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NMR and NBO Investigation of Dopamine Properties in Point View of Brain activities

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ABSTRACT

Dopamine dosage is the main reason for panic, fear as well as exhilaration. In this study, it has been shown that the electron negativity of Cl, Br and F ions plays an important role in binding of these ions to dopamine receptors. The nervous quartiles effective drugs have been calculated via NMR and NBO approach. Moreover, the HOMO-LUMO energy gap of dopamine and its halogenated derivatives have been calculated at the B3LYP/6-31G* level. These calculations are so important in order to investigate many other diseases since it can exhibit the ability and relation between electron acceptor represents and electron donation in any brain activities. Finally, the accuracy of calculated result has confirmed by comparing the results to the experimental data.

Key words: Dopamine; NMR; NBO;Brain activity.

INTRODUCTION

Dopamine is a nervous transporter which has a key role in the central nervous system. This nervous transporter has an important role in the normal functions of brain such as learning, memorizing (storage ability in mind), controlling the noise level and adjusting character. Also do-pamine is the brain's Cortex and this Cortex is responsible for human behaviors[1-9].

Through the decades, dopamine has been always attracted by scientists due to important roles in many diseases such as schizophrenia, Parkinson's and depression (e.g. increase or decrease dopamine dosage in the body can cause disorder dopamine depression[10].However the structure and reactivity of this molecule has not been investigated thoroughly[11-13].

Understanding the structure, reactivity and stability of dopamine derivateis important for understanding the acting mechanism in the body sincethey determine the bonding ability to receptors. In this paper, the effect of electronegativity of atoms in the binding ability to receptors has been investigated in order to improve drug treatment of this common drug.For this purpose, the energy levels of dopamine molecules and electronegativity atoms such as chlorine, fluorine, bromine ions are calculated via NMR and NBO method[14-17].

Computational Methods

The structures of dopamine and halogenated derivatives were designed primarily using Chem. Bio Draw 12.0 (Scheme 1). The geometry of the systems has been optimized at the B3LYP /6-31G* computational level [18-20]. The optimization, NBO and NMR calculations of all systems are done by density functional theory (DFT) using B3LYP method and the standard 6-31G* basis set, by Gaussian09 suit of programs (Gaussian 09, Revision A.02) in the gas phase[21-24].

Mullikan charges on the atoms, dipole moments, and geometry parameters such as bond lengths were also determined by the same method. The energy barrier for rotation around the tow bond in the dopamine moleculeis also assessed and the results are represented in Table 1 and Fig.1 [25-27].

RESULTS AND DISCUSSION

Energies

The E_{HOMO}, E_{LUMO} and HOMO-LUMO energygap (Eg;Δ) of dopamine and halogenated derivatives were calculated using the B3LYP method and 6-31G* basis set and the results are presented in Table 4-9 and Table S3-S8 (Supplementary materials)[28].

The energy levels are so important since the energy level for LUMO as an electron acceptor represents the ability to obtain an electron and the energy level of HOMOrepresentsthe ability to donate an electron. As shown in Table 4-9, the$(Cl)_2$-Dop moleculeh as the lowest energy gap is -175.7456 Kcal/mol and the dopamine molecule has the largest energy gap is-130.9417 Kcal/mol[29-31].

Geometries

The structures of dopamine and halogenated derivatives were designed primarily using of Chem. Bio Draw 12.0 in scheme 1 and the obtained results were compared to other derivate at the end. The optimization, NBO and NMR calculations of the whole systems are done by density functional theory (DFT) using B3LYP method and the standard 6-31G basis set using Gaussian 09. The optimized geometrical parameters, such as Dipole moment (Debye), energy of structure formation (HF;kcal/mol) and enthalpies (ΔH), Gibbs free energy (ΔG) are listed in Table 4-9.As shown in Table 4-9, the (Br)2 - Dop moleculehasthe lowest ΔG is 72.059013Kcal/mol and the dopamine molecule has the largest ΔG is 91.416315 Kcal/mol. The molecule has the lowest ΔH is 102.29162Kcal/mol and the dopamine molecule has the largest ΔH is 122.32726 Kcal/mol.

Table 1: The calculated energy barrier of rotation around bonds C_1-O_{10} and C_2-O_{11}

Rout 1(C_6-C_1-O_{10}-H_{21})		Rout 2(C_3-C_2-O_{11}-H_{22})	
Angstroms and Degrees	**E(k(cal/mol)**	**Angstroms and Degrees**	**E(k(cal/mol)**
-15.2	-2.32175	-166.77	-8.09475
-0.202	-1.8825	13.22	-2.259
14.8	-2.32175	28.22	-1.69425
29.8	-1.69425	43.22	-0.94125
44.8	-0.94125	58.22	-0.251
59.8	-0.251	73.22	0
74.8	0	88.22	-0.31375
89.8	-0.43925	103.22	-1.19225
104.8	-1.44325	118.22	-1.8825
119.8	-3.07475	133.22	-4.518
134.8	-4.95725	148.22	-6.4005
149.8	-6.83975	163.22	-7.781
164.8	-8.22025	178.22	-8.4085

Table 2: Computed chemical shifts for selected atoms

Structure	Atom number	σ11	σ22	σ33	σiso	Δσ
(OH)2-DOP*	C1	-6.7203	35.6456	129.586	52.8371	115.1234
(F)2-DOP*		-17.4526	17.9589	78.9894	26.4985	78.7362
F(OH)-DOP*		-16.694	22.9613	76.7965	27.68793333	73.66285
(Cl)2-DOP*		-22.6423	57.3594	114.0318	49.58297	96.67325
Cl(OH)-DOP*		3.7164	62.4586	123.6434	63.2728	90.5559
(Br)2-DOP*		-25.6558	56.5618	110.3614	47.08913333	94.9084
Br(OH)-DOP*		11.7828	69.3353	126.8483	69.32213333	86.28925
(OH)2-DOP*	C2	-4.2227	35.8531	130.5894	54.07326667	114.7742
(F)2-DOP*		-12.7193	18.0642	79.269	28.2	76.59
F(OH)-DOP*		-8.3722	24.9618	21.9099	12.83316667	13.6151
(Cl)2-DOP*		-17.9397	59.6516	114.7442	52.15203	93.88825
Cl(OH)-DOP*		8.0263	26.0354	122.4972	52.1863	105.4664
(Br)2-DOP*		-20.9239	59.6319	111.1917	49.96656667	91.8377
Br(OH)-DOP*		29.0368	34.451	131.1433	64.87703	99.3994
(OH)2-DOP*	C8	19.9281	32.2393	170.3295	74.16563333	144.2458
(F)2-DOP*		129.9135	36.9611	64.7332	143.86	31.29
F(OH)-DOP*		130.0042	36.7783	64.3277	77.03673333	-19.06355
(Cl)2-DOP*		129.945	36.9932	164.9629	110.6337	81.4938
Cl(OH)-DOP*		9.7885	36.8712	164.4894	70.38303	141.1596
(Br)2-DOP*		129.7864	36.9806	165.0564	110.6078	81.6729
Br(OH)-DOP*		20.2364	31.8799	170.9779	74.36473333	144.91975

The isotropic chemical shielding σ_{iso} parameters are average of parameters, σ_{11}, σ_{22} and σ_{33} > 33 > 22 >11 *Dop=dopamine

Table 3: Computed chemical shifts for selected atoms

Structure	Atom number	σ11	σ22	σ33	σiso	Δσ
(OH)2-DOP*	N	95.9945	29.4999	242.7177	122.7373667	179.9705
(F)2-DOP*		191.716	25.3634	41.97	219.68	33.43
F(OH)-DOP*		190.9571	25.0724	41.8411	85.95686667	-66.17365
(Cl)2-DOP*		191.5971	25.4218	241.9345	152.9845	133.4251
Cl(OH)-DOP*		0.6262	25.0737	241.9851	89.22833333	229.13515
(Br)2-DOP*		191.5634	25.4276	241.9487	152.9799	133.4532
Br(OH)-DOP*		96.2871	29.4256	243.2144	122.9757	180.3581
(OH)2-DOP*	H19	24.7994	28.992	41.3526	31.71467	14.4569
(F)2-DOP*		23.7725	29.4723	40.0824	31.1	13.46
F(OH)-DOP*		23.8236	29.5709	40.1099	31.16813333	13.41265
(Cl)2-DOP*		23.7761	29.5058	40.1742	31.15203333	13.53325
Cl(OH)-DOP*		3.8093	29.5853	40.1726	24.5224	23.4753
(Br)2-DOP*		23.7379	29.4884	40.2316	31.15263	13.61845
Br(OH)-DOP*		24.719	28.9215	41.4097	31.6834	14.58945
(OH)2-DOP*	H20	25.6399	31.2533	39.7743	32.2225	11.3277
(F)2-DOP*		25.2384	31.3865	38.977	31.86	10.66
F(OH)-DOP*		25.2569	31.4527	38.9689	31.89283333	10.6141
(Cl)2-DOP*		25.2443	31.4942	38.9987	31.9124	10.62945
Cl(OH)-DOP*		5.2442	31.5347	38.9681	25.249	20.57865
(Br)2-DOP*		25.2012	31.5541	38.9776	31.91097	10.59995
Br(OH)-DOP*		25.4854	31.2492	39.7694	32.168	11.4021

The isotropic chemical shielding σ_{iso} parameters are average of parameters, σ_{11}, σ_{22} and σ_{33} > 33 > 22 >11 *Dop=dopamine

Table 4: Occupancy of natural orbitals (NBOs) and hybrids of dopamine calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO a	Occupancy	E	Length (Å)
(OH)2-DOP*	-0.714676	91.416315	122.32726	-130.9417	324198.48	1.3422	σ(C_1-O_{10})	1.99428	-0.89263	1.367773
							σ(C_2-O_{11})	1.99428	-0.89158	1.368191
							σ(C_8-N_9)	1.99352	-0.69245	1.466979
							σ(N_9-H_{19})	1.98953	-0.59715	1.018841
							σ(N_9-H_{20})	1.99081	-0.59666	1.019841
							σ(o_{10}-H_{21})	1.98816	-0.72203	0.969679
							σ(o_{11}-H_{22})	1.98812	-0.72117	0.969655
							CR(1) N9	1.99967	-14.15973	-
							CR(1) O10	1.99978	-18.97620	-
							CR(1) O11	1.99978	-18.97565	-
							LP(1) N9	1.96300	-0.29819	-
							LP(1) O10	1.98058	-0.58666	-
							LP(2) O10	1.87668	-0.30619	-
							LP(1) O11	1.98052	-0.58625	-

Table 5: Occupancy of natural orbitals (NBOs) and hybrids of fluorine derivativescalculated by the B3LYP method with 6-31G*(d) basis set

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO a	Occupancy	E	Length (Å)
(F)2-DOP*	-0.715220	74.983818	103.11933	-140.8939	-354340.1	4.5494	σ(C_1-F_{10})	1.99254	-0.81360	1.490790
							σ(C_2-F_{11})	1.99255	-0.81275	1.490832
							σ(C_8-N_9)	1.99367	-0.72093	1.451545
							σ(N_9-H_{19})	1.98887	-0.60580	1.028165
							σ(N_9-H_{20})	1.98974	-0.60641	1.028052
							CR(1) N9	1.99964	-14.17086	-
							CR(1) F10	1.99997	-24.46188	-
							CR(1) F11	1.99997	-24.46132	-
							LP(1) N9	1.96365	-0.30046	-
							LP(1) F10	1.99189	-1.08634	-
							LP(2) F10	1.97365	-0.38268	-
							LP(3) F10	1.94114	-0.37902	-
							LP(1) F11	1.99191	-1.08530	-
							LP(2) F11	1.97357	-0.38209	-
							LP(3) F11	1.94223	-0.37828	-
F(OH)-DOP*	-0.715003	83.055426	111.34841	-131.2805	-339269.8	4.0068	σ(C_1-F_{10})	1.99517	-0.99874	1.348276
							σ(C_2-O_{11})	1.99430	-0.90590	1.365509
							σ(C_8-N_9)	1.99346	-0.69512	1.466480
							σ(N_9-H_{19})	1.98944	-0.59912	1.018767
							σ(N_9-H_{20})	1.99077	-0.59858	1.019799
							σ(o_{11}-H_{21})	1.98806	-0.73264	0.969690
							CR(1) N9	1.99967	-14.16175	-
							CR(1) F10	1.99994	-24.43437	-
							CR(1) O11	1.99978	-18.98781	-
							LP(1) N9	1.96271	-0.30007	-
							LP(1) F10	1.98935	-1.01194	-
							LP(2) F10	1.96580	-0.39358	-
							LP(3) F10	1.92036	-0.39107	-
							LP(1) O11	1.98027	-0.59669	-
							LP(2) O11	1.87676	-0.31674	-

Table 6: Occupancy of natural orbitals (NBOs) and hybrids of chlorine derivatives calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO a	Occupancy	E	Length (Å)
(Cl)2-DOP*	-0.715383	73.1948	102.2916	-175.7456	-806600.9	3.8253	$\sigma(C_1\text{-}Cl_{11})$	1.98950	-0.71181	1.765766
							$\sigma(C_2\text{-}Cl_{10})$	1.98955	-0.71140	1.765634
							$\sigma(C_8\text{-}N_9)$	1.99372	-0.71906	1.451624
							$\sigma(N_9\text{-}H_{19})$	1.98893	-0.60413	1.028213
							$\sigma(N_9\text{-}H_{20})$	1.98975	-0.60476	1.028091
							CR(1) N9	1.99964	-14.16918	-
							CR(1) Cl10	2.00000	-100.11360	-
							CR(2) Cl10	1.99979	-10.60753	-
							CR(3) Cl10	1.99992	-7.22659	-
							CR(4) Cl10	1.99998	-7.22023	-
							CR(5) Cl10	1.99999	-7.21960	-
							CR(1) Cl11	2.00000	-100.11534	-
							CR(2) Cl11	1.99979	-10.60669	-
							CR(3) Cl11	1.99995	-7.22386	-
							CR(4) Cl11	1.99995	-7.22419	-
							CR(5) Cl11	1.99999	-7.22024	-
							LP(1) N9	1.96370	-0.29880	-
							LP(1) Cl10	1.99350	-0.91875	-
							LP(2) Cl10	1.97008	-0.32085	-
							LP(3) Cl10	1.92962	-0.31899	-
							LP(1) Cl11	1.99348	-0.91970	-
							LP(2) Cl11	1.97021	-0.32132	-
							LP(3) Cl11	1.92814	-0.31955	-

Table 7: Occupancy of natural orbitals (NBOs) and hybrids of chlorine derivatives calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO[a]	Occupancy	E	Length (Å)
Cl(OH)-DOP*	-0.715707	82.385877	111.34527	-131.726038528	-565401.1	3.8764	$\sigma(C_1\text{-}Cl_{11})$	1.98873	-0.70060	1.764012
							$\sigma(C_2\text{-}O_{10})$	1.99426	-0.85575	1.412481
							$\sigma(C_8\text{-}N_9)$	1.99377	-0.71415	1.451525
							$\sigma(N_9\text{-}H_{19})$	1.98909	-0.59970	1.028174
							$\sigma(N_9\text{-}H_{20})$	1.98975	-0.60025	1.028130
							$\sigma(o_{10}\text{-}H_{21})$	1.98795	-0.71680	0.991190
							CR(1) N9	1.99964	-14.16442	-
							CR(1) O10	1.99980	-18.99604	-
							CR(1) Cl11	2.00000	-100.08973	-
							CR(2) Cl11	1.99979	-10.61420	-
							CR(3) Cl11	1.99994	-7.21411	-
							CR(4) Cl11	1.99996	-7.21266	-
							CR(5) Cl11	1.99999	-7.20958	-
							LP(1) N9	1.96402	-0.29433	-
							LP(1) O10	1.98244	-0.60464	-
							LP(2) O10	1.88683	-0.31522	-
							LP(1) Cl11	1.99388	-0.90538	-
							LP(2) Cl11	1.96992	-0.31106	-
							LP(3) Cl11	1.93318	-0.30943	-

Table 8: Occupancy of natural orbitals (NBOs) and hybrids of bromine derivatives

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO[a]	Occupancy	E	Length (Å)
(Br)2-DOP^*	-0.715441	72.059013	105.04574	-133.8847	-3456570	3.4846	σ(C_1-Br_{11})	1.98553	-0.65158	1.903692
							σ(C_2-Br_{10})	1.98570	-0.65260	1.902276
							σ(C_8-N_9)	1.99323	-0.70342	1.465402
							σ(N_9-H_{19})	1.98916	-0.60584	1.018617
							σ(N_9-H_{20})	1.99077	-0.60554	1.019651
							CR(1) N9	1.99967	-14.16868	-
							CR(1) Br10	2.00000	-476.72898	-
							CR(2) Br10	1.99997	-67.79805	-
							CR(3) Br10	1.99976	-8.48457	-
							CR(4) Br10	1.99997	-56.39273	-
							CR(5) Br10	1.99986	-6.53335	-
							CR(6) Br10	1.99999	-56.38965	-
							CR(7) Br10	1.99998	-6.52463	-
							CR(8) Br10	2.00000	-56.38971	-
							CR(9) Br10	1.99999	-6.52480	-
							CR(10)Br10	1.99993	-2.65294	-
							CR(11) Br10	1.99993	-2.65307	-
							CR(12) Br10	1.99999	-2.64361	-
							CR(13) Br10	1.99980	-2.65284	-
							CR(14) Br10	1.99993	-2.64676	-
							CR(1) Br11	2	-476.729	-
							CR(2) Br11	1.99997	-67.8139	-
							CR(3) Br11	1.99976	-8.47004	-
							CR(4) Br11	1.99998	-56.3925	-
							CR(5) Br11	1.99994	-6.5265	-
							CR(6) Br11	1.99998	-56.3935	-
							CR(7) Br11	1.99991	-6.5296	-
							CR(8) Br11	2	-56.3914	-
							CR(9) Br11	1.99999	-6.52368	-
							CR(10)Br11	1.99978	-2.65331	-
							CR(11) Br11	1.99998	-2.64705	-
							CR(12) Br11	1.99996	-2.65024	-
							CR(13) Br11	1.99994	-2.65346	-
							CR(14) Br11	1.99992	-2.64699	-
							LP(1) N9	1.96207	-0.30636	-
							LP(1) Br10	1.99455	-0.95276	-
							LP(2) Br10	1.97317	-0.2932	-
							LP(3) Br10	1.93321	-0.29197	-
							LP(1) Br11	1.99457	-0.95335	-
							LP(2) Br11	1.97342	-0.29365	-
							LP(3) Br11	1.93271	-0.29245	-

Table 8: Occupancy of natural orbitals (NBOs) and hybrids of bromine derivatives

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO[a]	Occupancy	E	Length (Å)
Br(OH)-DOP*	-0.715719	81.8983	113.7618	-166.013	-1890386	3.7584	σ(C_1-Br_{11})	1.98444	-0.63499	1.906622
							σ(C_2-O_{10})	1.99462	-0.91537	1.362391
							σ(C_8-N_9)	1.9934	-0.69646	1.466399
							σ(N_9-H_{19})	1.9894	-0.60025	1.018787
							σ(N_9-H_{20})	1.99075	-0.59973	1.019811
							σ(o_{10}-H_{21})	1.98841	-0.73754	0.969946
							CR(1) N9	1.99967	-14.163	-
							CR(1) O10	1.99977	-18.9888	-
							CR(1) Br11	2	-476.741	-
							CR(2) Br11	1.99997	-67.5907	-
							CR(3) Br11	1.99976	-8.65225	-
							CR(4) Br11	1.99998	-56.383	-
							CR(5) Br11	1.99992	-6.5152	-
							CR(6) Br11	1.99998	-56.3825	-
							CR(7) Br11	1.99993	-6.51377	-
							CR(8) Br11	2	-56.3811	-
							CR(9) Br11	1.99999	-6.51003	-
							CR(10)Br11	1.99978	-2.64137	-
							CR(11) Br11	1.99996	-2.6375	-
							CR(12) Br11	1.99998	-2.63583	-
							CR(13) Br11	1.99994	-2.64154	-
							CR(14) Br11	1.99992	-2.63499	-
							LP(1) N9	1.96266	-0.30132	-
							LP(1) O10	1.9786	-0.59815	-
							LP(2) O10	1.86962	-0.3204	-
							LP(1)Br11	1.9953	-0.93367	-
							LP(2)Br11	1.97324	-0.28394	-
							LP(3)Br11	1.93939	-0.28138	-

Table 9: Occupancy of natural orbitals (NBOs) and hybrids of bromine derivatives

Symbol	charge of nitrogen	ΔG	ΔH	Energy of band gap (kcal/mol)	E (kcal/mol)	Dipole Moment(D	NBO[a]	Occupancy	E	Length (Å)
Br(OH)-DOP*	-0.715719	81.8983	113.7618	-166.013	-1890386	3.7584	σ(C_1-Br_{11})	1.98444	-0.63499	1.906622
							σ(C_2-O_{10})	1.99462	-0.91537	1.362391
							σ(C_8-N_9)	1.9934	-0.69646	1.466399
							σ(N_9-H_{19})	1.9894	-0.60025	1.018787
							σ(N_9-H_{20})	1.99075	-0.59973	1.019811
							σ(o_{10}-H_{21})	1.98841	-0.73754	0.969946
							CR(1) N9	1.99967	-14.163	-
							CR(1) O10	1.99977	-18.9888	-
							CR(1) Br11	2	-476.741	-
							CR(2) Br11	1.99997	-67.5907	-
							CR(3) Br11	1.99976	-8.65225	-
							CR(4) Br11	1.99998	-56.383	-
							CR(5) Br11	1.99992	-6.5152	-
							CR(6) Br11	1.99998	-56.3825	-
							CR(7) Br11	1.99993	-6.51377	-
							CR(8) Br11	2	-56.3811	-
							CR(9) Br11	1.99999	-6.51003	-
							CR(10)Br11	1.99978	-2.64137	-
							CR(11) Br11	1.99996	-2.6375	-
							CR(12) Br11	1.99998	-2.63583	-
							CR(13) Br11	1.99994	-2.64154	-
							CR(14) Br11	1.99992	-2.63499	-
							LP(1) N9	1.96266	-0.30132	-
							LP(1) O10	1.9786	-0.59815	-
							LP(2) O10	1.86962	-0.3204	-
							LP(1)Br11	1.9953	-0.93367	-
							LP(2)Br11	1.97324	-0.28394	-
							LP(3)Br11	1.93939	-0.28138	-

Table S1: Computed chemical shifts for selected atoms

Structure	Atom number	η	κ	Charge
(OH)2-DOP*	C1	0.552007	0.378372093	0.327738
(F)2-DOP*		0.674621696	0.48806174	0.581972
F(OH)-DOP*		0.807502696	0.151672095	0.310302
(Cl)2-DOP*		1.241321	-0.17069	-0.07644
Cl(OH)-DOP*		-1.6284	0.02036739	-0.111033
(Br)2-DOP*		1.299425551	-0.208929459	0.048784
Br(OH)-DOP*		1.000457763	-0.000343283	0.047116
(OH)2-DOP*	C2	0.52375621	0.405457	0.315797
(F)2-DOP*		0.60278251	0.595417964	0.003529
F(OH)-DOP*		3.6724666	-1.201564621	0.305575
(Cl)2-DOP*		1.239633	-0.16957	-0.07595
Cl(OH)-DOP*		-52.3018	0.685351	0.362558
(Br)2-DOP*		1.315730904	-0.21947446	0.048189
Br(OH)-DOP*		0.081704	0.89395	0.328631
(OH)2-DOP*	C8	0.128023138	0.836289	-0.128391
(F)2-DOP*		-13.8256	-4.052946663	-0.340644
F(OH)-DOP*		7.335404476	-1.838942392	-0.133027
(Cl)2-DOP*		-1.710899479	6.308816348	-0.134595
Cl(OH)-DOP*		-67.0237	0.64987	-0.13307
(Br)2-DOP*		-1.70447	6.262591	-0.13434
Br(OH)-DOP*		0.1205167	0.845516994	-0.129605

Table S2: Computed chemical shifts for selected atoms

Structure	Atom number	η	κ	Charge
(OH)2-DOP*	N	-0.554212496	1.906395171	-0.714647
(F)2-DOP*		0.936090259	-3.280343256	-0.407913
F(OH)-DOP*		3.760213469	-1.224908125	-0.715729
(Cl)2-DOP*		-1.86819	7.602459	-0.7154
Cl(OH)-DOP*		-128.3092667	0.79741787	-0.715707
(Br)2-DOP*		-1.86735	7.594614	-0.71544
Br(OH)-DOP*		-0.55607	1.91013	-0.71502
(OH)2-DOP*	H19	0.43501	0.493439335	0.296342
(F)2-DOP*		0.634552	0.543629765	0.310717
F(OH)-DOP*		0.642747705	0.294216612	0.298807
(Cl)2-DOP*		0.635069181	0.301175136	0.300622
Cl(OH)-DOP*		10.1258	-0.417693114	0.298418
(Br)2-DOP*		0.633387	0.302703	0.300477
Br(OH)-DOP*		0.432076	0.496426	0.297998
(OH)2-DOP*	H20	0.743319474	0.20571089	0.290714
(F)2-DOP*		0.863861	0.199592525	0.2761
F(OH)-DOP*		0.875599438	0.096295216	0.293655
(Cl)2-DOP*		0.881969434	0.091214448	0.294312
Cl(OH)-DOP*		12.5714	-0.55916	0.293424
(Br)2-DOP*		0.899	0.077713	0.294229
Br(OH)-DOP*		0.758255	0.192971	0.293085

Table S3: Occupancy of natural orbitals (NBOs) and hybrids of dopamine calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	NBO a	Occupancy	Hybrid
(OH)2-DOP*	$\sigma(C_1\text{-}O_{10})$	1.99428	$0.5771(sp^{3})_{C1}+0.8166(sp^{1.93})_{O10}$
	$\sigma(C_2\text{-}O_{11})$	1.99428	$0.5774(sp^{2.98})_{C2}+0.8165(sp^{1.94})_{O11}$
	$\sigma(C_8\text{-}N_9)$	1.99352	$0.6368(sp^{3.17})_{C8}+0.7710(\ sp^{2.19})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98953	$0.8299(sp^{3.23})_{N9}+0.5579(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.99081	$0.8282(sp^{3.28})_{N9}+0.5605(s)_{H20}$
	$\sigma(o_{10}\text{-}H_{21})$	1.98816	$0.8625(sp^{3.92})_{O10}+0.5060(s)_{H21}$
	$\sigma(o_{11}\text{-}H_{22})$	1.98812	$0.8626(sp^{3.92})_{O11}+0.5059(s)_{H22}$
	CR(1) N9	1.99967	s
	CR(1) O10	1.99978	s
	CR(1) O11	1.99978	s
	LP(1) N9	1.96300	$sp^{3.62}$
	LP(1) O10	1.98058	$sp^{1.19}$
	LP(2) O10	1.87668	p
	LP(1) O11	1.98052	$sp^{1.19}$

Table S4: Occupancy of natural orbitals (NBOs) and hybrids of fluorine derivativescalculated by the B3LYP method with 6-31G*(d) basis set

Symbol	NBO a	Occupancy	Hybrid
(F)2-DOP*	$\sigma(C_1\text{-}F_{10})$	1.99254	$0.5385(sp^{3.64})_{C1}+0.8426(sp^{3.98})_{F10}$
	$\sigma(C_2\text{-}F_{11})$	1.99255	$0.5388(sp^{3.62})_{C2}+0.8424(sp^{3.98})_{F11}$
	$\sigma(C_8\text{-}N_9)$	1.99367	$0.6402(sp^{3.12})_{C8}+0.7682(sp^{2.08})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98887	$0.8317(sp^{3.14})_{N9}+0.5553*\ (s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.98974	$0.8298(sp^{3.17})_{N9}+0.5581(s)_{H20}$
	CR(1) N9	1.99964	p
	CR(1) F10	1.99997	s
	CR(1) F11	1.99997	s
	LP(1) N9	1.96365	$sp^{4.15}$
	LP(1) F10	1.99189	$sp^{0.26}$
	LP(2) F10	1.97365	p
	LP(3) F10	1.94114	p
	LP(1) F11	1.99191	$sp^{0.26}$
	LP(2) F11	1.97357	p
	LP(3) F11	1.94223	p
F(OH)-DOP*	$\sigma(C_1\text{-}F_{10})$	1.99517	$0.5260(sp^{3.45}d^{0.01})_{C1}+0.8505(sp^{2.30})_{F10}$
	$\sigma(C_2\text{-}O_{11})$	1.99430	$0.5786(sp^{2.93}d^{0.01})_{C2}+0.8156(sp^{1.94})_{O11}$
	$\sigma(C_8\text{-}N_9)$	1.99346	$0.6373(sp^{3.16}d^{0.01})_{C8}+0.7706(sp^{2.19})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98944	$0.8301(sp^{3.23})_{N9}+0.5576(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.99077	$0.8285(sp^{3.27})_{N9}+0.5600(s)_{H20}$
	$\sigma(o_{11}\text{-}H_{21})$	1.98806	$0.8635(sp^{3.89}d^{0.01})O11+0.5043(s)_{H21}$
	CR(1) N9	1.99967	s
	CR(1) F10	1.99994	s
	CR(1) O11	1.99978	s
	LP(1) N9	1.96271	$sp^{3.63}$
	LP(1) F10	1.98935	$sp^{0.44}$
	LP(2) F10	1.96580	$sp^{99.99}d^{0.31}$
	LP(3) F10	1.92036	p
	LP(1) O11	1.98027	$sp^{1.19}$
	LP(2) O11	1.87676	p

Table S5: Occupancy of natural orbitals (NBOs) and hybrids of chlorine derivatives calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	NBO[a]	Occupancy	Hybrid
(Cl)2-DOP*	$\sigma(C_1\text{-}Cl_{11})$	1.98950	$0.6793(sp^{3.31})_{C1}+0.7338(sp^{4.77}d^{0.03})_{Cl11}$
	$\sigma(C_2\text{-}Cl_{10})$	1.98955	$0.6794(sp^{3.28}d^{0.01})_{C2}+0.7338(sp^{4.77}d^{0.03})_{Cl10}$
	$\sigma(C_8\text{-}N_9)$	1.99372	$0.6400(sp_{3.12}d^{0.01})_{C8}+0.7684(sp^{2.08})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98893	$0.8315(sp_{3.14})_{N9}+0.5555(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.98975	$0.8297(sp_{3.17})_{N9}+0.5582(s)_{H20}$
	CR(1) N9	1.99964	s
	CR(1) Cl10	2.00000	s
	CR(2) Cl10	1.99979	s
	CR(3) Cl10	1.99992	p
	CR(4) Cl10	1.99998	p
	CR(5) Cl10	1.99999	p
	CR(1) Cl11	2.00000	s
	CR(2) Cl11	1.99979	s
	CR(3) Cl11	1.99995	p
	CR(4) Cl11	1.99995	p
	CR(5) Cl11	1.99999	p
	LP(1) N9	1.96370	$sp^{4.15}$
	LP(1) Cl10	1.99350	$sp^{0.21}$
	LP(2) Cl10	1.97008	$sp^{99.99}d^{0.11}$
	LP(3) Cl10	1.92962	p
	LP(1) Cl11	1.99348	$sp^{0.21}$
	LP(2) Cl11	1.97021	$sp^{99.99}d^{0.11}$
	LP(3) Cl11	1.92814	p

Table S6: Occupancy of natural orbitals (NBOs) and hybrids of chlorine derivatives calculated by the B3LYP method with 6-31G*(d) basis set

Symbol	NBO[a]	Occupancy	Hybrid
Cl(OH)-DOP*	$\sigma(C_1\text{-}Cl_{11})$	1.98873	$0.6777(sp^{3.29}d^{0.01})_{C1}+0.7353(sp^{4.71}d^{0.03})_{Cl11}$
	$\sigma(C_2\text{-}O_10)$	1.99426	$0.5792(sp^{3.11}d^{0.01})_{C2}+0.8152(sp^{2.18})_{O10}$
	$\sigma(C_8\text{-}N_9)$	1.99377	$0.6394(sp^{3.13}d^{0.01})_{C8}+0.7689(sp^{2.07})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98909	$0.8311(sp^{3.15})_{N9}+0.5561(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.98975	$0.8296(sp^{3.17})_{N9}+0.5584(s)_{H20}$
	$\sigma(o_{10}\text{-}H_{21})$	1.98795	$0.8645(sp^{3.93}d^{0.01})_{O10}+0.5026(s)_{H21}$
	CR(1) N9	1.99964	s
	CR(1) O10	1.99980	s
	CR(1) Cl11	2.00000	s
	CR(2) Cl11	1.99979	s
	CR(3) Cl11	1.99994	p
	CR(4) Cl11	1.99996	p
	CR(5) Cl11	1.99999	p
	LP(1) N9	1.96402	$sp^{4.15}$
	LP(1) O10	1.98244	$sp^{1.10}$
	LP(2) O10	1.88683	$sp^{99.99}d^{0.18}$
	LP(1) Cl11	1.99388	$sp^{0.21}$
	LP(2) Cl11	1.96992	$sp^{99.99}d^{0.07}$
	LP(3) Cl11	1.93318	p

NMR

Nuclear magnetic resonance (NMR) is very powerful tool in studying microscopic phenomena in physics, chemistry, biology and medicine. Determination of spectral parameters using the quantum-chemistry methods helps in the assignment and interpretation of the experimental data[32]. In this study, NMR has been used for

Table S7: Occupancy of natural orbitals (NBOs) and hybrids of bromine derivatives

Symbol	NBO[a]	Occupancy	Hybrid
(Br)2-DOP^*	$\sigma(C_1\text{-}Br_{11})$	1.98553	$0.7066(sp^{3.52})_{C1}+0.7076(sp^{6.23}d^{0.02})_{Br11}$
	$\sigma(C_2\text{-}Br_{10})$	1.98570	$0.7071(sp^{3.48})_{C2}+0.7071(sp^{6.21}d^{0.02})_{Br10}$
	$\sigma(C_8\text{-}N_9)$	1.99323	$0.6383(sp^{3.14})_{C8}+0.7698(sp^{2.19})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.98916	$0.8307(sp^{3.21})_{N9}+0.5567(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.99077	$0.8289(sp^{3.26})_{N9}+0.5594(s)_{H20}$
	CR(1) N9	1.99967	s
	CR(1) Br10	2.00000	s
	CR(2) Br10	1.99997	s
	CR(3) Br10	1.99976	s
	CR(4) Br10	1.99997	p
	CR(5) Br10	1.99986	p
	CR(6) Br10	1.99999	p
	CR(7) Br10	1.99998	p
	CR(8) Br10	2.00000	p
	CR(9) Br10	1.99999	p
	CR(10)Br10	1.99993	d
	CR(11) Br10	1.99993	d
	CR(12) Br10	1.99999	d
	CR(13) Br10	1.99980	d
	CR(14) Br10	1.99993	d
	CR(1) Br11	2	s
	CR(2) Br11	1.99997	s
	CR(3) Br11	1.99976	s
	CR(4) Br11	1.99998	P
	CR(5) Br11	1.99994	P
	CR(6) Br11	1.99998	P
	CR(7) Br11	1.99991	P
	CR(8) Br11	2	P
	CR(9) Br11	1.99999	P
	CR(10)Br11	1.99978	d
	CR(11) Br11	1.99998	d
	CR(12) Br11	1.99996	d
	CR(13) Br11	1.99994	d
	CR(14) Br11	1.99992	d
	LP(1) N9	1.96207	$sp^{3.65}$
	LP(1) Br10	1.99455	$sp^{0.16}$
	LP(2) Br10	1.97317	$sp^{99.99}d^{0.13}$
	LP(3) Br10	1.93321	p
	LP(1) Br11	1.99457	$sp^{0.16}$
	LP(2) Br11	1.97342	$sp^{99.99}d^{0.13}$
	LP(3) Br11	1.93271	p

determination of microscopic properties of dopamine and it halogenated derivate[33-35].

To discuss the magnitude of the shielding tensor, it is necessary to report the three principal eigenvalues of the chemical shielding anisotropy tensor (σ_{11}, σ_{22}, σ_{33})using following equations:

a) the isotropic value of the shielding tensor which is defined as:

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

a) the anisotropy ($\Delta\sigma$) of the tensor, given by:

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

b) the shielding tensor asymmetry parameter (η) given by:

$$\eta = \frac{|\sigma_{22} - \sigma_{11}|}{|\sigma_{33} - \sigma_{iso}|}$$

The optimization and NMR calculation are done by density functional theory (DFT) using B3LYP method and the standard 6-31G* basis set in the gas phase. Table 2 and 3 presents the computed chemical shift for selected hydrogen, nitrogen and carbon atoms. According to this Table, anisotropic shielding value ($\Delta\sigma$) for C_8 and N atom of F(OH)-Dopmolecule and N are negative values. Interestingly, among all of mentioned carbon atoms, C_2 of F(OH)-Dophas the lowest isotropic shielding value. The º, η and charges valuesare summarized in Table S1 and S2 [36-38].

NBO analysis

NBO method gives useful information about interactions in both filled and virtual orbital spaces which could enhance the analysis of intra

Table S8: Occupancy of natural orbitals (NBOs) and hybrids of bromine derivatives

Symbol	NBO[a]	Occupancy	Hybrid
Br(OH)-DOP*	$\sigma(C_1\text{-}Br_{11})$	1.98444	$0.7029(sp^{3.53})_{C1}+0.7113(sp^{6.18}d^{0.02})_{Br11}$
	$\sigma(C_2\text{-}O_{10})$	1.99462	$0.5776(sp^{2.98}d^{0.01})_{C2}+0.8163(sp^{1.90})_{O10}$
	$\sigma(C_8\text{-}N_9)$	1.9934	$0.6375(sp^{3.16}d^{0.01})_{C8}+0.7705(sp^{2.19})_{N9}$
	$\sigma(N_9\text{-}H_{19})$	1.9894	$0.8302(sp^{3.22})_{N9}+0.5574(s)_{H19}$
	$\sigma(N_9\text{-}H_{20})$	1.99075	$0.8286(sp^{3.27})_{N9}+0.5598(s)_{H20}$
	$\sigma(o_{10}\text{-}H_{21})$	1.98841	$0.8642(sp^{3.87}d^{0.01})_{O10}+0.5031(s)_{H21}$
	CR(1) N9	1.99967	s
	CR(1) O10	1.99977	s
	CR(1) Br11	2	s
	CR(2) Br11	1.99997	s
	CR(3) Br11	1.99976	s
	CR(4) Br11	1.99998	p
	CR(5) Br11	1.99992	p
	CR(6) Br11	1.99998	p
	CR(7) Br11	1.99993	p
	CR(8) Br11	2	p
	CR(9) Br11	1.99999	p
	CR(10)Br11	1.99978	d
	CR(11) Br11	1.99996	d
	CR(12) Br11	1.99998	d
	CR(13) Br11	1.99994	d
	CR(14) Br11	1.99992	d
	LP(1) N9	1.96266	$sp^{3.63}$
	LP(1) O10	1.9786	$sp^{1.22}$
	LP(2) O10	1.86962	p
	LP(1)Br11	1.9953	$spp^{0.16}$
	LP(2)Br11	1.97324	$sp^{99.99}d^{0.02}$
	LP(3)Br11	1.93939	p

and intermolecular interactions. This is carried out by considering all possible interactions between filled donor and empty acceptor NBOs and estimating their energy importance by second order perturbation theory[39].

NBO analysis is based on a method for optimally transforming a given wave function into localized form, corresponding to the one-center ("lone pairs") and two-center ("bonds") elements of the chemist's Lewis structure picture. In NBO analysis, the input atomic orbital basis set is transformed via natural atomic orbitals (NAOs) and natural hybrid orbitals (NHOs) into natural bond orbitals (NBOs)[40-43].

Table 4-9 lists the calculated occupancies of natural orbitals. The calculated Natural bond hybrids and are also given in this table[44-46].

Table S3-S8 show share of orbitals contribute in the bonds (BD for 2-center bond).

According to calculations, the nitrogen atom forms three single bond (sigma bond) with two hydrogen atoms H_{19} and H_{20} (σ_{N_9}-H_{19} and σ_{N_9}-H_{20}), and a carbon atom C_8 (σ_{C_9}-N_9) and a lon pair orbital (Lp). As seen from Table S3-S8, the LP on the nitrogen atom is formed from an $sp^{3.62}$ hybrid for the$(OH)_2$-DOP molecule, $sp^{4.15}$hybrid for the F_2-DOP molecule, $sp^{3.63}$ For the F(OH)-DOPmolecule, $sp^{4.15}$ hybrid for the Cl_2-DOP molecule, $sp^{4.15}$ hybrid For

Scheme 1: Optimized structure of dopamine and halogenated derivatives

Fig. 1: The scan of potential energy verses degrees changing of Dopamine

the Cl(OH)-DOP molecule, $sp^{3.65}$ hybrid for the Br_2-DOP molecule, and$sp^{3.63}$ hybrid For the Br (OH)-DOP molecule[47].

CONCLUSION

In the present work, atheoretical analysis of dopamine and its halogenated derivate has been performed in order to obtain the dipole moment (μ) and energy of structure formation (HF)of dopamine and it halogenated derivate. Also the thermodynamic parameters of this compound has been studied and according to the results, it has been found that the amount of Gibbs free energy(ΔG) and standard enthalpies (ΔH) of dopamine and its halogenated derivatearepositive value, therefore dopamine and its halogenated derivateareunstable structure. Moreover, the chemical shifts of these molecules have been simulated using quantum mechanics.Finally, the Natural Bond Orbital (NBO) analysis has provided the detailed insight into the type of hybridization and the nature of bonding in dopamine and its halogenated derivate.

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