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Study of the Effect of Halogens on the Asymmetric Parameters, Coating Constants and Chemical Disposition of Carbon Atoms in the $C_{17}H_2ON_2S$ Compound with Quantum Chemistry Calculations

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Abstract

In this study, the combination of Phenergan $C_{17}H_2ON_2S$, in which two aromatic rings are present, are attached to the rings at carbon position 5 and 13 halogens, and the changes in the asymmetric parameter, the convex constants, and the chemical displacement of the lateral carbon atoms are calculated. It shows that with the change of halogen based on the electronegativity of the fluorine atom, the contiguous constants always have the lowest values and chemical displacement in most of the carbon atoms studied.

Keywords: Phenergan, Fullerenes, Chemical potential, Nano drug carriers.

1. Introduction

Phenergan is well absorbed through the oral route and from the injection site. Its metabolism is liver. Its onset of oral or intramuscular injection is approximately 20 minutes and is about 3-5 minutes after consumption. The duration of its sedative effect is about 8-2 The time and duration of the anti-histamine effect is 6-6 hours. This drug is slowly excreted in the kidneys and stools, mainly in the form of passive metabolites. In this study, with the change of substitutions at positions 5 and 13 simultaneously, the

changes of the asymmetric parameter, the convex constants and the chemical displacement of the lateral carbon atoms are considered [1-12].

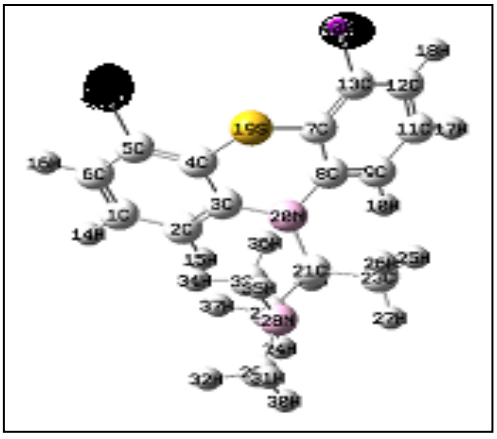


Fig 1. View of Phenergan In the case of X = F, Cl, Br

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [13-15]. 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 Phenergan 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 Phenergan 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.

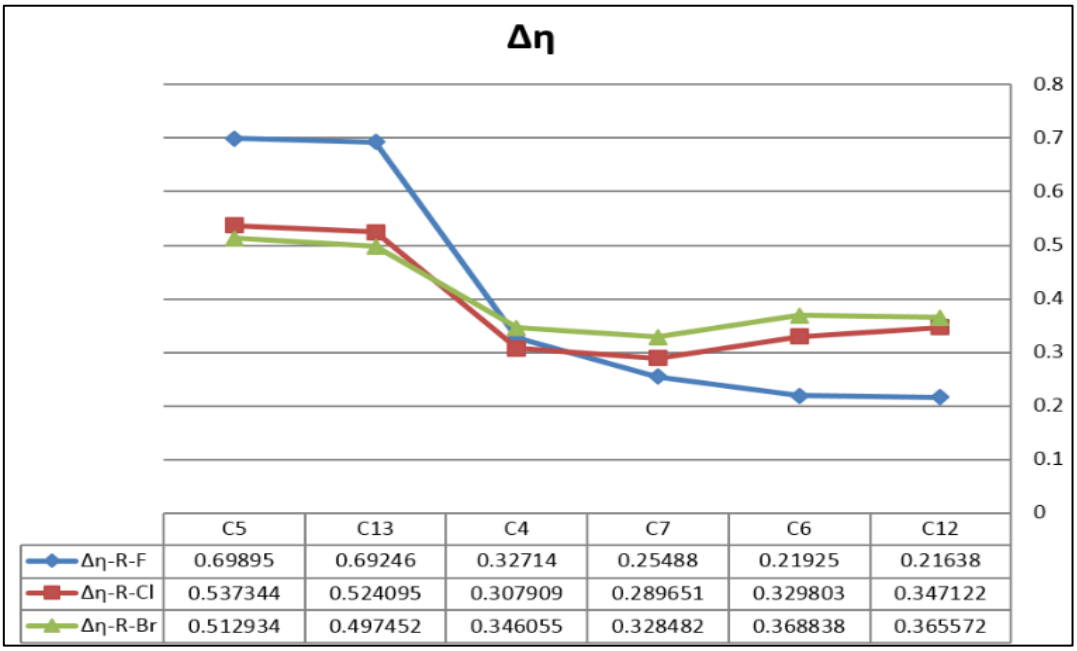
3. Results

In this paper, computer computing in the $C_{17}H_{20}N_2S$ composition using Gaussian Winogens 98 software
The compounds were first optimized with the Hartree method and were optimized in the G * 6-31 base series, and then studies were done on the changes in the fixation constants in the ipsum-related state of the compound. By changing the halogen on the rings of this compound, the process of variation Coating constants were evaluated in the ring, and the results of the convex constants indicate that the values of ηΔ or the asymmetric parameter of the anisotropy of the chemical displacement depend on the electronegativity and atomic shape and increase with the increased electronegativity of the atomized atom (halogen). The values of δ, or the displacement of the isotropic Chemical decreases with increasing electronegativity and amounts The term σΔ or the fixed coating depends on the atomic atom and the negative integer. Chlorine has the highest content and the fluorine atom has the lowest value. The results are shown in tables and charts (1, 2 and 3).

The values of Δη: for the positions of 5 and 13 carbon according to the halogen on it, are as follows: F> Cl> Br

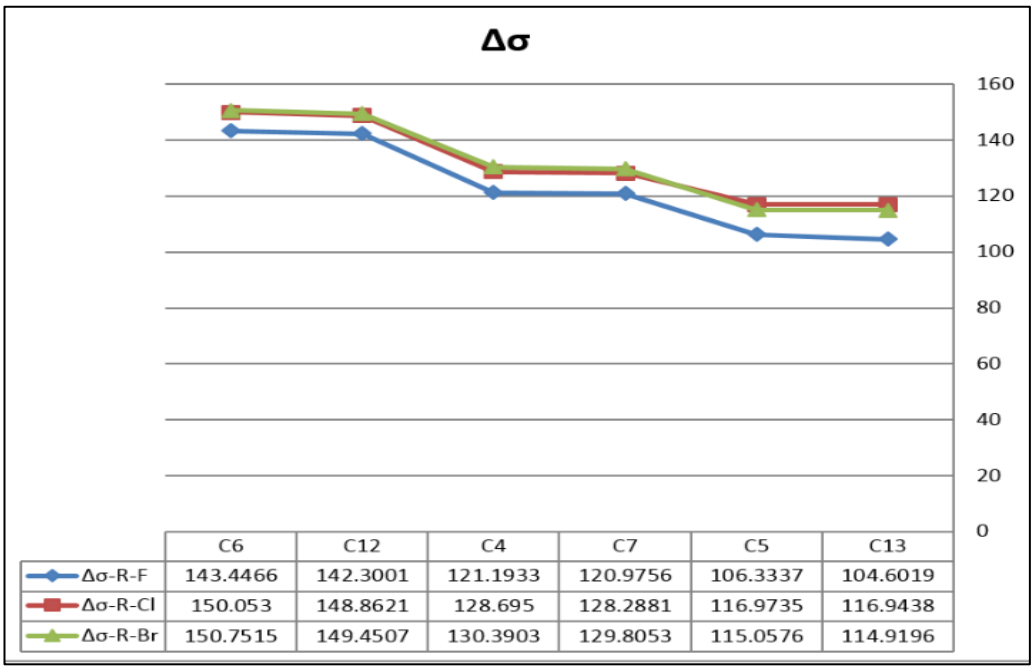
The values of δ: for the positions of 5 and 13 carbon, according to the halogen on it, are as follows: Br> Cl> F

The values of Δσ: for the positions of 5 and 13 carbon according to the halogen on it, the following is true: F> Br> Cl



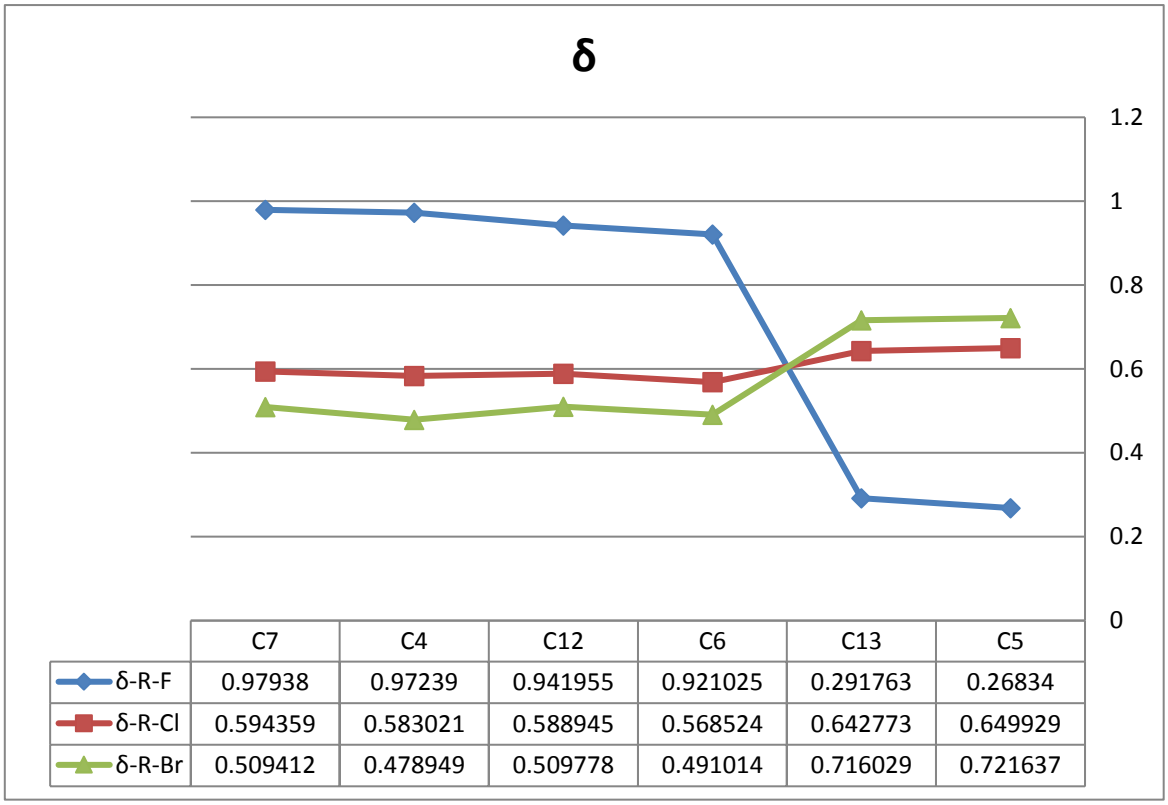
	C5	C13	C4	C7	C6	C12
Δη-R-F	0.69895	0.69246	0.32714	0.25488	0.21925	0.21638
Δη-R-Cl	0.537344	0.524095	0.307909	0.289651	0.329803	0.347122
Δη-R-Br	0.512934	0.497452	0.346055	0.328482	0.368838	0.365572

Fig2: Comparison of the values of Δη for positions of 5, 4, 7, 6, 12, and 13 with respect to the halogen placed on it by the Hartree Factor method and in the base series 6-31 G*



	C6	C12	C4	C7	C5	C13
Δσ-R-F	143.4466	142.3001	121.1933	120.9756	106.3337	104.6019
Δσ-R-Cl	150.053	148.8621	128.695	128.2881	116.9735	116.9438
Δσ-R-Br	150.7515	149.4507	130.3903	129.8053	115.0576	114.9196

Fig 3. Comparison of the values of Δσ for the positions of 5, 4, 7, 6, 12, and 13 with respect to the halogen placed on it using the Hartree Factor method and in the base series 6-31 G *



	C7	C4	C12	C6	C13	C5
δ-R-F	0.97938	0.97239	0.941955	0.921025	0.291763	0.26834
δ-R-Cl	0.594359	0.583021	0.588945	0.568524	0.642773	0.649929
δ-R-Br	0.509412	0.478949	0.509778	0.491014	0.716029	0.721637

Fig 4. Comparison of the values of δ for the positions of 5, 4, 7, 6, 12, and 13 with respect to the halogen placed on it by the Hartree Factor method and in the base series 6-31 G*

4. Conclusion:

The presence of halogen causes changes in the CSA coverage rates. The amount of these changes in the halogen content loop varies depending on the type of halogen. As the halogen has a higher electronegativity, the higher the Δη value, the lower the amount δ and the chlorine Δσ. Bromine and fluorine is altered due to the induction of halogens and their shape. The contents in tables and diagrams (1) and (2) and (3) are shown using the calculations of the HF technique in the base series 6-31G.*

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