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Computational Survey on the Effect of Changes in Halogenated Compounds on the structural properties in Chlorpromazine

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Abstract

In this study, on the combination of chlorpromazine with two aromatic rings, halogens are attached to the rings, and changes in the angles and lengths of the ipsos are calculated. Calculations show that by changing the halogen based on the amount of electronegativity, the magnitude and variation of the angular lengths The lengths of the links also change in the following order. The angles of the IPSO mode: RF <R-Cl <R-Br. In addition, the length of the bonds in C5-C4: R-F <R-Br <R-Cl and the length of the C5-C6: R-F <R-Cl <R-Br. Similarly, bipolar moments changes in states where the halide is connected to two loops and into a loop. Calculations show that by varying the halogen based on the electronegativity and the factor occupancy, the bipolar momentum changes as follows.

Pro + 2F> Pro + 2Cl> Pro + 2Br> Pro + F> Pro + Cl> Pro + Br>

chlorpromazine

Keywords: Chlorpromazine, Chemical potential, Bipolar Moment

1. Introduction

Allergies or allergies often appear to be skin or respiratory illnesses, and various factors, such as pollen, of plants or some of the foods affect it. The root of the French scientist was the first to recapture the

disease and found that in some people, The contact with the Marine Corps was made in 1937, and the French scholar Stube found that some phenol ethers could in certain cases prevent the effects of histamine with the receptor in the cells. The French scientists, as a result of their continued research and studies, discovered A string of materials is null and void They received histamine, all of which were highly toxic. The first drug of this category, which was less effective at the same time as its toxicity, was discovered and introduced by Halper in 1949. The compounds of the antlers were recognized as the most effective and useful compound, and for the first time used as an antihistamines The test compound is an organic compound and antihistaminic drugs. It is a combination of phenothiazine derivatives.

In this project, by changing the refractories in position 5, changes in the length of the C5-C4 and C5-C6 bonds of the substitution change zone The complex ring has been investigated (Fig. 1) [1-9].

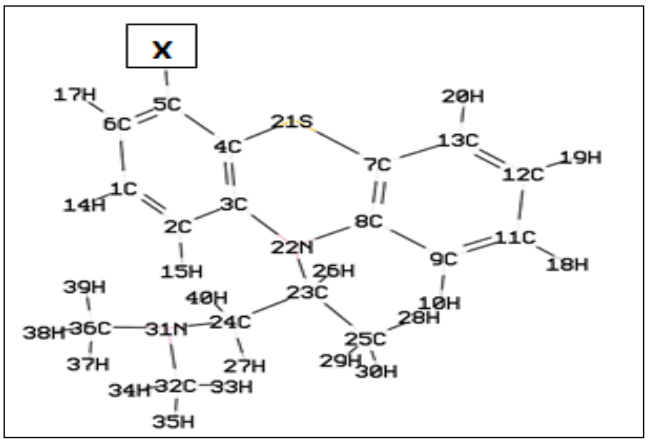


Fig 1. View of Chlorpromazine, . C17H20N2S composition image in carbon position 5

X= F, Cl, Br

Also, by changing the refluxes in position 5 alone, the positions 5 and 13 simultaneously examined with respect to the chlorampromazine combination cluster with the closed formula C17H20N2S and the existing heterotrams of bipolar moments. (figure 2)

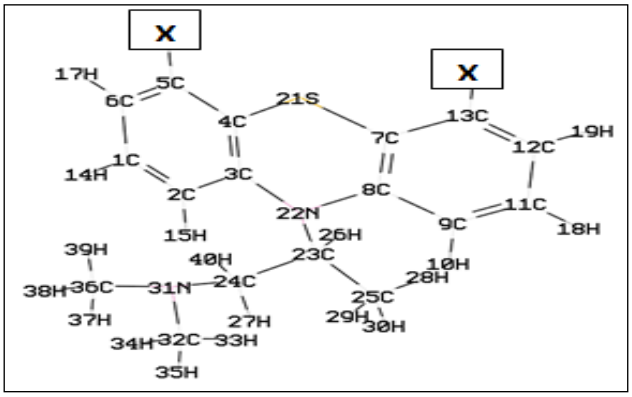


Fig 2. shows the composition of C17H20N2S in the position of carbon 5 and 13

X = F, Cl, Br

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [10]. 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[11-15]. For all atoms, the standard 6-31G basis set is utilized. The structures of Chlorpromazine 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 Chlorpromazine 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[15-19].

3. Results

In this paper, computational calculations were performed on the C17H20N2S composition using Gaussian 98 software. The compounds were first optimized with the Hartree Factor method in the G * 6-31 base series, and then studies on the angular and longitudinal changes in the ipsw state of the compound The changes in the length of the links and the changes in the angles in the ring were evaluated by changing the halogen on one of the rings of the compound, and the results indicate that the length of the links and angles in the ring is shortened for the time when the fluorine halogen is on the table.

Table (1) Calculates the length of the connections in the C17H20N2S composition by changing the type of halogen in the carbon position 5 at the level HF / 6-31G *

atom	C5-C6	C5-C4
R-F	1.37436	1.37887
R-Cl	1.37903	1.38303
R-Br	1.37955	1.38263

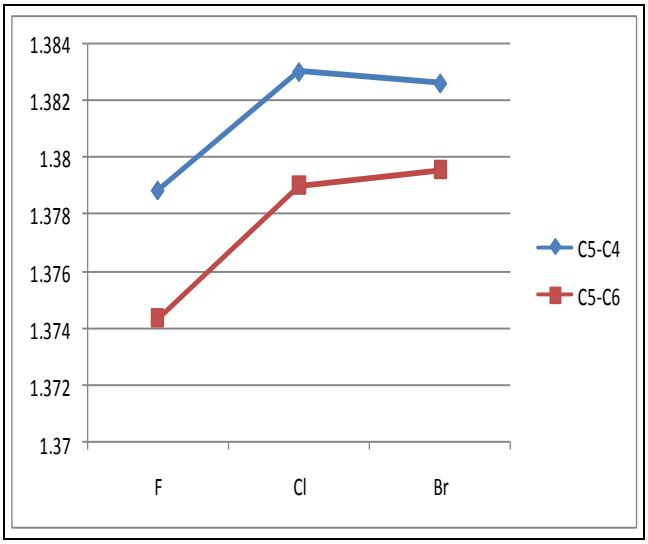


Fig 3.The variations in the length of the bond for the carbon atoms bonded to the complex ring with a halide substrate at position 5 in the HF method

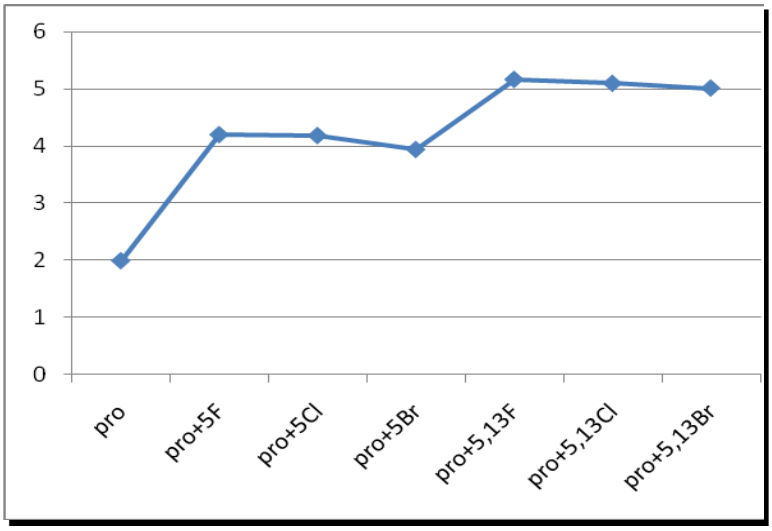
And then studies on bipolar momentum variations in the case of halides

Is connected to a ring and two-rings. In this compound, by changing the halogen on the two rings and a ring of this composition, the trend of bipolar moments in the ring was evaluated and the results indicate an increase in the bipolar momentum in the two halides It is attached to the halogen component, depending on the type of halogen and the location of the halide substrate on it. Table and graph (2)

Table 2: Calculating the dipole moment in the chlorampromazine C17H20N2S composition by changing the type of halogen

	Dipole moment (deby)			
Compound	H	F	Cl	Br
Chlorpromazine	1.9834			
Chlorpromazi +C5-X	1.9834	4.2003	4.1828	3.9388
Chlorpromazi +C5-XC13-X	1.9834	5.1704	5.1013	5.0183

Table 3. bipolar momentum changes for the carbon atoms attached to the complex ring, and with a halide solvent in position 5 and 5.13



5. Conclusion:

The presence of halogen causes changes in the length of the bonds and as a result of the strength of the bonds. The amount of these changes in the halogen-containing ring varies depending on the type of halogen. The more the halogen has a greater electronegativity, the greater the length of the bundle, which is due to the induction of halogens, i.e. bonds Case Study

C5-C4, C5-C6 are stronger. The contents of the table and diagram (1). Also, the presence of halogen causes bipolar moments to change. The amount of these changes in the halogen-containing ring varies depending on the type of halogen and the presence of halogen. The more halogen Electronegativity and on one side of the loop, the amount of dipole moment is increased as a result of the induction of halogens. Table and diagram (2). The data are based on quantum chemistry calculations at the HF / 6-31G * level.

Reference

[1] B. Acemioglu, *Journal of Colloid and Interface Science*, 274, 371 (2004).

[2] Z.Jianjun, L. Bingwei, Y. Chenxuan, R. Xiangdong, *J. Rare Earths*, 28, 37 (2010).

[3] APHA-AWWA, WPCF, "*Standard Methods for the Examination of Water and astewater*",21st ed., American Public Health Association,Washington, DC (2005).

[4] X.Li,Q.Xu,G.Han, W.Zhu, Z.Chen, X.He,X.Tian, *J. Hazard. Mat*., 165, 469 (2009).

[5] F.Colak, N.Atar, A.Olgun, *Chem. Eng. J.*,150, 122 (2009).

[6] R. Nadeem, M.H. Nasir, M.S. Hanif, *Chem. Eng. J.*, 150, 40 (2009).

[7] K. Li, X. Wang, *Bioresour. Technol*., 10,2810 (2009).

[8]Y.S Ho, G. McKay, *Process Biochem*., 34, 451 (1999).

[9]A. Gucek, S. Sener, S. Bilgen, M. A. Mazmanci, *J. Colloid Interf. Sci.*, 286, 53 (2005).

[10] F. Geiger, M. Stoldt, H. Schweizer, P. Bauerle, E. Umbach, *Adv. Mat*., 5, 922 (1993).

[11] F. Garnier, G. Horowitz, X. Peng, D. Fichou, *Adv. Mat*., 2, 592 (1990).

[12] P. bäurele In: K. Müllen and G. Wegner, Editors, Electronic Materials : The oligomer

Approach, Wiley-VCH, Weinheim, NY, 105- 197 (1998)

[13] G. Horowitz, M.E. Hajlaoui, *Adv. Mater*., 12, 1046 (2000); H. Meng, J. Zheng, A.J. Lovinger, B.-C. Wang, P.G. Van Patten, Z. Bao, Chem. Mater., 15, 1778 (2003);

[14] M. Mushrush, A. Facchetti, M. Lefenfeld, H.E. Katz, T.J.Marks, J. Am. Chem. Soc., 125, 9414 (2003).

[15] M. Pasini, S. Destri, W. Porzio, C. Botta, U. Giovanella, *J. Mater. Chem.*, 13, 807 (2003);

[16] M. Suzuki, M. Fukuyama, Y. Hori, S.Hotta, *J. Appl. Phys.*, 91, 5706 (2002).

[17] D. Pisignano, M. Anni, G. Gigli, R. Cingolani, M. Zavelani-Rossi, G.Lanzani, G.Barbarella, L. Favaretto, *Appl. Phys. Lett*., 81, 3534 (2002).

[18] L. Torsi, A.J. Lovinger, B. Crone, T. Someya, A. Dodabalapur, H.E. Katz, A.Gelperin, J. Phys. Chem. B., 106, 12563 (2002); J. Roncali, *J. Mater. Chem.*, 9, 1875 (1999).

[19] N. Noma, T. Tsuzuki, Y. Shirota, Adv. Mater., 7, 647 (1995); C. Videlot, A. El Kassmi, D. Fichou, *Solar Energy Mater. Solar Cells*, 63, 69 (2000); K. Hara, M. Kurashige, Y. Dan-Oh, C. Kasada, A. Shinpo, S. Suga,K. Sayama, H. Arakawa, New J. Chem., 27, 783 (2003); J. Ackermann, C. Videlot, A. El Kassmi, R. Guglielmetti, F. Fages, *Adv.Mater*., 16, 1709 (2004).