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A Theoretical Study on Dopamine: Geometry, energies and NMR

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ABSTRACT

The Dopamine has been studied theoretically at the B3LYP/6-31G* level were performed in gas phase. We calculated physical parameters like atomic charges, energy (ΔE), asymmetry parameter (η), chemical shift σ_{iso}, dipole moment and isotropic NMR determinant and in this work we used Gaussian 03 at NMR and calculation by using B3LYP methods with 6-31G* basis set.

Keywords: Dopamine; NMR; Theoretical

INTRODUCTION

Dopamine, like most amines, is an organic base. A dopamine molecule consists of a benzene ring with two hydroxyl side groups. Dopamine is a hormone and neurotransmitter that plays a number of important roles in the human brain and body [1,2]. In the brain, dopamine functions as a neurotransmitter—a chemical [3] released by nerve cells to send signals to other nerve cells [4].

Several important diseases of the nervous system are associated with dysfunctions of the dopamine system. Parkinson's disease (PD), causing tremor and motor impairment, is caused by loss of dopamine-secreting neurons in the midbrain area [4,5,6]. There is evidence that schizophrenia (SPh) involves altered levels of dopamine activity [7] that are frequently used to treat it have a primary effect of attenuating dopamine activity [8]. Attention deficit hyperactivity disorder (ADHD) be associated with decreased dopamine activity [9].

We will focus here on the mesencephalic dopamine centers and Energy Levels of dopamine molecules, the reaction of chlorine and bromine, and iodine atoms with the molecule dopamine.

COMPUTIONAL METHODS

The structure of dopamine was designed primarily using of Chem. Bio Draw 12.0 (Fig 1). The geometry of the systems has been optimized at the B3LYP [10,11] and 6-31G* [12] computational level. Mullikan charges on the nitrogen atom and the dipole moments, and geometry parameters

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such as bond lengths were also determined and the data are listed in Table 1. All the calculations have been performed with the Gaussian-09 program [13].

RESULTS AND DISCUSSION

The optimized structural parameters of dopamine has been calculated by DFT/B3LYP level with the 6-31G* basis set and are listed in Table 1. The optimized molecular structure along with the numbering atom of dopamine is as shown in Fig. 1.

The reported geometry and molecular properties, such as the equilibrium energy, HOMO-LUMO band gap, dipole moment etc. after the geometry optimization. The basic electronic parameters related to the frontier orbitals in a molecule are the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and their resulting energy gap. Both the HOMO and LUMO are the main orbital take part in chemical stability [14].

The optimization and NMR calculation of all systems are done by density functional theory (DFT) using B3LYP method and the standard 6-31G* basis set, by Gaussian03 suit of programs were done in the gas phase. Quantum chemical calculations yield chemical shielding tensors in the principal axis system with the order of $\sigma_{33} > \sigma_{22} > \sigma_{11}$; hence, Eqs. (1) And (2) are used to convert the calculated chemical shielding tensors to the absolute isotropic (σ_{iso}) and anisotropic ($\Delta\sigma$) chemical shielding parameters:

$$\sigma_{iso} = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 \quad (1)$$

$$\Delta\sigma = \sigma_{33} - (\sigma_{11} + \sigma_{22})/2 \quad (2)$$

Table 2 presents the computed chemical shift for selected hydrogen, nitrogen and carbon atoms. The shielding tensor asymmetry parameter (η) which is given by:

$$\eta = \frac{|\sigma_{22} - \sigma_{11}|}{|\sigma_{33} - \sigma_{iso}|} \quad (3)$$

The span (Ω) describes the maximum width of the powder pattern. The skew (κ) of the tensor is a measure of the amount and orientation of the asymmetry of the tensor [15, 16].

$$Span: \quad \Omega = \sigma_{11} - \sigma_{33} \;\; ; \;\; \Omega \geq 0 \quad (4)$$

$$Skew: \quad \kappa = \frac{3(\sigma_{22} - \sigma_{iso})}{\Omega} \;\; ; \;\; (-1 \leq \kappa \leq +1) \quad (5)$$

Table 2 presents the computed chemical shift for selected hydrogen, nitrogen and carbon atoms. The graphs of calculated isotropic shielding values, anisotropic chemical shift tensor ($\Delta\sigma$), asymmetry parameter (η), skew (the amount and orientation of the asymmetry of the tensor) and total atomic charge of propose atoms versus the atomic number are also drawn in Figure 2a to e, respectively. As shown in Figure 2, the N nucleus has more negative total atomic charge and a larger isotropic chemical shift tensor (σiso), anisotropic chemical shift tensor (Δσ) and the amount and orientation of the asymmetry of the tensor (κ) for the N atom (Fig 2a, b and d).

CONCLUSION

The optimized structure of dopamine that studied in this work, has been shown in Fig 1. Dipole moment, E, HOMO, and LUMO, band gap, ΔG and ΔH reported in Table 1. We calculated chemical shifts for each atom and these parameters are reported in Table 2.

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Table 1. Hybrids, geometry and molecular properties of dopamine by the B3LYP method with 6-31G*(d) basis set

Symbol	charge of nitrogen(a.u)	ΔG (kcal/mol)	ΔH (kcal/mol)	Energy of band gap (kcal/mol)	E(kcal/mol)	Dipole Moment(D)
$(OH)_2$-DOP*	-0.71468	91.41632	122.3273	-130.942	324198.5	1.3422

* $(OH)_2$-DOP: dopamine

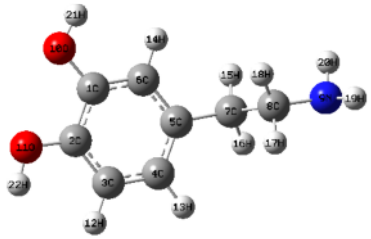

Fig. 1. The Structure of dopamine.

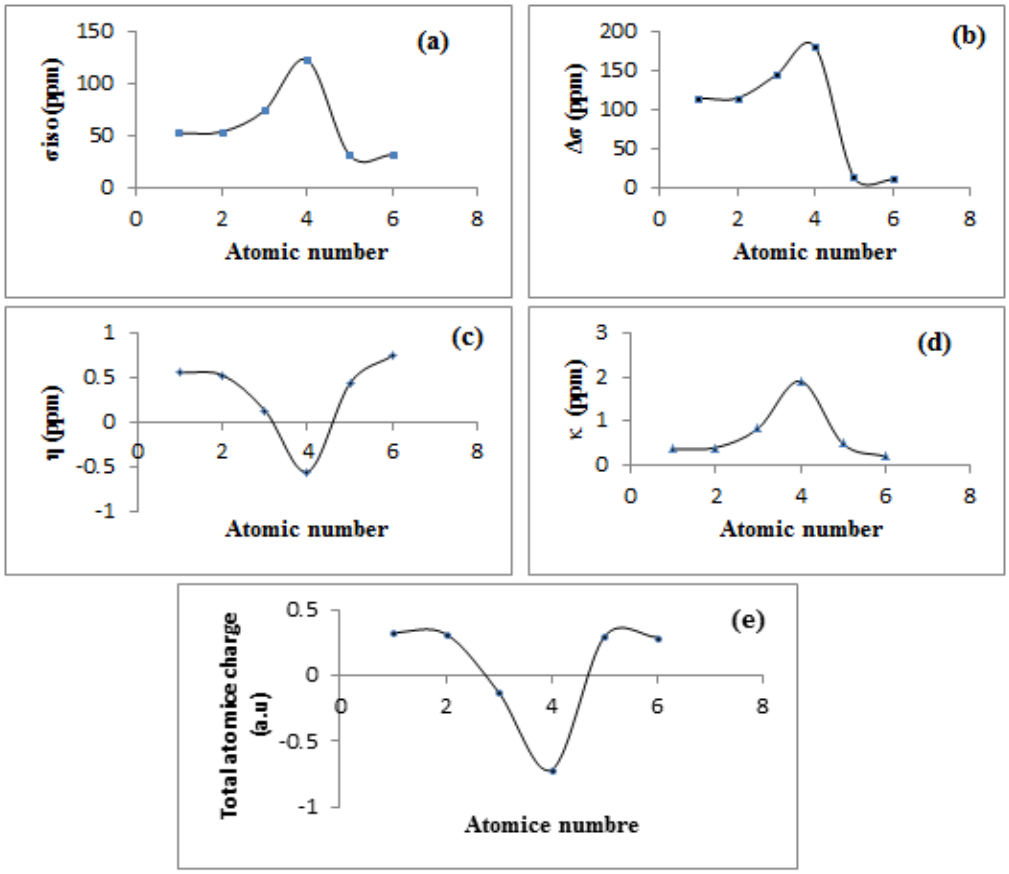

Fig. 2. Graphs of the isotropic shielding values (σ_{iso}) versus atomic number; (a) anisotropic shielding value($\Delta\sigma$) versus atomic number; (b) η versus atomic number; (c) skew (the amount and orientation of the asymmetry of the tensor)(κ) versus atomic number; (d) total atomic charge (a.u) versus atomic number; (e) for selected atoms of dopamine at the level of B3LYP/6-31G* theories in GIAO method.

Table 2. Computed chemical shifts for selected atoms

atom number	σiso(ppm)	Δσ(ppm)	η(ppm)	κ(ppm)	Charge(a.u)
C1	52.8371	115.1234	0.552007	0.378372093	0.327738
C2	54.07326667	114.7742	0.52375621	0.405457	0.315797
C8	74.16563333	144.2458	0.128023138	0.836289	-0.128391
N	122.7373667	179.9705	-0.554212496	1.906395171	-0.714647
H19	31.71467	14.4569	0.43501	0.493439335	0.296342
H20	32.2225	11.3277	0.743319474	0.20571089	0.290714

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