



## Evaluation of the Effect of Changes in Halogenated Compounds on NICS of Promethazine

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### Abstract

In this research at the first Promethazine drug and its fullerene derivative were optimized. NMR calculations for the complexes were carried out at the B3LYP/6-31G\* quantum chemistry level. Promethazine is not used as an antihistaminic drug for anyone. In the pharmaceutical composition of promethazine (RS) - N, N-dimethyl-1- (10H-Phenothiazin-10 yl) -propen-2-amino, two aromatic rings In this study, halogens are connected to one of their loops and the changes in the type of halogen at the surface \* HF / 6-31G are calculated. The calculations show that, by changing the type of halogen based on the variation of electronegativity of halogens, the aromatase level is as follows increase. R-F > R-Cl > R-Br. The data in tables and graphs and shapes were compared and discussed.

**Keywords:** Promethazine, Hallucination Aromatization, Level HF / 6-31G

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### 1. Introduction

Promethazine's drug is thought to slow down the stimulation of the cerebrospinal lattice system indirectly by stopping it with competition with histamine for binding to the hormone receptor in the head cell, spasticity and histamine-induced congestion. It is a drug that is only reacted It prevents histamine, but it does not eliminate if it occurs. By preserving its chemical antimicrobial receptors (CTz), its anti-vomiting effect may be applied. Its anti-vertigo effects are likely to be exerted by central antimuscarinic effect. In this study, the flow Aromatitiste Promethazine [1-42].

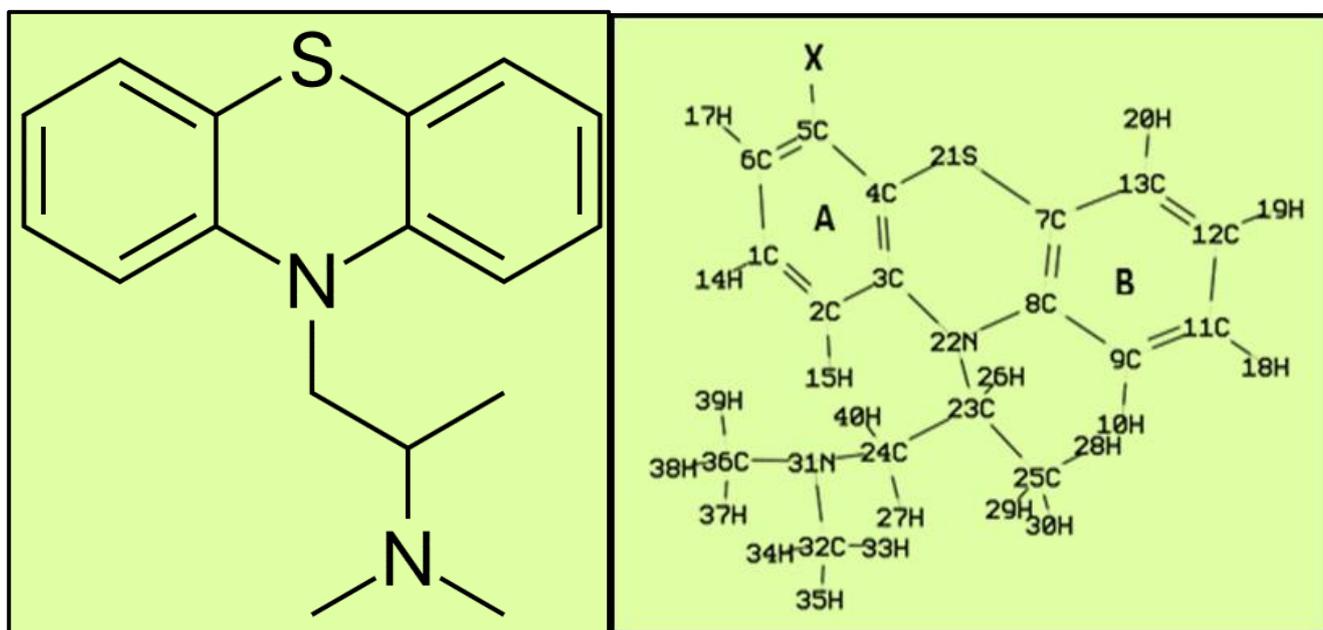


Fig 1. Optimized image of promethazine ((C<sub>17</sub>H<sub>20</sub>N<sub>2</sub>S X = F, Cl, Br. And loops A and B.

## 2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [9]. 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 Promethazine with different Halogen were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Halogen on Promethazine were investigated. Through attachment to same position. 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, computational calculus was performed on the C<sub>17</sub>H<sub>20</sub>N<sub>2</sub>S composition using Gaussian Winogens 98 software. The compounds were first optimized with the Hartree Fake method in the G \* 6-31 base series, and then NICS studies were conducted to investigate the aromatic character of the rings present in this compound. By changing the halogen on the

One of the rings of this composition was evaluated for the aromatic changes in the ring (A) and the results indicate that the amount of aromatase in the ring (A) is greater than the type of halogen on which the primary promethazine composition is. Table (1) F>Cl>Br>H

Table 1: Calculation of NiCS (0) and NiCS (1) Combination of C<sub>17</sub>H<sub>20</sub>N<sub>2</sub>S by changing the type of halogen at HF / 6-31G \*

|         | R+F      | R+Cl     | R+Br     | R+H      |
|---------|----------|----------|----------|----------|
| NICS(0) | -10.3599 | -9.7266  | -9.5222  | -8.7743  |
| NICS(1) | -12.4755 | -12.3839 | -12.3052 | -11.2070 |

Investigating the H NMR spectrum of these compounds showed that, by changing the amount of halogen on the ring A, the amount of latency on the A-ring hydrogens, in particular the adjacent halogen halides, is altered at the side positions of carbon 5 and 13, where the comparison of the displacement of the peaks is shown in Fig.

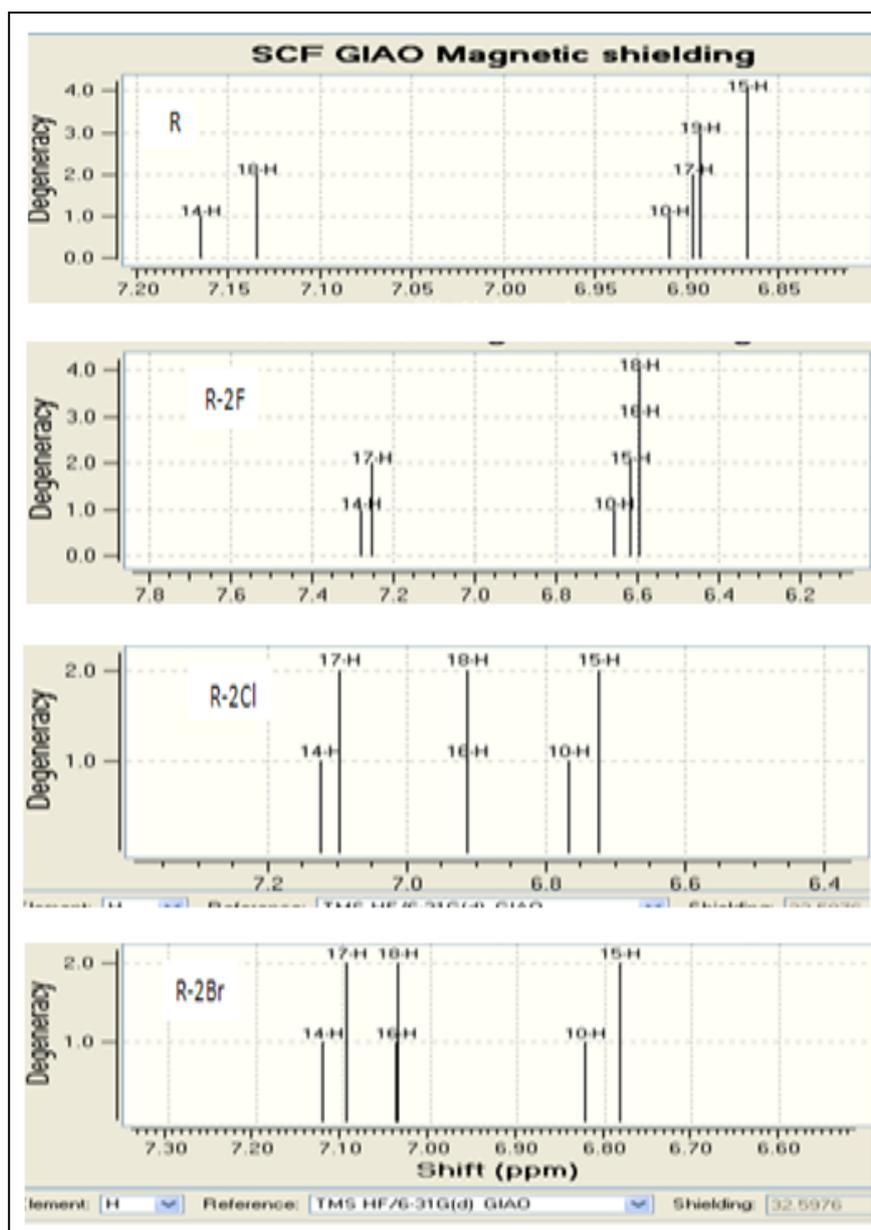


Fig 2. Spectrum of 1H NMR Compounds of R-2X include dualoguanium with the primary composition of promethazine X = F, Cl, Br calculated in HF / 6-31G\*

#### 4. Conclusion:

The presence of halogen causes changes in the anisotropic effects of the aromatic ring flow. The amount of these streams in the halogen containing ring is greater than halogen-like loops. In addition, by increasing the electronegativity of halogen from bromine to fluorine, the flow rate of the rings increases as a result of the induction of halogens. The comparison of the 1H NMR spectrum of the R-2X compositions including dual halogen with the initial promethazine compound shows that by increasing the amount of atomic atomic electrostatics, on the carbon numbers 5 and 13, the chemical displacement of the

adjacent hydrogens is shifted to the weak field due to the lower electron density density on it. Figure (2).

Data using calculations in HF / 6-31G \* levels are shown.

## References

- [1] S.F. Yin, B.Q. Xu, S.J. Wang, C.F. Ng, C.T. Au, *Catal. Lett.*, 96, 113 (2004).
- [2] M.T. Drexler, M. D. Amiridis, *Catal. Lett.*, 79, 175 (2002).
- [3] R.S. Varma, *Green. Chem.*, 1, 43 (1999).
- [4] S. Samantaray, D.K. Pradhan, G. Hota, B.G. Mishra, *Chem. Eng. J.*, 193, 1 (2012).
- [5] S. Li, W. Zhang, M.H. So, C.M. Che, R. Wang, R. Chen, *J. Mol. Catal. A: Chem.*, 359, 81 (2012).
- [6] J. Albadi, A. Razeghi, A. Mansournezhad, H. Abbaszadeh, *J. Nanoparticles*, 9, 83 (2013).
- [7] J. Albadi, N. Iravani, F. Shirini, F. Dehghan, *J. Chem. Res.*, 36 (10), 610 (2012)
- [8] A.M. Donia, A.A. Atia, W.A. Al-Amrani, A.M. EiNahas, *J. Hazard. Mater.*, 161, 1544 (2009).
- [9] A. Hou, B.Chen, J. Dai, K.Zhang, *J. Cleaner Prod.*, 18, 1009 (2010).
- [10] A.Afkhami, M.S. Tehrani, H.Bagheri, *Desalination*, 263, 240 (2010).
- [11] G. Crini, *Bioresour. Technol.*, 97, 1061(2006).
- [12] R. Ahmadi, E. Farajpour, *Ce. N.*, 37, 6 (2015).