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Molecular docking, spectroscopic studies and simulation of the dopamine molecule by the DFT and MP2 methods

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The FTIR and Raman spectra of dopamine were also recorded in the spectral region 20 - 4000 cm^{-1} and 400 - 4000 cm^{-1} respectively. The optimized molecular geometry and fundamental vibration frequencies are interpreted using structural optimizations based on the DFT method. The B3LYP / 6-311G (d, p) was used to determine the calculations of the chemical descriptor. The dopamine (DA) molecule can acquire a maximum charge of 0.513 eV from its environment. To understand the molecular interactions of Dopamine, the MEP is a crucial tool. Nonlinear optical descriptors (NLO) and the lengths, bond angles are also determined by DFT and MP2 methods. The DFT method was used to determine the chemical shifts of ^{1}H and ^{13}C of the product. These constants have been calculated by employing the GIAO (Gauge-Including-Atomic-Orbit), CSGT (Continuous Set of Gauge Transformations) and IGAIM (Individual Gauges for Atoms In Molecules) methods at the B3LYP/6-311G (d, p). The comparison of the theoretical chemical shifts with the experimental ones shows that the CSGT method is the best.

1. Introduction

DA (**Fig. 1**) is a neurotransmitter, a biochemical molecule that enables communication within the nervous system, and one that directly influences behavior. DA reinforces usually beneficial actions such as eating healthy food by inducing the sensation of pleasure, which thus activates the reward/reinforcement system.[1] It is therefore essential for the survival of the individual. More generally, it plays a role in motivation and risk-taking in mammals, and therefore in humans as well.[2] This molecule belongs to the group of catecholamines and is derived from two amino acids tyrosine or phenylalanine. In the central nervous system, it activates postsynaptic and presynaptic dopamine receptors. It is mainly produced in the substantia nigra and in the ventral tegmental area, located in the midbrain.[3] Although dopamine, along with norepinephrine and serotonin, is very minor in the brain, since together they concern less than 1% of neurons, they play an essential final modulating role of motor and psychic outputs. It is also a neurohormone produced by the hypothalamus. Its main hormonal function is to inhibit the release of prolactin from the anterior lobe of the pituitary gland.[4] Dopamine was designated with a motivational function based on the Ungerstedt 18 report that food and drink deficits similar to those induced by pains of the lateral hypothalamus can be caused by damage selective to the dopamine fibers that pass through this region, while selective deterioration to the mesolimbic dopamine fibers diminishes the forward locomotion that is similar to majority rewards. The development of dopamine antagonists has found that the compromise in dopaminergic function affects the instrumental response to food more adequately than it alleviates free eating.[5] The density functional theory (DFT) plays an interesting role in studies on freezing and melting transitions.[6,7] The liquid-crystal interface,[8] nucleation,[9] glass transition,[10] and quasi-

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crystals [11] are also treated within the framework of the DFT. NMR spectroscopy has become an extraordinary tool for studying molecular structure. The DFT computing of shielding NMR has very precise levels of approximation and is available in the literature.[12] There are many more methods to calculate chemical shifts such as: Continuous Set of Gauge Transformations (CSGT), a slight variation on the CSGT method (IGAIM) and gauge independent gold invariant gold including atomic orbital (GIAO). The GIAO/DFT approach is known to give acceptable chemical shifts for different nuclei with larger molecules.[13,14]

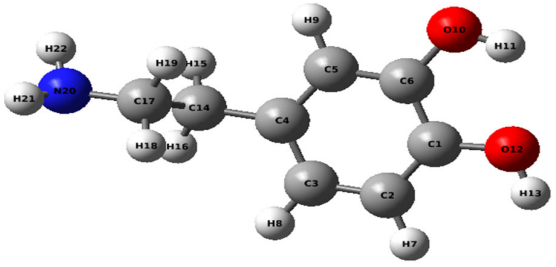

Fig. 1. Optimized molecular structure of dopamine

This work investigated the structural and spectroscopic properties of DA. We used the DFT method with different functionalities to calculate the lengths and angles of the links. Determining molecular orbitals, the MEP surface can lead to an understanding of the properties and activity of DA. We calculate the chemical shifts by different methods to find the most reliable.

2. Results and discussion

2.1 Infrared vibration spectra of the dopamine molecule

FT-IR is a method founded on the vibrations of the atoms of a molecule.[15] The infrared (IR) spectrum of the dopamine neurotransmitter has been registered in the range of fingerprints (0–4000 cm^{-1}). Spectroscopic studies are supplemented by quantum chemical calculations at the levels of the B3LYP theory by the basic set 6-311G (d, p).[16]

FT-IR spectrum (**Table 1**) shows characteristic vibrational peaks at wavenumber 3657 cm^{-1} and 2047 cm^{-1} that were assigned to N-H and C-H stretching, respectively. Further, IR peaks that appeared at 1558 cm^{-1} were attributed to C=C (phenolic) multiple peaks. The C-C stretching peaks were observed at 1287 cm^{-1}. The C-OH (phenolic) stretching was assigned to IR peaks that appeared at 1117 cm^{-1}. The vibrational peaks that appeared at 485 cm^{-1} were attributed to =C-H bending. The FT-IR data observed for dopamine by the DFT method are similar to their experimental counterparts.

Table. 1. Calculated and experimental vibrational low frequencies in the region up to 4000 cm^{-1} for dopamine (ν, stretching; δ, in-plane bending). [17]

ν, stretching (cm^{-1}) / δ, in-plane bending	Calculated ''FT-IR''	Experimental ''FT-IR''
ν_{N-H}	3657	3348
ν_{C-H}	2047	2954
$\nu_{C=C}$	1598	1640
ν_{C-C}	1287	1287
ν_{C-O}	1117	1145
ν_{C-OH}	485	475

2.2 Theoretical chemical displacements ^{1}H and ^{13}C NMR of the dopamine molecule

NMR spectroscopy is a method that exploits the magnetic properties of certain atomic nuclei. It is based on the phenomenon of nuclear magnetic resonance (NMR), also utilized in medical imaging under the name of MRI, NMR is a property of certain atomic nuclei with nuclear spin (for example ^{1}H, ^{13}C, …), placed in a magnetic field. The molecular structure of dopamine is optimized by B3LYP/6-311G (d, p) method with the Gaussian 09 program. Then, the ^{13}C and ^{1}H NMR chemical shifts of DA are calculated and compared to the experimental data are shown in **Table 2**. It has been confirmed from **Table 2** that the calculated values are similar to experimental values.

According to the data of **Table 2** we managed to draw a curve of the experimental displacements according to the theoretical displacements, we obtained a line of the following equation: Y = a X + b (**Fig. 3**). It seems that the chemical shifts calculated for the carbon and hydrogen atoms are similar to experimental results.

Table. 2. The theoretical ^{13}C NMR and ^{1}H NMR chemical shifts of the molecule calculated using GIAO/CSGT/IGIAM / B3LYP, (Experimental values for the dopamine structure).[18]

Nuclei ^{13}C , ^{1}H	ca δ_{exp} l	δ_{GIAO}	δ_{CSGT}	δ_{IGIAM}
C1	145.19	144.5	144.0	144.6
C2	117.53	115.9	115.1	115.5
C3	122.18	122.8	121.0	121.0
C4	130.27	131.5	131.8	131.0
C5	117.56	116.4	115.9	115.6
C6	148.98	145.6	144.9	143.9
C14	32.93	39.3	38.6	37.6
C17	41.62	41.9	41.2	41.5
H7	6.90	6.73	6.72	6.52
H8	6.84	6.68	6.75	6.65
H13	3.22	5.15	5.01	5.04
H16	2.86	2.83	2.54	2.14

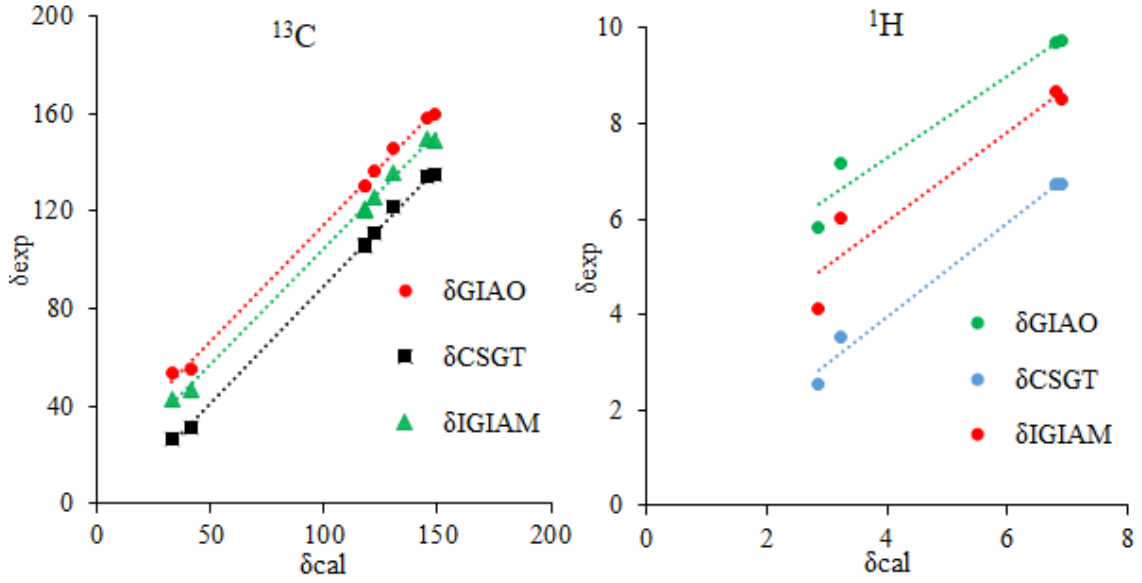

Fig. 2. Graphic correlation of the chemical shift between the values calculated at basic level 6-311G (d, p) and experimental

Regression analysis was used to determine a, b and R^2 parameters of the linear correlation shown in **Fig. 3** between the experimental and the theoretical chemical shifts of ^{1}H and ^{13}C calculated according to GIAO, CSGT and IGIAM methods for the dopamine. The obtained slope, intercept and the correlation coefficients, R^2, are summarized in Table 3. It is shown that the correlation coefficients R^2 for the CSGT are closer to one than that of the GIAO and IGIAM method. From these results, it appears that the CSGT method better describes the NMR ^{13}C ($R^2 = 0.9982$) and ^{1}H ($R^2 = 0.984$) chemical shifts calculation for the dopamine compound investigated in this work.

Table 3. The parameters of the equation a, b and R^2 of the GIAO, IGAIM, CSGT methods at the level of the basis set 6-311G (d, p)

Method	Nuclei	Equation /Correlation	GIAO	CSGT	IGAIM
DFT/6-311G (d,p)	^{13}C	a	0.9559	0.9652	0.9568
		b	9.0279	6.9952	18.744
		R^2	0.9979	0.9982	0.9975
	^{1}H	a	0.8563	0.9762	0.9359
		b	3.8633	0.0625	2.2093
		R^2	0.9541	0.984	0.9108

2.3 Quantum chemical calculation

Quantum chemical calculations have been executed using the DFT with a basic set 6-311G (d, p) implemented in the Gaussian 09 software package. The distribution of charges of NBO in B3LYP / 6-311G (d, p) of the DA molecule shows that the most negative charges are found on the oxygen atom and nitrogen. This observation is due to the electronegativity of the oxygen atom (O10, O12) and nitrogen (N20). Border molecular orbitals (FMO) (HOMO and LUMO) are interesting for describing chemical reactivity. The HOMO which does not have electrons represents the capacity of (E_{HOMO}) to give an electron, while the LUMO does not have electrons, which represents the capacity of (E_{LUMO}) to accept an electron .[19] Distribution charges, HOMO and LUMO calculated for dopamine are presented in (**Fig. 4**).

The electrostatic potential is a physical observable which can be obtained by calculation. It has been used to predict regioselectivity.20 In the electrostatic potential, the regions of potential rich in electrons represent the sites of protonation and nucleophilic attack, the regions of potential poor in electrons represent the electrophilic sites. **Fig. 5** indicates the molecular electrostatic potential (MEP) and the electrostatic potential of the potential Maps. It seems that the electrostatic potentials on the surface of the molecule are represented by different colors. The red regions represent the negative electrostatic potential, the blue parts indicate the positive electrostatic potential and the green color indicates the zero potential. On the other hand, the red-colored regions indicate the electrophilic reactivity and the nucleophilic reactivity for the positive parts.

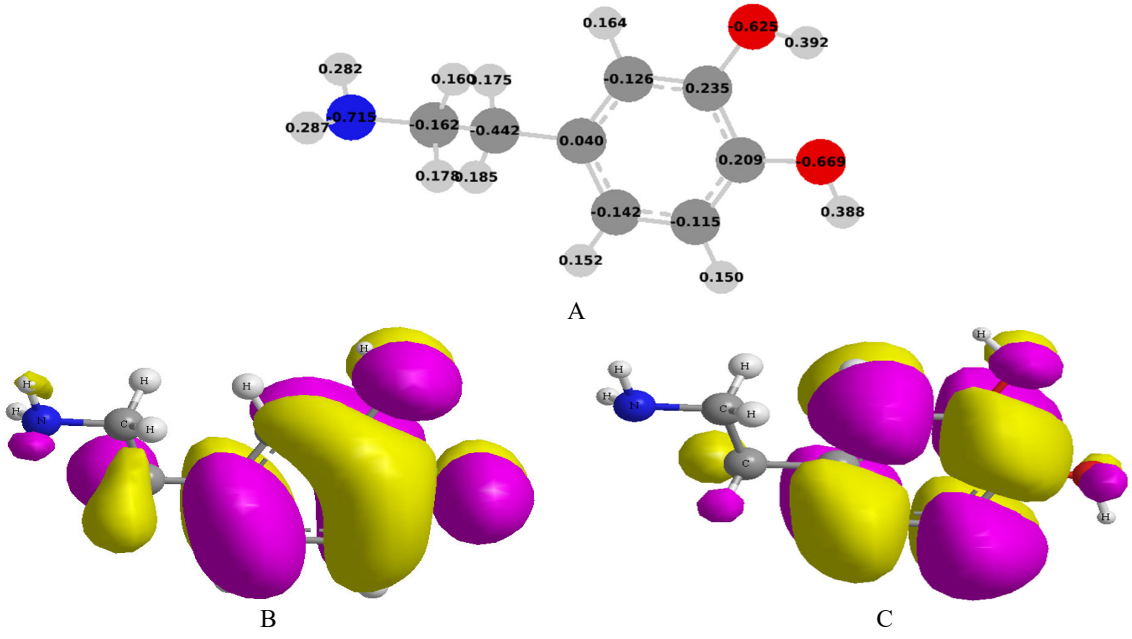

Fig. 3. (A) NBO charges distribution, (B) HOMO and (C) LUMO of dopamine

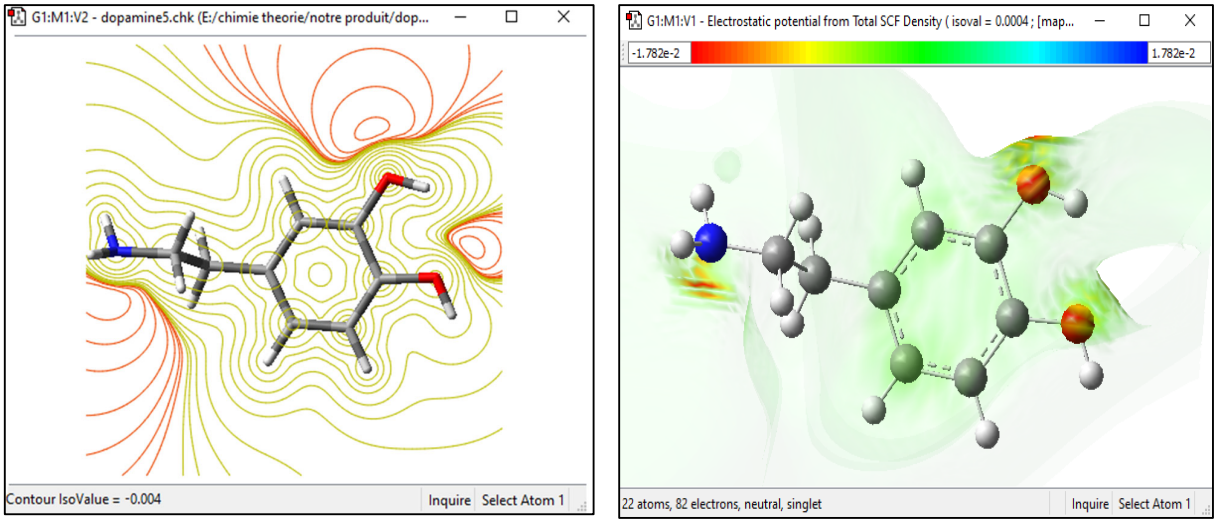

Fig. 4. Contour electrostatic potential and electrostatic potential maps around the DA

Based on the functional density theory, several properties of dopamine are represented in **Table 4**. [21]

Ionization potential: $I = -E_{HOMO}$

Electronic affinity: $A = -E_{LUMO}$

Absolute electronegativity : $\chi = \frac{I+A}{2}$

Overall hardness: $\eta = I - A$

Overall softness: $\sigma = \frac{1}{\eta} = \frac{1}{E_{LUMO} - E_{HOMO}}$ Electronic chemical potential: $\mu = -\frac{(I+A)}{2}$

Maximum charge transfer: $\Delta Nmax = -\frac{\mu}{\eta}$ Overall electrophilicity: $\omega = \frac{\mu^2}{2\eta}$

Overall nucleophilia N: $N = E_{HOMO} - E_{HOMO(TCE)}$ with $E_{HOMO(TCE)}$ = -9.3686 eV calculated by DFT/B3LYP 6-311G (d, p).

Table. 4. Quantum theoretical parameters of dopamine calculated by B3LYP/6-311G (d, p)

Parameters	E_{LUMO} (eV)	E_{HOMO} (eV)	ΔE (eV)	I (eV)	A (eV)	μ (eV)
dopamine	-0.143	-11.060	10.917	11.060	0.143	-5.601
Parameters	**χ (eV)**	**η (eV)**	**σ (eV^{-1})**	**ω (eV)**	**N (eV)**	**ΔN_{max}(eV)**
dopamine	5.601	10.917	0.091	1.436	-1.691	0.513

In this paper, an alternative approach to the evaluation of local electric dipole moments (μ), the polarizability (α), first hyperpolarizability (β) and second hyperpolarization are calculated using a basic set of DFT and MP2 (**Table 5**). Complete equations to calculate the amplitude of the total static dipole moment, the average polarizability, and the first and second hyperpolarizability (γ), using the x, y, z components of 09W The Gaussian exit is as follows.[22]

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \qquad \alpha = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})}{3} \qquad \beta = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$$

$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz} \qquad \beta_y = \beta_{yyy} + \beta_{xxy} + \beta_{yzz} \qquad \beta_z = \beta_{zzz} + \beta_{xxz} + \beta_{yyz}$$

$$< \gamma > = \frac{1}{5} \left(\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2\left[\gamma_{xxyy} + \gamma_{yyzz} + \gamma_{xxzz}\right]\right)$$

The μ of the DA is calculated using DFT / MP2 and method B3LYP with a basic set 6-311G (d, p). μ reflects the distribution of molecular charges and is given as a three-dimensional vector. Consequently, it can be utilized as a descriptor to represent the charge movement through the molecule as a function of the negative and positive charge centers. Dipole moments are necessarily determined for neutral molecules. For charged molecules, its values depend on the orientation and the choice of the origin of the molecule. The value of the μ and the first polarizability calculated by the DFT method is greater than that calculated by the MP2 method. The polarizability calculated by the two methods is almost the same. The second hyperpolarizability obtained by the DFT method is lower than that found by the MP2 method. The difference sometimes in the values calculated by the two methods is explained by the MP2 method is an Ab initio method based on the calculation of the wave function which depends on 4N variables (three spatial coordinates and the fourth of spin) and energies of molecular orbitals. While the density functional theory (DFT) goes beyond reducing the number of variables by replacing the wave function with a function which is the electronic density ρ (x, y, z) which does not depend on 3 variables only.

Table 5. Electric dipole moments (Debye) by two methods DFT and MP2 of dopamine calculated using B3LYP / 6-311G (d, p)

	Parameters	DFT	MP2
Dipole moment (Debye)	μ_x	0.5428	0.5013
	μ_y	-1.7468	-1.7050
	μ_z	1.0655	1.0233
	μ	2.1168	2.0507
Polarizability (Debye)	α_{xx}	-54.8451	-50.7512
	α_{yy}	-63.7261	-63.7051
	α_{zz}	-67.9888	-66.5811
	α	-57.260	-60.3458
First hyperpolarizability (Debye)	β_{xxx}	40.2463	38.2463
	β_{xyy}	9.7492	8.4062
	β_{xzz}	-4.5695	-4.2134
	β_{yyy}	-14.4696	-13.5621
	β_{xxy}	7.6557	8.5648
	β_{yzz}	3.4453	3.2215
	β_{zzz}	6.4694	5.9875
	β_{xxz}	27.6194	20.6548
	β_{yyz}	2.3612	3.0001
	β	58.144	51.7967
Second hyperpolarizability (Debye)	γ_{xxxx}	-2057.8593	-200.8453
	γ_{yyyy}	-509.5370	-501.1470
	γ_{zzzz}	-153.9081	-150.5621
	γ_{xxyy}	-405.7996	-410.5686
	γ_{yyzz}	-114.7490	-100.7490
	γ_{xxzz}	-389.3145	-356.5625
	γ	-908.206	-517.6603

2.5 Bond length and angle properties of dopamine

Their lengths and connections to the angles were optimized at B3LYP / CAMB3LYP / HCTH / HSEH1PBE / WB97XD by the DFT method based on levels 6-311G (d, p), the purpose of which is to describe the molecular chemical and physical properties. The optimized geometric parameters are listed in **Table 6**, **Table 7** and **Table 8**, respectively, as experimental results available for comparison. As we can see on these tables the results of the band lengths and band angles of the same molecule at the DFT level (B3LYP/ CAMB3LYP / HCTH / HSEH1PBE / WB97XD) are very similar and in good condition according to the experimental structure. The C4-C14 bond length is longer than the C5-C6 bond length and these were optimized to 1.514 Å and 1.389 Å respectively because the C6 bond is bound by OH. The length of the C3-C4-C14-C17 bond is 95.2° in the side chains constitutes 4 carbons and is consistent with the experimental value. The study of the geometric product, therefore, showed excellent agreement between experimental[23] and theoretical results.

Table 6. Bond lengths (Å) of dopamine by the DFT based on 6-311G (d, p).

Bond length (Å)	B3LYP	CAMB3LYP	HCTH	HSEH1PBE	WB97XD	Exp
C_5-C_4	1.405	1.405	1.399	1.404	1.401	1.399
C_5-C_6	1.389	1.389	1.382	1.39	1.384	1.393
C_6-C_1	1.401	1.400	1.393	1.402	1.396	1.403
C_1-C_2	1.388	1.388	1.393	1.389	1.384	1.389
C_2-C_3	1.400	1.400	1.395	1.398	1.396	1.396
C_3-C_4	1.402	1.402	1.394	1.402	1.397	1.395
C_6-O_{10}	1.388	1.388	1.380	1.385	1.379	1.357
C_1-O_{12}	1.406	1.406	1.398	1.401	1.396	1.372
C_4-C_{14}	1.514	1.514	1.508	1.509	1.505	1.510
C_{14}-C_{17}	1.543	1.543	1.534	1.539	1.533	1.521
C_{17}-N_{20}	1.469	1.467	1.458	1.459	1.456	1.490

Table 7. Bond angle (°) of dopamine by the DFT based on 6-311G (d, p)

Bond angle (°)	B3LYP	CAMB3LYP	HCTH	HSEH1PBE	WB97XD	Exp
C_5-C_6-C_1	119.87	119.87	119.91	119.71	119.85	119.91
O_{10}-C_5-C_6	119.93	119.93	120.20	119.58	120.20	118.63
C_6-C_1-C_2	120.39	120.39	120.47	120.13	120.44	119.78
C_2-C_1-O_{12}	114.29	125.30	125.37	125.10	125.41	116.73
C_1-C_2-C_3	119.50	119.50	119.42	119.77	119.49	119.93
C_2-C_3-C_4	120.90	120.90	120.87	120.97	120.85	120.89
C_3-C_4-C_5	118.60	120.90	118.69	118.33	118.68	118.87
C_4-C_{14}-C_{17}	112.98	112.98	112.74	113.52	112.62	110.75
C_{14}-C_{17}-N_{20}	110.52	110.52	110.55	111.01	110.53	110.84
C_3-C_4-C_{14}	120.85	120.85	120.85	120.93	120.86	120.73
C_4-C_5-C_6	120.71	120.71	120.61	121.06	120.67	120.6

Table 8. Dihedral angle (°) of dopamine by the DFT based on 6-311G (d, p)

Dihedral angle (°)	B3LYP	CAMB3LYP	HCTH	HSEH1PBE	WB97XD	Exp
O_{10}-C_6-C_5-C_4	179.85	179.85	179.84	179.87	179.81	179.98
C_5-C_6-C_1-O_{12}	179.86	179.86	179.85	179.85	179.85	177.53
C_6-C_1-C_2-C_3	-0.1157	-0.1157	-0.0836	-0.1433	-0.1983	-0.21
C_2-C_3-C_4-C_{14}	-178.14	-178.14	-178.10	-178.24	-177.93	-176.20
C_3-C_4-C_{14}-C_{17}	95.21	95.21	95.60	94.19	96.45	100.47
C_4-C_{14}-C_{17}-N_{20}	-178.32	-178.32	-178.77	-177.44	-178.29	-171.77
C_{14}-C_4-C_5-C_6	178.10	178.10	178.08	178.16	177.90	176.67
O_{12}-C_1-C_2-C_3	-179.88	-179.88	-179.85	-179.90	-179.87	-177.85

3. Conclusion

In this work, we have studied the determination of theoretical molecular structures of dopamine by B3LYP / 6-311G (d, p) with DFT and MP2 methods. We have given a good approach to calculating the dipole moments. According to the tables, the results of the lengths and angles of the connections of the same molecule at the DFT level (B3LYP/ CAMB3LYP / HCTH / HSEH1PBE / WB97XD) are very similar and in good condition according to the experimental structure. The study of the geometric product has therefore shown an excellent agreement between the experimental and theoretical results. We used the DFT method to reproduce the nuclear magnetic properties of the ^{13}C and ^{1}H of dopamine. The theoretical calculation of chemical shifts of dopamine compounds shows that the theoretical values calculated by the CSGT method are similar to the experimental results. The density functional theory can be used as an effective approach to chemical shift calculations to NMR ^{13}C and NMR ^{1}H. The FT-IR data observed for dopamine by the DFT method are similar to their experimental counterparts.

4. Theoretical section

In this work, our objective is to analyze all the density functions implemented in the Gaussian 09 program suite - a more widely used quantum chemistry program. Quantum molecular descriptors (QMD) and the following quantum chemical

indices have been taken into account: the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest occupied molecular orbital (E_{LUMO}), the energy band gap $\Delta E = E_{LUMO} - E_{HOMO}$, The electrostatic potential Contour and the potential maps electrostatic. [24,25,26] The IR and vibrational simulation spectra of dopamine have been done on the DFT using the Gaussian program 09.

The ^{1}H and ^{13}C chemical shifts were calculated by the B3LYP/6311G (d, p) at optimized geometries by GIAO/CSGT/IGAIM methods. [27,28] Water was used as a reference in calculating the ^{1}H and ^{13}C chemical shifts. Linear correlation analyses were performed by the program and the visualization of the output files is carried out by the software Gauss-View 09. The quality of each correlation was given by the value R (Pearson's correlation coefficient).[29,30]

The isotropic chemical shift calculation δ_{iso} can be found as:

$$\sigma_{iso}^{molécule} = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

where, σ_{xx}, σ_{yy} and σ_{zz} are the main normal constraints coefficients. The isotropic chemical shifts were calculated from the following formula:

$$\delta_{iso} = \sigma_{iso}^{réf} - \sigma_{iso}^{molécule}$$

where σ_{ref} is the tensor of corresponding electronic form a reference water substance.

References

1 Rossi-Fernández A.C., Meier L.A., and Castellani N.J. (**2019**) Neutral and zwitterionic dopamine species adsorbed on silver surfaces: A DFT investigation of interaction mechanism, *Int. J. Quantum Chem., 119*, 1-18.
2 Vatrál J., Boča R., and Linert W. (**2015**) Oxidation properties of dopamine at and near physiological conditions, *Monatshefte fur Chemie, 146* (11) 1799-1805.
3 Schultz W. (**2007**) Behavioral dopamine signals, *Trends Neurosci., 30* (5) 203-210.
4 Madadi Mahani N. (**2019**) Dopamine detection by doped single-walled carbon nanotube biosensors: A theoretical study, *J. Res. Pharm., 23* (7) 785-791.
5 Wise R.A. (**2004**) Dopamine, learning and motivation, *Nat. Rev. Neurosci., 5* (6) 483-494.
6 Scuseria G.E., Janssen C.L., and Schaefer H.F. (**1988**) An efficient reformulation of single and double excited equations coupled to a closed-shell cluster (CCSD). *J. Chemi. Physi., 89* (4) 7382-7387.
7 Miehlich B., Savin A., Stoll H., and Preuss H. (**1989**) Results obtained with the correlation energy density functionals of Becke and Lee, Yang and Parr. *Chemi. Physi. Lett., 157* (3) 200-206.
8 Lipari N.O., and Duke C.B. (**1975**) The electronic structure of dialkylbenzenes. *J. Chemi. Physi. 63* (5) 1748-1757.
9 Purvis G.D., and Bartlett R.J. A (**198**2) complete coupled single and double cluster model: the inclusion of disconnected triples. *J. Chemi. Phys., 76* (4) 1910-1918.
10 Norman R.O.C., and Taylor R. (**1963**) Electrophilic substitution in benzenoid compounds. Else. *Publis. Comp., 3* (3) 3562-3570.
11 McLean A.D., and Chandler G.S. (**1980**) Sets of contracted Gaussian bases for molecular calculations. I. Second row atoms, Z = 11–18. *J. Chemi. Physi., 72* (10) 5639-5648.
12 Cakmak I. (**2005**) GIAO calculations of chemical shifts in enantiometrically pure 1-trifluoromethyl tetrahydroisoquinoline alkaloids. *Journal of Molecular Structure: Theochem, 716* (1-3) 143-148.
13 Tahmassebi D. (**2003**) Substituent effects on 13C chemical shifts of ketenimines: a GIAO/HF and DFT study. *Magne. Resona. Chemis., 41* (4) 273-277.
14 Jaroszewska-Manaj J., Maciejewska D., and Wawer I. (**2000**) 1H, 13C and 15N NMR and GIAO CPHF calculations on two quinoacridinium salts. Magne. *Resonan. Chemis., 38*(6), 482-485.
15 Othmer K. (**2005**) Infrared spettroscopy, *Encycl. Chemic. Techno., 14* (10) 1-20.
16 Lagutschenkov A., Langer J., BerdenOomens G., and Dopfer J. (**2011**) Infrared spectra of protonated neurotransmitters: Dopamine. *Physi. Chemis. Chemi. Physi., 13* (7) 2815-2823.
17 Yadav T., and Mukherjee V. (**2018**) Interpretation of IR and Raman spectra of dopamine neurotransmitter and effect of hydrogen bond in HCl. *J. Molecu. Struc., 1160* (3) 256-270.
18 Wishart D.S., Knox C., Guo A.C., Eisner R., Young N., Gautam B., Hau D.D., Psychogios N., and Dong E. (**2008**) HMDB: une base de connaissances pour le métabolome humain. *Nucle. Aci. Resea., 37* (2) 12-27.
19 Bouayad K., Rodi Y.K., Elmsellem H., Abdel-Rahman I., El Ghadraoui E.H., and Chakroune S. (**2018**) Density-functional theory and experimental evaluation of inhibition mechanism of Novel imidazo [4,5-b] pyridine derivatives, *J. Materi. Environ. Scie., 9* (2) 474-486.
20 Zoubir M., Zeroual A., Bkiri F., Benharref A., Mazoir N., and El Hajbi A. (**2017**) Experimental and theoretical analysis of the reactivity and regioselectivity in esterification reactions of diterpenes (totaradiol, totaratriol, hinikione and totarolone), *Mediterra. J. Chemis., 6* (5) 98-107.

21 El-Ghozlani M., El-Haib A., and El-Ajlaoui R. (**2018**) Theoretical investigation of the mechanism, stereoselectivity and regioselectivity of the epoxidation reaction of γ-himachalene : MEDT screening, Résultats de recherche Résultats Web, *J. Chemi. Techno. Appli., 2* (1) 4-9.
22 Luber S. (**2014)** Local electric dipole moments for periodic systems via density functional theory embedding, *J. Chemi. Physi., 141* (23) 234110-234121.
23 Mohammad-Shiri H., Ghaemi M., Riahi S., and Akbari-Sehat A. (**2011**) Computational and electrochemical studies on the redox reaction of dopamine in aqueous solution, *Inte. J. Electrochemi. Scie. 6* (3) 317-336.
24 Remya K., and Suresh C.H. (**2013**) Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small non-covalent dimers? A benchmark study using gaussian 09, *J. Compu. Chemis., 34* (15) 1341-1353.
25 Soltani A.R., and Baei M.T. (**2019**) A DFT study on structure and electronic properties of BN nanostructures adsorbed with dopamine, *Comput. 7* (4) 1-13.
26 Zhou L., Lv Y.L., Hu YX.., Zhao J.H., Xia X., and Li X. (**2018**) Experimental and theoretical investigations of 1,3,5-tris (4-aminophenoxy) benzene as an effective corrosion inhibitor for mild steel in 1 M HCl, *J. Molec. Liq., 249* (22) 79-187.
27 Becke A.D. (**1993**) A new mixing of Hartree-Fock and local density-functional theories, *J. Chemi. Physi., 98* (2) 1372–1377.
28 Lee C., Yang W., and Parr R.G. (**1988**) Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density, *Physi. Revi. B*, *37* (2) 785-789.
29 Womacott T.M., and Womacott R.J. (**1990**) *Introductory Statistics*, fifth ed., Wiley. New York.
30 El Idrissi M., Abdennouri M., Jorio S., and El Hajbi A. (**2017**) DFT Approach Chemical Shift Calculations to 13C for Bicyclical Epoxy-Himachlene Compound in the Presence of a Lewis Acid. *J. Comput. Metho. Molec. Desi., 7* (2) 1-8.