Available online at www.derpharmachemica.com

ISSN 0975-413X
CODEN (USA): PCHHAX

Der Pharma Chemica, 2016, 8(11):207-215
(http://derpharmachemica.com/archive.html)

Analysis of Molecular Structure, Vibrational spectra and Electronic Properties of 2-amino-3-nitro-6-picoline by Density Functional Methods

DAVID PEGU

Department of Physics, Haflong Govt. College, Haflong, Assam, India

---

ABSTRACT

In the present study the geometrical parameters and vibrational spectroscopic properties of the compound 2–amino-3-nitro-6-picoline (2A3N6P) have been calculated by using Harteree-Fock and Density functional method (B3LYP) with 6-311++G(d,p) basis set. The calculated optimized structural parameters and the scaled frequencies are investigated and compared with earlier reported data. The complete vibrational assignment and analysis of the fundamental modes of the molecule were carried out. In addition, molecular electrostatic potential and total electron density has been analyzed to investigate size, shape, charge density distribution and site on chemical reactivity of the molecule. Finally the Mullikan atomic charges of the compound have been studied.

Key words: FT-IR, FT-Raman, MESP, DFT.

INTRODUCTION

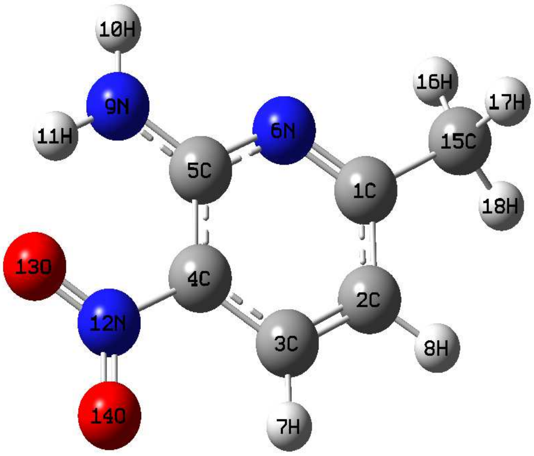
Pyridines and its derivatives are heterocyclic compounds occurring naturally a large number that are building blocks of biologically important molecules and important industrial, pharmaceutical and agricultural products [1,2]. The chemistry and applications of pyridine compounds have recently received much attention due to their efficacy as synthetic intermediates and biological importance. Pyridine derivatives exhibited various types of biological activities antimicrobial [3], antimalarial [4], antitumorial [5,6] and antidiabatics [7]. Pyridine derivatives act as anesthetic agents, drugs for certain brain diseases, and prodrugs for treating neuronal damage caused by stroke [9-10]. They also underpin analgesics for acute and chronic pain, treatment for tinnitus, depression, and even diabetic neuropathy. The literature survey reveals that vibrational and electronic spectra of pyridine and its derivatives have been investigated by many authors [11-14]. A A Dahy et al. evaluated structure and vibrational assignments of 2-amino-3-nitro pyridine based on ab initio (MP_2) and DFT calculations [15]. The harmonic frequencies of amino and methyl substituted pyridine were calculated by many authors and the anharmonicity was estimated by N. Sundaraganesan et al [16].

It appears that structural and vibrational assignments of alkyl amino, nitro and methyl substituted pyridines have not been subjected to a systematic study using *ab-initio* and DFT calculations. The theoretical *ab-initio* and DFT calculations give information regarding the nature of the electronic structure, the functional groups, orbital interactions and mixing of skeletal frequencies. A comprehensive investigation of geometrical structure, spectral analysis and along with molecular electrostatic potential surfaces of may lead to the better understanding of structural and spectral characteristics. Therefore, in the present study theoretical analysis of the title compound 2A3N6P have been carried out using *ab-initio* and DFT calculations. The main objective of the present study is to investigate structure and vibrational frequencies in order to obtain a complete description of vibrational assignments along with normal mode analysis of the title compound.

MATERIALS AND METHODS

Computational Details

All calculations were performed at HF and B3LYP levels on a Pentium IV personal computer using Gaussian 03W program Package [17] and Gauss-View molecular visualization program package. Initial geometry generated from standard geometrical parameters was minimized without any constraint in the potential energy surface at the Hartee - Fock level, adopting the standard 6-311G ++ (d, p) basis set. This geometry was then reoptimized again at Becke–Lee–Parr (B3LYP) [18-20] hybrid exchange–correlation three-parameter functional level, using basis set 6-311++G (d, p). The optimized structural parameters were used to calculate the vibrational frequencies of the compound at HF and DFT levels with same basis set to characterize all stationary points as minima. As a result, the unscaled frequencies, force constants, infrared intensities and Raman activities are obtained. To overcome the negligence of electron correlation we have used uniform scaling factor values 0.96 for B3LYP / 6-311++G (d,p) and 0.89 for the HF / 6-311++G(d,p) basis set.



Figure(i): Opimized molecular structure of 2A3N6P

Table (i): Optimized geometrical parameters of 2-amino-3-nitro-6-picoline

Bond length in (angstroms)			Bond angles in (degrees)			Dihedral angles in (degrees)		
	HF	B3LYP		HF	B3LYP		HF	B3LYP
C1-C2	1.398	1.399	C2-C1-N6	122.79	122.8	N6-C1-C2-C3	0.0104	0.0223
C1-N6	1.313	1.313	C2-C1-C15	121.19	121.18	N6-N1-N2-H8	179.994	179.983
C1-C15	1.504	1.504	N6-C1-C15	116.02	116.02	C15-C1-C2-C3	179.971	179.932
C2-C3	1.373	1.373	C1-C2-C3	117.62	117.62	CC2-C1-N6-C5	0.0029	0.0139
C2-H8	1.072	1.072	C2-C3-C4	119.92	119.89	C15-C1-N6-C5	179.979	179.929
C3-C4	1.388	1.388	C3-C4-C5	119.00	119.05	N6-C1-C15-H16	58.6678	58.6848
C3-H7	1.072	1.072	C3-C4-N12	118.01	117.97	C1-C2-C3-C4	0.0044	0.0144
C4-C5	1.414	1.413	C5-C4-N12	123.02	122.98	C2-C3-C4-N12	179.989	180.00
C4-N12	1.44	1.441	C4-C5-N6	119.65	119.63	C7-C3-C4-N12	0.0098	0.0032
C5-N6	1.333	1.333	C4-C5-N9	125.18	125.2	C3-C4-C5-N6	0.0158	0.0086
C5-N9	1.339	1.339	N6-C5-N9	115.18	115.16	C3-C4-C5-C9	179.953	179.914
C9-H10	0.992	0.992	C1-N6-C5	121.03	121.01	N12-C4-C5-N6	179.981	179.991
C9-C11	0.991	0.993	C5-N9-H10	116.93	116.93	C12-C4-C5-N9	0.0504	0.0858
C12-O13	1.197	1.197	C10-N9-H11	121.52	121.52	C3-C4-N12-O13	179.911	179.876
C12-O14	1.189	1.189	C4-N12-O13	118.48	118.48	C5-C4-N12-O13	0.0861	0.1238
C15-H16	1.085	1.085	O13-N12-O14	123.42	123.42	C4-C5-N6-C1	0.0103	0.0018
C15-H17	1.085	1.085	C1-C15-H16	109.56	109.56	C9-C5-N6-C1	179.961	179.917
C15-H18	1.083	1.083	C16-C15-H17	107.65	107.65	C4-C5-N6-C1	179.961	179.865

Geometrical Parameters

The optimized molecular structure of the title molecule calculated by ab-initio HF and DFT-B3LYP with 6-311++G(d,p) basis set are listed in Table (i) in accordance with the atom numbering scheme shown in the fig. (i). The comparisons among the HF and DFT (B3LYP) are given in order and the results shows that both levels predict consistent results.

MULLIKEN ATOMIC CHARGES

The computed of Mulliken atomic charges play an important role in the application of quantum mechanical calculations of the molecular system. The Mulliken atomic charges of title molecule obtained by HF and B3LYP method with 6-311++G(d,p) basis set are presented in Table (ii) and the graphical representation of the results are shown in Fig. (ii).

Table (ii): Mulliken atomic charges of 2-amino-3-nitro-6-picoline

Atoms	HF/6-311++ G(d,p)	B3LYP/6-311++G(d,p)
C1	-0.22583	-0.316886
C2	-0.460668	-0.175212
C3	0.187974	0.171964
C4	-0.277859	-0.088511
C5	0.448166	-0.084269
N6	-0.291657	-0.143565
H7	0.320555	0.268773
H8	0.215794	0.185451
N9	-0.509241	-0.323927
H10	0.343353	0.302033
H11	0.353519	0.316505
N12	-0.16949	-0.229709
O13	-0.094638	-0.058151
O14	-0.070329	-0.021695
H15	0.230353	0.197199

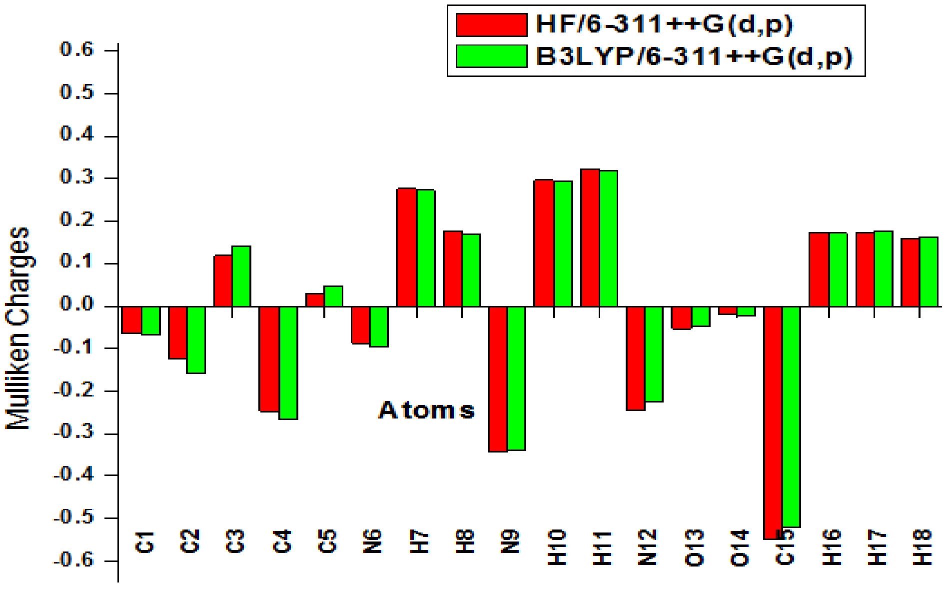


Figure (ii): Mulliken atomic charge distributributions of 2-amino-3-nitro-6-picoline

As can be seen in Table (ii) and Figure (ii), all hydrogen atoms and two carbon atoms in the ring C3, C5 have a net positive charge. It is interesting to see all the nitrogen atoms (N6, N9 and N12) and two oxygen atoms (O13 and O14) have a net negative charge. The maximum negative charges attained by C4, C15, N9 which are more donor atoms. Tendency to behave more acceptor atoms are C3, C5 and all hydrogen atoms which are positively charged. The donor and acceptor atoms may suggest the population of electron distribution of each atom in the compound.

Table(iii): Vibrational wavenumbers obtained for 2-amino-3-nitro-6—picoline at HF and B3LYP using 6311++ G(d,p) basis set [harmonic frequency (cm^{-1}), IR intensities (km mol^{-1}), Raman scattering activities (A^0 amu^{-1})]

		HF/6-311++G(d,p)				B3LYP/6-311++G(d,p)				
Obs. nos.	Sym. Species	Unsld. (cm^{-1})	Scaled (cm^{-1})	IR intensity	Raman activity	Unsld. (cm^{-1})	Scaled (cm^{-1})	IR intensity	Raman activity	Assignments
1	A´´	52	46	0.013	0.2981	23	22	0.1108	0.6126	τ (CH3)
2	A´´	58	52	3.817	0.2185	67	64	1.8447	0.0348	τ (NO2)+ φ (ring)
3	A´´	97	86	0.006	0.1133	85	82	0.0027	0.1145	φ(ring) + φCH3
4	A´´	218	194	3.884	0.0012	203	195	0.0437	0.0041	φC-NH2+φ(ring)
5	A´	266	236	1.962	0.5765	249	239	1.7418	0.4881	βCH3+βNO2
6	A’’	273	243	106.2	0.7236	259	249	23.0725	0.6897	τNH2
7	A’’	312	278	149.8	1.1919	319	306	187.225	0.4325	τNH2
8	A´	362	322	6.379	0.9489	339	325	6.0993	2.4175	βNH2+βCH3
9	A´	397	353	0.643	4.1851	369	354	0.1505	8.1468	βCCC+βCH3
10	A´	458	408	2.888	1.9387	421	404	2.549	2.8391	βNH2
11	A´´	468	417	0.169	0.6415	435	418	3.2491	0.7937	φCH
12	A´	605	538	8.272	3.0274	561	539	7.4607	2.6154	βNH2+s(ring)
13	A´	634	564	9.372	5.1506	587	564	2.2022	11.364	S(ring)
14	A´	642	571	0.556	0.2524	619	594	1.4272	0.4552	tNH2
15	A´	682	607	1.611	4.1825	634	609	1.0494	3.3769	ωNO2+γC-CH3+s(ring)
16	A´	696	619	0.181	0.4568	653	627	1.9984	0.0495	tNH2
17	A´	792	705	11.04	22.7421	715	686	11.4399	0.3273	ωNO2+φCH
18	A´	812	723	47.65	1.4033	744	714	3.1574	16.282	γC-CH3+ ring deformation
19	A´´	826	735	1.161	0.026	745	715	4.581	1.3203	φCNC(ring)+φ(ring)
20	A´´	881	784	26.94	1.3124	810	778	25.2489	0.6672	φCH
21	A´	956	851	54.42	11.7825	853	819	23.8985	27.896	sNO2+βCH
22	A´	1038	924	15.81	5.4176	967	928	11.9151	1.7443	sNH2+β(ring)
23	A´´	1097	976	2.53	2.1176	990	950	1.0293	0.1955	φCH
24	A´´	1113	991	0.051	0.2808	1004	964	0.5779	4.4878	rCH3+βNH2
25	A´´	1154	1027	6.953	0.078	1054	1012	6.1638	0.2245	φC-CH3
26	A´	1174	1045	72.01	6.9189	1097	1054	16.7751	3.5069	βCH+γCN
27	A´	1214	1080	64.29	42.1996	1113	1068	44.2496	35.758	βNH2+γCN+rNH2
28	A´	1268	1129	23.03	20.9569	1184	1137	13.3704	5.9776	βCH+γNO
29	A´	1310	1166	160	9.3067	1254	1204	4.6941	11.41	βCH+γCCH3
30	A´	1359	1210	17.16	3.8054	1290	1238	463.209	140.65	γ(ring)+γCN+γNO2+ωNH2
31	A´	1442	1283	40.22	23.3219	1343	1289	0.9824	1.145	βCH+γ(ring)
32	A´	1530	1362	1.356	8.5169	1357	1303	158.133	183.53	γring+sNO2+γCN
33	A´	1545	1375	64.4	129.5	1407	1351	36.5011	36.677	ωCH3
34	A´	1593	1418	273.1	103.347	1447	1389	128.429	11.241	γNO2+ωCH3+ωNH2
35	A´´	1595	1420	7.698	9.1498	1476	1417	8.3251	9.0618	δCH3
36	A´	1610	1433	305.8	53.0619	1486	1427	19.3092	4.9251	γNO2+δCH3
37	A´	1622	1444	96.41	1.8832	1489	1429	44.1458	1.844	βCH + γCCC
38	A´	1710	1522	62.05	7.2204	1540	1478	167.431	17.075	γNO2+δCH3
39	A´	1766	1572	347.1	47.3054	1595	1531	57.7084	21.547	sNH2
40	A´	1776	1581	188	21.2667	1617	1552	182.682	41.372	Γ(ring)+sNH2
41	A´	1813	1614	981.4	8.4603	1648	1582	572.215	9.9589	γCCC+sNH2
42	A´	3183	2833	14.22	209.65	3038	2916	9.3231	304.8	γ_{sy}CH3
43	A´	3246	2889	11.54	78.9536	3094	2970	6.7905	95.598	γ_{as} CH3
44	A´	3263	2904	21.19	58.6393	3122	2996	15.2349	63.842	γ_{as} CH3
45	A´	3366	2996	2.446	70.6242	3199	3071	3.3629	86.472	γ_{as}CH
46	A´	3393	3019	2.517	71.0105	3220	3091	3.1957	83.568	γ_{sy}CH
47	A´	3841	3418	112.7	127.19	3575	3432	85.8479	181.9	γ_{sy}NH2
48	A´	3985	3547	123.7	23.789	3718	3570	101.254	35.976	γ_{as}NH2

Notes : A´- in plne, A´´-out of plne, τ- twisting, ϕ - out-of-plane bending, β- in-plane-bending, ω- wagging, r-rocking, γ- stretching, s-scissoring, γ_{as}-asymmetric stretching, γ_{sy}-symmetric stretching, Γ- torsion, sym.- Symmetry, unsld.-unscaled

Vibrational Analysis

The maximum number of potentially active observable fundamentals of a non-linear molecule, which contains N atoms, is equal to 3N-6 apart from three rotational degrees of freedom. The molecule 2A3N6MP has 18 atoms which are distributed as Γ= 3N-6 = 48 fundamental modes of vibrations. The molecule belongs to C_1 point group symmetry and 48 normal modes of vibrations are distributed as 35 in- plane and 13 out of plane vibrations. The detailed vibrational assignment of the fundamental modes of 2A3N6MP along with the calculated IR intensity and Raman activity and normal descriptions are reported in the Table (iii)**.** The comparative graph of the calculated IR intensities and Raman activities for the title molecule are presented in Figure (iii) and (iv). Some important modes of vibrations along with scaled wave nos. and observation nos. have been discussed as follows.

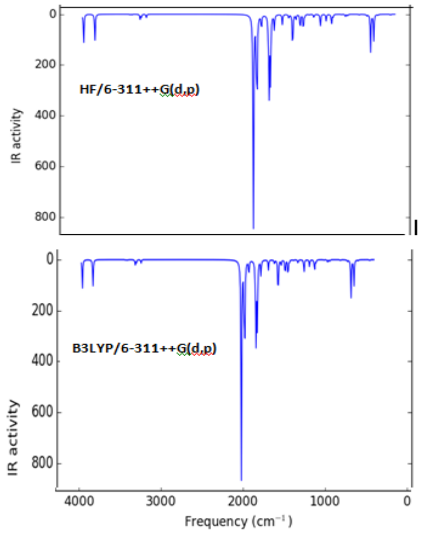


Figure (iii): Calculated FT-IR spectrum of 2A3N6P

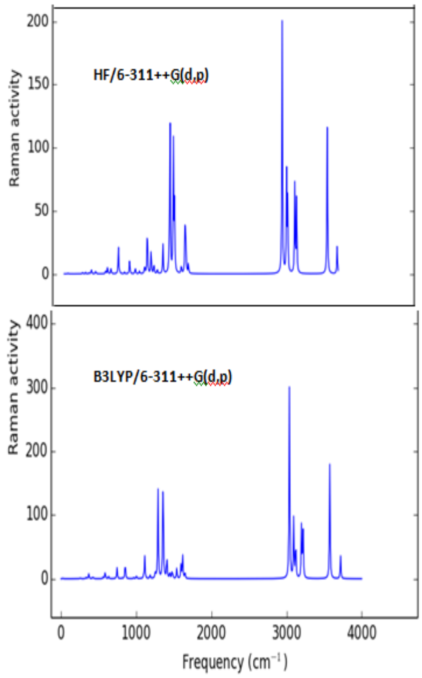


Figure (iv): Calculated FT-Raman spectrum of 2A3N6P

Methyl group vibrations: The title compound possesses only one methyl group at the 6th position with respect to the nitrogen in the pyridine ring. For methyl substituted benzene derivative the CH_3 asymmetric stretching vibration normally expected in the region 2900-3000 cm^{-1} and symmetric stretching appear between 2800-2900 cm^{-1} [28-30].The symmetric CH_3 vibrations observed around 2980 cm^{-1} and asymmetric CH_3 vibration in the region 2870 cm^{-1} for similar molecules.[31-34].

The asymmetric C-H stretching vibration in methyl group appears higher than the symmetric stretching. The asymmetric CH_3 vibrations are observed at 2890(43), 2905(44) for HF/6-311++G (d,p) and2970(43), 2997(44) for B3LYP / 6-311++G (d,p). One CH_3 symmetric stretching vibration observed at 2916(42) by B3LYP/6-311++G (d,p) and for HF/6-311++G(d,p) this stretching vibration observed at 2833(42). Bellamy suggested that each CH_3 group gives rise to three C-H oscillations (2800-3000 cm^{-1}) and three C-H deformations. The CH_3 torsional modes observed at 22 (1) by B3LYP / 6-311++G(d,P) and 46 (1) by HF /6-311++G(d,P) are below 400 cm^{-1} as expected . The rocking CH_3 vibrations at 965(24) and 1028(25) by B3LYP and HF are well agree with the Long et al [35-36] within the region (974-1041 cm^{-1}). Two CH_3 wagging at 1375 (33), 1418(34) at HF and 1352 (33), 1389 (34) at B3LYP vibrations are observed which are also similar with earlier results. In our present investigations some in plane C-H vibrations are also observed with ring stretching vibration. Two in-plane bending C-CH_3 at 326(8), 239(5) and 237(5), 323(8**)** are within the range (390-260 cm^{-1}) in both B3LYP and HF and out- of- plane C-CH3 bending appears at 249 and 243 cm^{-1} in both level in mode no.6. The assignments are in good agreement obtained for methyl substituted pyridine derivatives [37].

C-N and C-C (ring vibrations) :

The description of the C-N stretching pyridine ring and C-C stretching bands of aromatic ring usually observed in the same frequency range 1450-1600 cm^{-1} and 950- 1450 cm^{-1} **[**38-39**].** The C-N stretching vibrations for aromatic amine observed in the region 1266-1382 cm^{-1}**.** In our present study C-N and C-C stretching vibrations are varied together which occur in the frequency region 1238- 1362 cm^{-1}. The stretching ring vibrations both CCC and CNC appears at 1239(30), 1290(31), 1303(32) and 1210(30), 1284(31), 1362(32) in B3LYP and HF respectively. Some out of plane ring vibrations are observed at 715 (19), 196(4), 81(3) and one in-plane vibration at 408(10) in B3LYP and similar vibrations are observed at 736(19), 194(4), 87(3) and 408(10) in HF method.

NO_2 Vibrations:

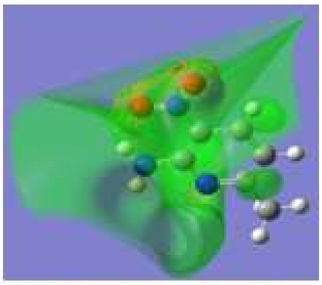
The vibrations of nitro groups are vibrate with strong intensity and relatively independent with rest of the molecules [40]. The various vibration associated with nitro groups are symmetric and asymmetric stretching, in plane vibrations (scissoring and rocking), out of plane vibration (wagging and twisting). The asymmetric and symmetric NO_2 stretching vibrations of the aromatic nitro compounds gives a band in the range 1570-1485 cm^{-1} and 1370-1320 cm^{-1} **[**41] respectively. The NO_2 stretching vibrations are observed at 1647 and 1595 cm^{-1} for 2-amino-3-nitro pyridine by A A Dahy et. al. and our computed results symmetric and asymmetric NO_2 stretching vibrations are occurs at 1418, 1433, 1523 (mode nos. 34, 36, 38) and 1389, 1427, 1479 (mode nos. 34, 36, 38) by HF and B3LYP method. A very strong NO_2 stretching vibrations are occurs at mode nos. 36 in both HF and B3LYP may be due to the electronic effects of the substituted methyl group. The deformation vibration of NO_2 group (scissoring, wagging, rocking and twisting) contributes to several modes in the low frequency region [42]. In our present calculation NO_2 twisting vibration occurs at 64 (2) cm^{-1} by B3LYP and at 52 (2) by HF and NO_2 scissoring at 851, 925 at mode nos. 21 and 22 in HF and frequencies 820, 929 cm^{-1} for B3LYP are nearly within the region 890- 835 cm^{-1} reported by C Brian Smith et al. **[**43]. In the present investigation NO_2 wagging vibrations are appears at 634 and 608 at mode nos. 15 for both B3LYP and HF in which γ C-H_3 are also active. The NO_2 rocking vibrations are active in the region 515- 590 cm^{-1} [44] and in 2A3N6MP it appears at 564 cm^{-1} and 563 cm^{-1} for HF and B3LYP respectively. Besides stretching and deformation of nitro group C-NO_2 in-plane-and out-of-plane vibrations are also observed in both HF and B3LYP within the expected region [45] which is presented in the Table (iii).

C-H Vibrations:

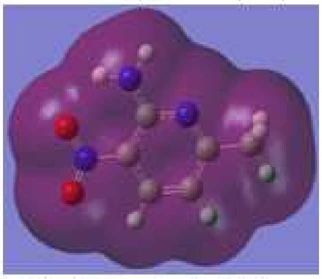
The heteroaromatic substituted pyridine compound shows the presence of C-H stretching, in-plane and out-of-plane bending vibrations. The titled molecules has only two C-H moieties give rise to two C-H stretching vibrations and these stretching vibrations are observed around 3100-3000 cm^{-1} which is their characteristics region [46]. The C-H in-plane vibration usually occur in the region (1000-1300 cm^{-1}) [47] and out-of-plane bending modes in the region (950-600 cm^{-1}) [48]. The title molecule 2A3N6MP the C-H symmetric and asymmetric stretching found to be present at scaled frequencies 3092(46) and 3072 (45) cm^{-1} in case of B3LYP. At the HF level these two stretching vibrations are observed at 3020 (46) and 2996 (45). The stretching vibration corresponds to the C_3-H_7 and C_2-H_8 in both the level of theory are in agreement with the theoretical and experimental value in the literature [49]. At HF level of theory C-H in plane vibrations contaminated with other modes of vibration are observed at 1444(37), 1284(31), 1167 (29), 1129(28) and 1045(26) and at B3LYP level these vibrations are observed at 1430(37), 1290(31), 1204(29), 1054(26). The C-H in plane vibrations assigned in the title molecule is found to be in the region in the literature **[**50]. In the present investigation, in HF method the bands at 784(20), 991(24) and at B3LYP the bands at 951(23), 778(20) are appear as out-of-plane bending C-H vibrations occur in the region (978-990 cm^{-1}) which are within the range found in literature [51].

NH_2 vibrations:

In our present observation two NH_2 stretching vibrations in each B3LYP and HF methods are observed. Asymmetric and symmetric stretching modes are observed at 3418 and 3547 at HF level and at B3LYP level these vibrations are observed at 3432 and 3569 cm^{-1}. Thus the asymmetric vibrations are higher than the symmetric and the above NH_2 stretching vibrations are in agree with the literature data [52]. In addition to the stretching vibration NH_2 group has occurred scissoring at frequencies 1553(40), 1583(41) in B3LYP and 1572(39), 1581(40) in HF. It is found that the NH_2 scissoring vibrations are within the range (1590- 1650) reported by Thompson [53]. The NH_2 rocking vibrations has been identified in the mode nos. 27 with frequency 1069 for B3LYP and at frequency 1080 in HF at mode no 27 are excellent agreement with predicted results within the region 1077-1057 reported by N. Sundaraganesan et al for 2-amino-6-methyl pyridine. The NH_2 wagging computed at 408, 539 cm^{-1} (mode nos. 10 and 12) in HF and for B3LYP 404, 539 cm^{-1} (mode nos. 10 and 12) which are nearly expected value [54]. Two torsional modes are observed at 249, 307 cm^{-1} in B3LYP and at 243, 279 in HF with same mode nos. 6 and 7 respectively.



Electro static potential (ESP)



Total electron density (ED)

Molecular electrostatic potential (MEP)

Figure (v): Electrostatic potential (ESP), electron density (ED) and the molecular electrostatic potential (MEP) map of 4F4HBP molecule.

OTHER MOLECULAR PROPERTIES

Electrostatic potential, electron density and molecular electrostatic potential and electrostatic potential are useful quantities to illustrate the charge distributions of molecules are used to visualize variably charged regions of a molecule. Therefore, the charge distributions can give the information about how the molecules interact with another molecule. In the present study, electrostatic potential, electron density (ED) and the molecular electrostatic potential (MESP) of the molecule under investigation are constructed to predict reactive sides for electrophilic and nucleophilic attack at B3LYP/6-311++ G(d,p) method. The electrostatic potential, total electron density surface and the molecular electrostatic potential mapped into the constant electron density surface are shown in the Fig. v and Fig. v (b). The ED plots for the title molecule show a uniform distribution. MESP helps to predict molecular shape, size as well as reactive sites for electrophonic and nucleophilic attack in terms of color grading of a molecule. The different values of the electrostatic potential at the surface are represented by different colors. Red and blue areas in the MESP refer to the regions of positive and negative potentials and correspond to the electron rich and electron-poor regions, respectively, whereas the green color signifies the neutral electrostatic potential. The electrostatic potential increases in order red<orange<yellow<geen<blue. The intensity of the color scheme for the MESP surface is red, electron rich, partially negative charge; blue, electron deficient, partially positive charge; light blue, slightly electron deficient region; yellow, slightly electron rich region; green, neutral; respectively [55]. It can be seen from the MESP figures v(b), that the yellowish blob localized more over the oxygen in the nitro group indicates negative ESP, while the positive ESP is localized on the rest of the molecules. From the figure it is found that the region around the nitro group represents the most negative potential region (red), while regions around hydrogen atoms represent positive potential (blue). However, the hydrogen atoms at the CH_3 group and in the ring have smaller value than the hydrogen in the NH_2 group.

CONCLUSION

In the present work, the molecular structure parameters of the compound 2-amino-3-nitro-6-picoline have been obtained using HF and density functional theory computed optimized geometric parameters of the molecule were compared and analyzed with available experimental data. The vibrational frequencies of the fundamental modes of the compound have been precisely assigned and analyzed, and the theoretical results were compared with earlier reported literature results. The calculated MESP, total electron density provides the information of size, shape and charge distribution which further lead to the understanding of properties reactive side of the title molecule. Mulliken's net charges have been calculated and interpreted.

Acknowledgements
I would like to thank Dr. Utpal Sarkar, Department of Physics, Assam University, Silchar, Assam, for his help in various ways to carry out this research work.

REFERENCES

[1] T. Anderson, J. Liebigs *Ann. Chem*.,**1846**, 60, 86-103.,
[2] Pyridine And Pyridine Derivatives Vol 20; Kirk-Othmer Kirk-Othmer Encyclopedia of Chemical Technology (4th Edition).
[3] S. Tomaru, S. Matsumoto, T. Kurihara, H. Suzuki, N. Oobara, T. Kaino, *Appl. Phys. Lett*. 58 **1991,** 2583–2585.
[4] C. Kaneko, S. Yamada, I. Yokoe, N. Hata, Y. Ubata, *Tetrahedron Lett*. 7 **1966,** 4729–4733.
[5] C. Kaneko, I. Yokoe, S. Yamada, *Tetrahedron Lett*. 8 **1967,** 775–778.
[6] 6 . N. Hata, E. Okutsu, I. Tanaka, *Bull. Chem. Soc. Jpn* 41, **1968,** 1769–1775.
[7] N. Hata, I. Ono, T. Tuchiya, *Bull. Chem. Soc. Jpn* 45, **1972,** 2386–2391.
[8] I. Ono, N. Hata, *Bull. Chem. Soc. Jpn* 45, **1972,** 2951–2953.
[9] D. Doplp, Davidson (Ed.) 55, Springer, Berlin, **1975**, p. 49.
[10] K. C. Medhi, R.N. Medhi, *Spectrochim. Acta* 49A **1993,** 1024–1029.
[11] S. P. Jose, S. Mohan, Spectrochim. Acta 64A, **2006,** 240–245.
[12] D. Gandolfo, J. Zarembowitch, *Spectrochim. Acta* 33A, **1977**, 158-164
[13] J.H.S. Green, W. Kynaston, H.M. Paisley, *Spectrochim. Acta* 19, **1963**, 549
[14] D.A. Long, W.O. George, *Spectrochim Acta* 19, **1963**, 1777
[15] A. A. Dahy, S. T. Akriche, M Rzaigui, N. S. Al-Hokbany, N. M. Abd El-Salam, U. Karama, *Journal of Chemistry* **2012**, 9(4), 2191-2204
[16] N. Sundaraganesan, C. Meganathan, M. Kurt; *Journal of Molecular Structure* 891, **2008**, 284-291
[17] M. J. Frisch, et al., Gaussion 03 Program, Gaussian, Inc., Wallingford, CT, **2004**.
[18] A. D. Becke, *J. Chem. Phys*. 98 (**1999**) 5648.
[19] 19. J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, second ed., Gaussian Inc., Pittsburgh, USA, **1996**.

[20] 20. C. Lee, W. Yang, R.G. Parr, *Phys. Rev*. B 37, **1988**, 785‑789.

[21] D. Buckingham, *Adv. Chem. Phys*.,1967, 12,107-142.B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett.* 157, **1989**, 200–206.

[22] A. Domenicano, A. Vaciago, *Acta Crystallogr*. B 35, **1979**, 1382.

[23] A. Domenicano, P. Murray–Rust, C.A. Vaciago, *Acta Crystallogr*. B 39, **1983**.

[24] A. Domenicano, P. Murray–Rust, *Tetrahedron Lett*., **1979**, 2283.

[25] R. I. Deniiington, T. Keith, J. Milliam, K. Eppinnett, W. Hovell, Gauss View Version, **2003**.

[26] I. Nahringbauer, Ake Kvick, *Acta Cryst*. B33, **1977**, 2902.

[27] C. B. Aakeroey, A M Beatty, M Nievwenhuyzen, M. Zou, *J. Mat. Chem*., **1988**, 8, 1385

[28] D. A. Kleinman, *Phys. Rev*. 126, **1962**, 1977.

[29] B. Smith, Infrared spectral interpretation, A Systematic Approach, CRC Press, Washington, DC, **1999**.

[30] N. B. Colthup, L.H. Daly, S.E. Wiberly, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, **1990**.

[31] G. Socrates, Infrared Characteristic Frequencies, Wiley-Interscience Publication, New York, **1990**.

[32] D. A. Long, W.O. George, *Spectrochim. Acta* 19, **1963**, 1777

[33] J. F. Arenas, I. Tocon, J.C. Otero, J.I. Marcos, *J. Mol. Struct*., 1**997**, 443, 410–411

[34] H. F. Hameka, J.O. Jensen, *J. Mol. Struct. (Theochem*.), 362, **1996**, 325.

[35] F. P. Urena, M.F. Gomez, J.J.L. Gonzalez, E.M. Torres, *Spectrochim. Acta A* 59, **2003**, 2815.

[36] G. Varsanyi, S. Szoke, Vibrational Spectra of Benzene Derivatives, Acdemic Press, Budapest, New York, London, **1969**.

[37] H. Ji Singh & P. Srivastava, Indian Journal of Pure & Applied Physics, Vol.47, August **2009**, 557-562.

[38] G. Socrates, Infrared and Raman Characteristic group Frequencies, Tables and Charts, Wiley, Chichester, **2001**.

[39] S. Kalaiselvan, N. Sundaraganesan and B. Dominic Joshua, *Indian. J. Chem*. 47A, 1632- 1641.

[40] C. Brian Smith, Infrared Spectral Interpretation A Systematic Approach, CRC press, USA, **1999**.

[41] B. S. Yadav, Israt Ali, Pradeep Kumar & Preeti Yadav, *Indian Journal of Pure & Applied Physics*, Vol. 45, December **2007**, pp. 979-983.

[42] V. Krishnakumar, N. Jayamani, R. Mathammal, K. Parasuraman, *J. Raman Spectrosc*. 40, **2009**, 1551–1556.

[43] N.B. Colthup, L.H. Daly, S.E. Wiberley, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, **1964**, 226.

[44] G. Socrates, Infrared and Raman Characteristic Group Frequencies – Tables andCharts, 3rd ed., Wiley, New York, **2001**.

[45] I. F. Shishkov, N. I. Sadova, V. P. Novikov, L.V. Vilkov, Zh. Strukt. Khim. 25, **1984**, 98.

[46] K. Raslogi, M. A. Plalfox, R. P. Tanwar, L. Mithal, *Spectrochim. Acta* A58, **2002**, 1989.

[47] M. Pagannone, B. Formari, G. Mattel, *Spectrochim. Acta* 43A, **1986**, 621.

[48] M. Jag, Organic Spectroscopy – Principles and Applications, second edn., Narosa Publishing House, New Delhi, **2001**.

[49] H. Rostkowska, M. J. Nowak, L. Lapinski, M. Bertner, T. Kulikowski, A. Les, L.Adamowicz, *Spectrochim. Acta* 49A, **1993**, 551.

[50] L. J. Bellamy, R. L. Williams, *Spectrochim. Acta* 9, **1957,** 311.

[51] J. C. Evans *Spectromica Acta*, 16, **1960**, 428.

[52] J. M. Seminario, Recent Developments and Applications of Modern Density Functional Theory, vol. 4, Elsevier, **1996**, 800–806.

[53] B. Kosar, C. Albayrak, *Spectrochim. Acta* A 78, **2011**, 160–167.

[54] P. Thul, V.P. Gupta, V.J. Ram, P. Tandon, *Spectrochim. Acta* 75, **2010**, 251–260.

[55] P. Politzer, J.S. Murray, *Theor. Chem. Accts*. 108, **2002,** 134–142.