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A quantum chemical comparative study of Epinine and Hordenine

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Abstract
Epinine, is an organic compound and natural product that is structurally related to the important neurotransmitters dopamine and epinephrine while Hordenine, is an alkaloid of the phenethylamine class that occurs naturally in a variety of plants. These have nearly similar type of structures so we have done a comparative study of epinine and hordenine with B3LYP with 6-311 G (d, p) as the basis set. Here we have done a relative study of their structures, vibrational assignments, thermal and electronic properties of epinine and hordenine. We have plotted frontier orbital HOMO- LUMO surfaces, Molecular electrostatic potential surfaces to explain the reactive nature of epinine and hordenine.

Keywords: Epinine and Hordenine, vibrational analysis, DFT, HOMO-LUMO, MESP.

1. Introduction
Deoxyepinephrine, also known by the common names N-methyldopamine and epinine, is an organic compound and natural product that is structurally related to the important neurotransmitters dopamine and epinephrine. All three of these compounds also belong to the catecholamine family. The pharmacology of epinine largely resembles that of its "parent", dopamine. Epinine has been found in plants, insects and animals. It is also of significance as the active metabolic breakdown product of the prodrug ibopamine, which has been used to treat congestive heart failure [1, 2]. One of the most prominent pharmacological characteristics of epinine, its ability to raise blood pressure [3]. Tainter quantified the pressor activity of epinine in the atropine-treated and anesthetized intact cats [4].
Hordenine, or N, N-dimethyltyramine, is an alkaloid of the phenethylamine class that occurs naturally in a variety of plants, taking its name from one of the commonest, barley (Hordeum species). Chemically, hordenine is the N-methyl derivative of N-methyltyramine, and the N, N-dimethyl derivative of the well-known biogenic amine tyramine, from which it is biosynthetically derived. Currently, hordenine is widely sold as an ingredient of nutritional supplements, with the claims that it is a stimulant of the central nervous system, and has the ability to promote weight loss by enhancing metabolism. In experimental animals, given sufficiently large doses parenterally (i.e. by injection), hordenine does produce an increase in blood pressure, as well as other disturbances of the cardiovascular, respiratory and nervous systems. These effects are generally not reproduced by oral administration of the drug in test animals, and there are virtually no scientific reports of the effects of hordenine in human beings. The first report of the isolation from a natural source of the compound which is now known as hordenine was made by Arthur Heffter in 1894, who extracted this alkaloid from the cactus Anhalonium fissuratum (now reclassified as Ariocarpus fissuratum), naming it "anhalin" [5]. Hordenine has been found to act as a feeding deterrent to grasshoppers (*Melanoplus bivittatus*), [6] and to caterpillars of *Heliothis virescens* and *Heliothis subflexa* [7].
As a part of our ongoing research work [8-14], we report the comparative study of epinine and hordenine by DFT study. To the best of our knowledge, no comparative quantum chemical calculations of these molecules have been reported so far in the literature.

2. Material and methods
All the calculations were performed by the B3LYP [15, 16] method using the 6-311 G (d, p) basis set of Density functional theory [17]. All computations were carried out with the GAUSSIAN 09 package [18]. By combining the results of the GAUSSVIEW'S program [19] with symmetry considerations, vibrational frequency assignments were made with a high degree of accuracy. Vibrational frequencies of these molecules were calculated by these methods and then scaled [20] by 0.9613.

3. Results and Discussion

3.1 Geometry Optimization

Optimized parameters of epinine and hordenine calculated by B3LYP method with 6-311 G (d, p) basis set is listed in Table 1 in accordance with the atom numbering scheme as shown in Figures 1. Local minimum energies are -0.04300894 a.u. and -0.05260001 a.u. for epinine and hordenine respectively. For epinine and hordenine, C–C bond distances are found to be in the range from 1.3677-1.4879 A^0, and 1.3876-1.4936 A^0 while for C-N, these values are 1.4855 A^0 and 1.4927 A^0 respectively. In case of C-H bond distances, they lie in the range from 1.0935-1.1088 A^0 and 1.0958-1.1145 respectively, while for C-O, these values are 0.9485 A^0 and 0.949 A^0 respectively.

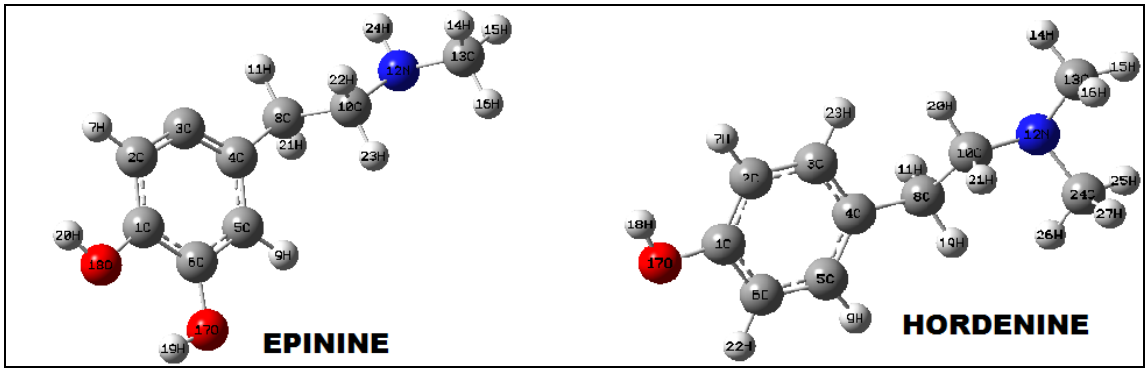

Fig 1: Model molecular structures of EPININE and HORDENINE

Table 1: Optimized geometrical parameters of Epinine and Hordenine by (B3LYP)/ 6-311 G (d, p) Method

Epinine		Hordenine	
Parameters	**6-311 G (d, p)**	**Parameters**	**6-311 G (d, p)**
Bond Length			
R(1,2)	1.4102	R(1,2)	1.4014
R(1,6)	1.4263	R(1,6)	1.4013
R(1,18)	1.3696	R(1,17)	1.3688
R(2,3)	1.3677	R(2,3)	1.3876
R(2,7)	1.0935	R(2,7)	1.0958
R(3,4)	1.3762	R(3,4)	1.3961
R(4,5)	1.4051	(3,23)	1.1001
R(4,8)	1.4879	R(4,5)	1.3963
R(5,6)	1.411	R(4,8)	1.4936
R(5,9)	1.0967	R(5,6)	1.3882
R(6,17)	1.3667	R(5,9)	1.0962
R(8,10)	1.5271	(6,22)	1.0957
R(8,11)	1.1084	R(8,10)	1.5274
R(8,21)	1.1088	R(8,11)	1.1092
R(10,12)	1.4855	R(8,19)	1.1145
R(10,22)	1.1118	R(10,12)	1.4927
R(10,23)	1.109	R(10,20)	1.1133
R(12,13)	1.4726	R(10,21)	1.1115
R (12.24)	0.9988	R (12,13)	1.4786
R (13,14)	1.1013	R (12,24)	1.4808
R (13,15)	1.0973	R (13,14)	1.0976
R (13,16)	1.0981	R (13,15)	1.0975
R (17,19)	0.9482	R (13,16)	1.1011
R (18,20)	0.9485	R (17,18)	0.949
-	-	R (24,25)	1.0967
-	-	R (24,26)	1.1025
-	-	R (24,27)	1.1007
Bond Angles			
A(2,1,6)	119.6748	A(2,1,6)	120.8153
A(2,1,18)	123.1098	A(2,1,17)	123.0221
A(6,1,18)	117.2153	A(6,1,17)	116.1625
A(1,2,3)	114.5009	A(1,2,3)	119.0333
A(1,2,7)	123.7535	A(1,2,7)	121.015
A(3,2,7)	121.7457	A(3,2,7)	119.9517
A(2,3,4)	130.025	A(2,3,4)	120.7939
A(3,4,5)	114.86	A(2,3,23)	120.66
A(3,4,8)	122.534	A(4,3,23)	118.5421
A(5,4,8)	122.6057	A(3,4,5)	119.5633
A(4,5,6)	119.7293	A(3,4,8)	120.043
A(4,5,9)	120.0603	A(5,4,8)	120.3779

A(6,5,9)	120.2104	A(4,5,6)	120.6405
A(1,6,5)	121.2098	A(4,5,9)	119.849
A(1,6,17)	123.8644	A(6,5,9)	119.5104
A(5,6,17)	114.9258	A(1,6,5)	119.1529
A(4,8,10)	110.3433	A(1,6,22)	120.3556
A(4,8,11)	109.6461	A(5,6,22)	120.4915
A(4,8,21)	109.2092	A(4,8,10)	111.5447
A(10,8,11)	110.8133	A(4,8,11)	108.4621
A(10,8,21)	110.6804	A(4,8,19)	111.2525
A(11,8,21)	106.049	A(10,8,11)	110.5139
A(8,10,12)	110.5468	A(10,8,19)	109.4221
A(8,10,22)	110.1597	A(11,8,19)	105.4736
A(8,10,23)	110.1617	A(8,10,12)	110.6337
A(12,10,22)	112.209	A(8,10,20)	109.1639
A(12,10,23)	107.453	A(8,10,21)	110.2812
A(22,10,23)	106.1784	A(12,10,20)	109.0117
A(10,12,13)	112.9354	A(12,10,21)	111.4528
A(10,12,24)	109.5252	A(20,10,21)	106.1684
A(13,12,24)	109.8403	A(10,12,13)	112.2805
A(12,13,14)	114.1411	A(10,12,24)	112.1627
A(12,13,15)	108.9036	A(13,12,24)	112.3173
A(12,13,16)	109.3421	A(12,13,14)	109.3667
A(14,13,15)	108.2899	A(12,13,15)	109.0365
A(14,13,16)	107.8832	A(12,13,16)	113.5272
A(15,13,16)	108.118	A(14,13,15)	108.179
A(6,17,19)	108.7623	A(14,13,16)	108.3357
A(1,18,20)	107.3608	A(15,13,16)	108.2612
-	-	A(1,17,18)	107.8101
-	-	A(12,24,25)	109.0038
-	-	A(12,24,26)	108.6977
-	-	A(12,24,27)	113.5353
-	-	A(25,24,26)	108.7433
-	-	A(25,24,27)	108.499
-	-	A(26,24,27)	108.2661

3.2 Assignment of Fundamentals

Epinine has the 24 atoms with 66 normal modes of vibration while hordenine has the 27 atoms with 75 normal modes of vibration. The model molecular structure of these compounds is given in figure-1. The theoretical spectrum of epinine and hordenine are drawn in a figure-2. Assignments are done using the animated views of normal mode description. Calculated vibrational frequencies for epinine and hordenine are given in Tables 2 & 3 which are useful for the experimentalists in absence of its experimental data.

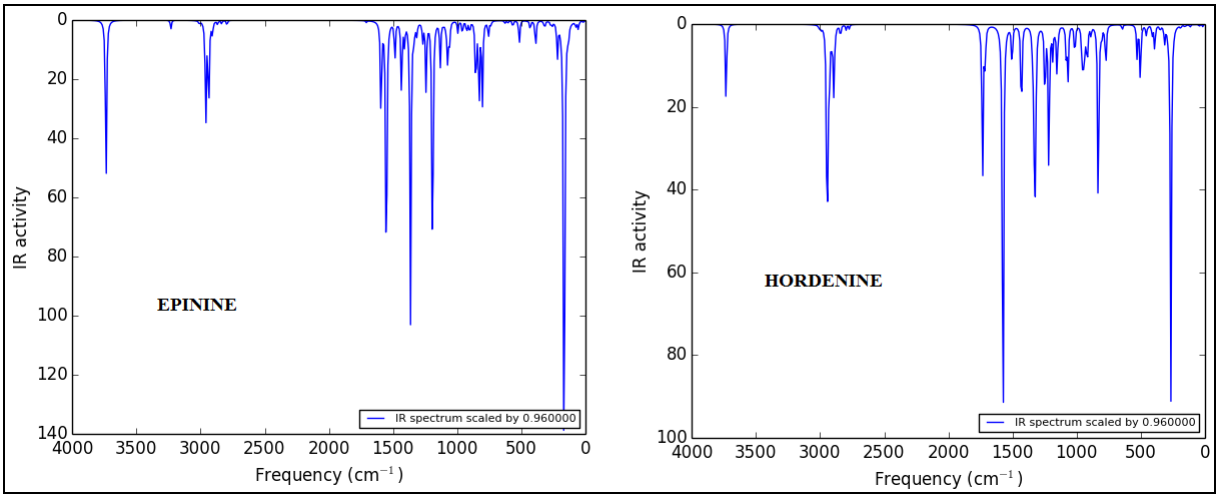

Fig 2: Calculated Spectrum of EPININE and HORDENINE

3.3 Vibrational Modes Description

The O–H stretching vibrations are normally viewed in the region 3400-3700 cm^{-1}. For epinine, a strong O-H stretching vibration, presented at 3739 cm^{-1} in calculated spectrum while 3733 cm^{-1} for hordenine. The N–H stretching vibrations are normally viewed in the region 3200-3600 cm^{-1}. For epinine, the N-H stretching vibration, presented at 3232 cm^{-1} in calculated spectrum. Some strong in plane and out of plane bending vibrations, are also seen in the assignment of epinine and hordenine. We have seen in literature that the C–H stretching vibrations are usually observed in 2800– 3200 cm^{-1} region. In the study of epinine, the (C–H) functional group, presented at 2937 and 2960 cm^{-1} in calculated spectra while 2940 and 2949 cm^{-1} for hordenine respectively in calculated data. For epininem, a strong scissoring vibration {S (H-C-H)}, presented at 1333

cm^{-1} but in case of hordenine, the {S (H-C-H)} vibration is at 1320 cm^{-1} in theoretical vibrational spectra. Some in and out of plane bending and rocking vibrations due to C-H are also presented in the assignment of epinine and hordenine.

In epinine, in the middle region, a twisting modes (CH_2 and CH_3) are calculated at 1075 and 1087 cm^{-1} while for hordenine, these modes are at 1144 and 1168 having appropriate IR intensity. As expected, torsion modes along with wagging modes appear in the lower frequency range. For epinine, strong torsion mode of C-C-C-C is at 515 cm^{-1} in calculated spectrum while strong torsion modes are at 528 cm^{-1} in calculated spectrum for hordenine respectively.

There are some frequencies in lower region having appreciable IR intensity. Furthermore, the study of low frequency vibrations are of great significance, because it gives information on weak intermolecular interactions, which take place in enzyme reactions [21]. Knowledge of low frequency mode is also essential for the interpretation of the effect of electromagnetic radiation on biological systems [22]. The aim of vibrational analysis is to acquire direct information on lower and higher frequency vibrations of such epinine and hordenine. No experimental FTIR spectrum is available for comparison of epinine and hordenine so it will provide a suitable path for experimental researchers.

Table 2: Vibrational assignments of Epinine with B3LYP/6-311G (d, p)

B3LYP (Calculated) Unscaled	B3LYP (Calculated) Scaled	IR (Int.)	Vibrational Assignments
15.4178	15	0.4768	molecule Bend from middle
57.0494	55	2.6941	molecule twist from middle
59.9741	58	0.1014	molecule twist from middle
77.1738	74	1.8165	w (N-H)
137.4468	132	5.2245	Rock CH_2
171.8873	165	38.6893	Twist CH_3
172.0984	166	155.2247	β (C-C-H)
202.728	195	0.5606	Twist CH_2
227.0199	218	12.3776	β (C-C-H)
269.3595	259	1.4083	w (O-H)
281.6088	270	1.0871	Twist CH_2
328.2021	315	1.8509	β (C-C-H)
336.9387	323	0.9859	Rock CH_2
403.662	388	9.9812	γ (C-C-C)
447.643	430	3.2598	Twist CH_2
474.366	455	0.1691	τ (C-C-C-C)
536.1963	515	8.2519	τ (C-C-C-C)
588.8655	565	2.3071	τ (C-C-C-C)
629.2074	604	0.9375	γ (C-C-C)
653.6895	628	1.0742	γ (C-C-H)
766.2203	736	1.4073	Rock CH_2
787.097	756	5.6858	γ (C-C-H)
836.1461	803	29.2644	β (C-C-H)
862.598	828	31.0981	γ (C-C-C)
886.1892	851	10.1488	Rock CH_2
892.4643	857	13.4953	γ (C-C-H)
939.3368	902	4.0439	β (C-C-H) + β (C-C-C)
963.6705	925	4.0407	γ (C-C-C)
998.4211	958	4.7382	β (C-C-N) + β (C-C-C)
1035.495	994	4.0251	β (C-C-N) + β (C-C-C)
1098.024	1054	1.5077	Rock CH_2
1105.689	1061	9.8574	β (C-C-H) + β (C-C-C)
1120.133	1075	13.9036	Twist CH_2 in whole
1132.382	1087	1.3347	Twist CH_2 in whole
1140.864	1095	0.6578	β (C-C-H) + β (C-C-C)
1154.519	1108	0.7976	β (C-C-H) + β (C-C-C)
1178.163	1131	15.4697	β (C-C-H)
1237.014	1188	26.8225	Twist CH_2
1242.392	1193	67.7885	Rock CH_2
1293.328	1242	23.6888	Rock CH_2
1320.243	1267	6.5263	Twist CH_2
1367.998	1313	4.0045	Twist CH_2
1374.472	1319	0.5755	S (H-C-H)
1377.083	1322	0.1495	S (H-C-H)
1388.374	1333	2.1001	S (H-C-H)
1395.677	1340	3.5831	Twist CH_2
1419.056	1362	100.6808	β (C-O-H)
1423.698	1367	3.8935	β (C-N-H)
1468.296	1410	7.5048	β (C-O-H)
1492.62	1433	25.9249	n(C-C)
1546.812	1485	13.483	β (C-O-H)

1616.243	1552	105.9633	n(C-O) + n(C-C)
1658.917	1593	36.1524	n(C-C)
1778.939	1708	0.6475	n(C-C)
2910.747	2794	1.7954	n(C-H)
2954.263	2836	1.1317	n(C-H)
2987.358	2868	1.2671	n(C-H)
3026.359	2905	1.833	n(C-H)
3031.328	2910	2.8773	n(C-H)
3059.168	2937	32.9622	n(C-H)
3061.835	2939	0.6767	n(C-H)
3082.837	2960	36.2677	n(C-H)
3135.64	3010	1.0146	n(C-H)
3366.211	3232	3.0707	n(N-H)
3891.208	3736	27.1226	n(O-H)
3894.421	3739	34.7049	n(O-H)

Where- n: stretching; β: in plane bending; γ: out of plane bending; τ: torsion, w: wagging, S: scissoring

Table 3: Vibrational assignments of Hordenine with B3LYP/6-311G (d, p)

B3LYP (Calculated) Unscaled	B3LYP (Calculated) Scaled	IR (Int.)	Vibrational Assignments
17.1363	16	0.5681	molecule Bend from middle
44.9251	43	44.9251	molecule twist from middle
73.6314	71	0.0226	molecule twist from middle
119.7227	115	0.6897	Twist CH_2
150.7202	145	0.1328	Twist CH_3
163.1725	157	0.4698	Twist CH_3
196.7266	189	0.7062	Twist CH_3
251.9938	242	0.4734	τ (C-C-C-N)
275.7309	265	91.0653	w (O-H)
298.3695	286	1.3121	τ (C-C-N-C)
327.0627	314	4.2244	Out of plane bending in whole
363.1349	349	1.2221	γ (C-C-H)
407.0025	391	6.5068	S (CH_2-N-CH_2)
427.9059	411	2.7105	τ (C-C-N-CH_3)
464.2355	446	0.6018	S (CH_2-N-CH_2)
477.1003	458	2.48	β (C-C-C)
523.6656	503	15.0055	β (C-C-C)
550.4992	528	8.0374	τ (C-C-C-C)
646.1409	620	0.0788	Ring deformation
670.5979	644	1.342	γ (C-C-H)
803.0084	771	8.2511	β (C-C-H)
810.8922	778	2.5089	Ring deformation
838.3001	805	2.9107	γ (C-C-H)
865.708	831	51.3479	γ (C-C-H)
924.9486	888	2.3792	Rock CH_2
952.1981	914	5.2088	Twist CH_3
958.5255	920	4.4963	Twist CH_3
971.6331	933	1.4946	γ (C-C-H)
975.7658	937	5.0366	Twist CH_3
989.0258	949	5.157	Ring breathing
989.6936	950	9.0098	Rock CH_3
1000.644	961	4.3054	γ (C-C-H)
1044.804	1003	0.1421	β (C-C-H)
1056.427	1014	8.1716	β (C-C-H)
1107.926	1064	0.463	Twist CH_2
1111.852	1067	13.1923	Twist CH_2
1125.588	1081	7.73	β (C-C-H)
1143.273	1098	0.1103	β (C-C-H)
1163.259	1117	0.1	β (C-C-H)
1191.872	1144	2.5203	Twist CH_3
1202.145	1154	10.7587	β (C-C-H)
1216.417	1168	1.0403	Twist CH_3
1236.134	1187	7.4771	β (C-C-C) + β (C-C-H)
1266.954	1216	39.1641	β (C-C-C) + β (C-C-H)
1298.926	1247	19.8244	β (C-C-H) in whole
1369.051	1314	0.836	β (H-C-H) in whole
1373.348	1318	0.5543	β (H-C-H) in whole

1374.507	1320	12.0084	β (H-C-H) in whole
1375.881	1321	10.5762	Twist CH_2
1380.845	1326	10.0379	β (H-C-H) in whole
1382.955	1328	28.8527	β (C-O-H) + S (H-C-H)
1389.6	1334	2.3412	β (C-O-H)
1394.38	1339	2.8364	S (H-C-H)
1397.827	1342	4.123	S (H-C-H)
1402.051	1346	0.895	S (H-C-H)
1490.265	1431	24.9539	Ring breathing
1566.365	1504	10.8977	n(C-C)
1639.723	1574	123.8541	n(C-O)
1784.559	1713	9.8246	n(C-C)
1805.873	1734	42.557	n(C-C)
2888.214	2773	1.0798	n(C-H)
2914.05	2797	1.2766	n(C-H)
2960.004	2842	2.9278	n(C-H)
3003.745	2884	1.8535	n(C-H)
3013.864	2893	15.4371	n(C-H)
3020.39	2900	2.3339	n(C-H)
3032.4	2911	2.7441	n(C-H)
3045.71	2924	1.7704	n(C-H)
3050.15	2928	9.7564	n(C-H)
3061.438	2939	0.4769	n(C-H)
3062.871	2940	32.9292	n(C-H)
3071.52	2949	30.7015	n(C-H)
3117.514	2993	0.9997	n(C-H)
3133.527	3008	0.6796	n(C-H)
3889.038	3733	20.2203	n(O-H)

Where- n: stretching; β: in plane bending; γ: out of plane bending; τ: torsion, w: wagging, S: scissoring

3.4 Electrical, Dipole moment and Thermo-dynamical properties

Frontier orbital energy gap, i.e. the gap between HOMO and LUMO shows the interaction of that molecule with other species. Frontier orbital energy gap helps to differentiate the chemical reactivity of the molecules. For epinine and hordenine, the frontier orbital energy gap is 8.5236 and 9.1604 eV, respectively and are given in table 4. So it can be concluded that epinine is the more reactive than hordenine. The pictures of HOMO, LUMO, and electrostatic potential for epinine and hordenine are shown in Figures 3. Dipole moment (μ), can be expressed in terms of *x*, *y* and *z* components and are given by following equations –

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1\backslash 2}$$

and dipole moment is given in table 4. Internal thermal energy (*E*), constant volume heat capacity Cv, and entropy *S***,** calculated at B3LYP/6-311G (d, p) level, are listed in Table 5. We know that, conduction band is almost empty at the room temperature, so the electronic contribution in total energy is negligible. Hence, thermodynamic properties show that vibrational motion plays an important role.

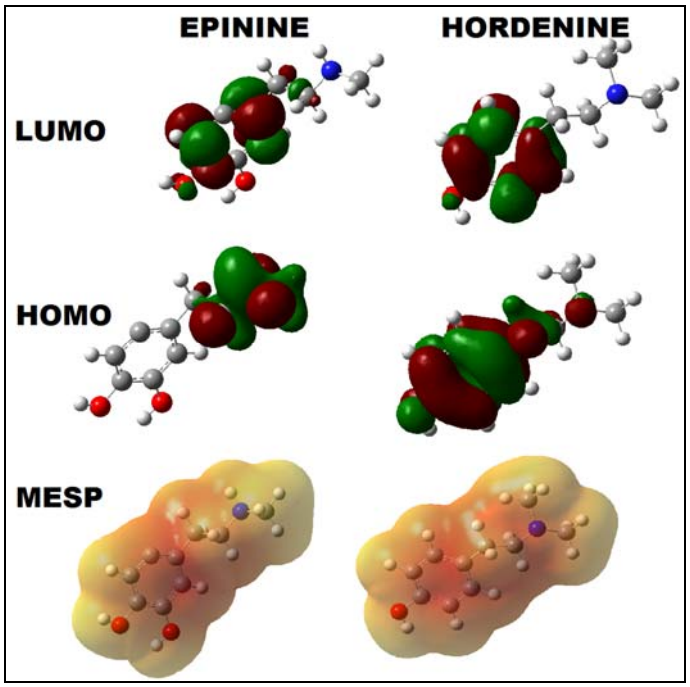

Fig 3: LUMO-HOMO and MESP pictures of EPININE and HORDENINE

Table 4: Lowest Energy, HOMO- LUMO Gap (Frontier orbital energy gap) and Dipole Moment of Epinine & Hordenie by (B3LYP)/ 6-311 G (d, p) method

Parameters	Epinine	Hordenine
Energy (in au)	-0.04300894	-0.05260001
Dipole moment (in Debye)	2.579	1.491
HOMO	-0.30461	-0.32952
LUMO	0.00876	0.00726
Frontier orbital energy gap (eV)	8.5236	9.1604

Table 5: Calculated Thermodynamic Properties of Epinine & Hordenine by B3LYP/6-311 G (d, p) methods

Parameters	E (Thermal) (kcalmol^{-1})	
	Epinine	**Hordenine**
Total	130.826	152.476
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	129.048	150.699
	CV (cal K^{-1}mol^{-1})	
Total	46.752	47.533
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	40.790	41.572
	S (cal K^{-1}mol^{-1})	
Total	117.816	113.583
Translational	41.230	41.213
Rotational	31.316	31.216
Vibrational	43.892	41.154

4. Conclusions

All calculated wave numbers are real in nature of the both molecules, thus all the compounds are stable. We have done density functional calculations on epinine and hordenine. Normal modes are discussed in detail with the help of gauss view program. The chemical reactivity of molecules shows the supremacy of epinine over hordenine. Dipole moment shows the solvency properties of these molecules while, Thermodynamic properties show that vibrational motion plays an important role in the field of this research. No experimental FTIR spectrum is available for comparison of epinine and hordenine so it will provide a suitable path for experimental researchers.

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