing the halogen type at HF / 6-31G * and B3LYP / 6-31G *

	A		B		C		D	
	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(0)
F	-12.1376	-8.7869	-0.4336	-2.1159	-6.8304	-7.5731	-0.5046	-1.8782
Cl	-11.1953	-8.798	-0.5374	-1.9104	-6.8829	-7.6129	-0.4652	-2.1469
Br	-10.9135	-8.7175	-0.5281	-1.9015	-6.8751	-7.6033	-0.4558	-2.1381
I	-10.2999	-8.8844	-0.4216	-1.8303	-6.7285	-7.5448	-0.3586	-2.0566

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 hydrogen of the ring A, in particular the adjacent halogen halides (3 and 10). The comparison of the displacement of the peaks in Fig. 2 is presented. [16-21].
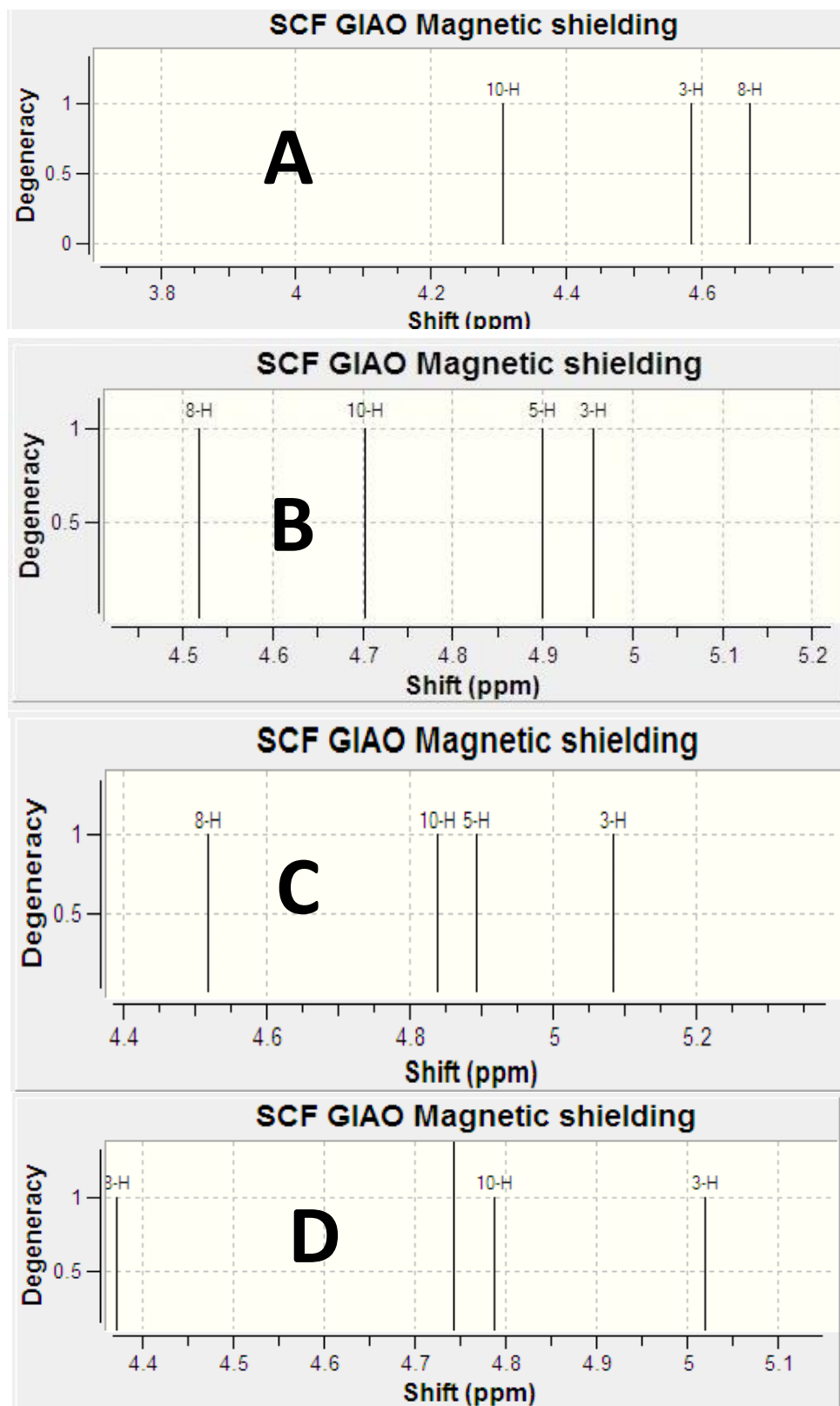
Fig (1) NMR spectra of compounds containing halogen a) F b) Cl d) Br d) I calculated in HF / 6-31G *

Conclusion

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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