

Determination of Vibrational Frequencies, Homo-Lumo Energy And IR-Spectra of Nucleobases (Adenine, Cytosine, Guanine, Thymine And Uracil)

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Abstract

Nucleic acid bases are fundamental biological entities, as building blocks of the genetic code. The five nucleic acid bases, cytosine, thymine, uracil, adenine, and guanine, found in DNA and RNA control the replication of DNA, store information required to synthesize proteins, and translate this information to the protein. This paper reports the vibrational frequencies, HOMO-LUMO energy, zero point vibrational energy and IR-spectra of the five nucleobases calculated from FHI-aims Code. Local Density Approximation of the Perdew-Wang, (pw-LDA) and Generalized Gradient Approximation of the Perdew-Burke-Ernzerhof (pbe-GGA) exchange correlations were employed to perform the task. The ultimate goal is to compare the performance of the two exchange correlations; LDA and GGA and to show how they relate to previously reported experimental and theoretical works. Results obtained for vibrational frequencies, HOMO-LUMO energy and zero point vibrational energy were found to be in good agreement with previously reported works. For instance, zero point vibrational energy for guanine in this work were found to be 3.11eV (LDA) and 3.08eV (GGA) while from a previously reported work, it was found to be 3.19eV. The HOMO-LUMO energy gap obtained in cytosine for this work are 3.46eV (LDA) and 3.41eV (GGA) whereas a previously reported work was 3.53eV. Guanine has the largest HOMO-LUMO gap implying that it is the most stable in chemical reactions. This is followed by adenine, uracil, thymine and cytosine being the least stable. The IR-spectra of these molecules were plotted and various frequencies corresponding to the most intense peaks have been identified.

Keywords: Nucleobases, HOMO-LUMO, RNA, DNA and IR-spectra.

1.0 Introduction

Deoxyribonucleic acid (DNA) is a naturally occurring biological macromolecule, containing thousands of nucleic acid bases known as nucleobases, and it is of prime importance in genetic determination [1]. The five nucleic acid bases, cytosine, thymine, uracil, adenine, and guanine, found in DNA and RNA control the replication of DNA, store information required to synthesize proteins, and translate this information to the protein. Nucleic acid bases are fundamental biological entities, as building blocks of the genetic code [1]. Apart from their presence in DNA and RNA nucleosides, the purine bases adenine and guanine, in particular, play a major role as structural constituents of the second messengers cAMP and cGMP, and are often involved in mutations leading to carcinogenesis. In addition, they are the preferred biological targets of platinum-based drugs (such as cisplatin, carboplatin or oxaliplatin), thus mediating the cytotoxic effect of these anticancer agents [2]. Spectroscopic investigations of the nucleic acid (NA) bases contained in non-interacting environments may help clarify the role of these molecules in biological systems. The spectra of the isolated bases, for example, may serve as reference data for the interpretation of results obtained in more complex surroundings. Indeed, gas-phase infrared studies of one class of biological molecules, the metalloporphyrins, have indicated that it may be possible to distinguish between thermal and solvent

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effects on the optical spectra of these molecules [3]. The spectroscopy of the isolated NA bases also maybe used to probe the molecular underpinning of point mutations. It has been proposed [3] that mutations occur when minor tautomers of the NA bases form nonstandard base pairs; if left uncorrected, the mispairs may lead to changes in the genetic code.

Previous investigations in the infrared region include both gas-phase and matrix-phase work. The absorption spectra of gas-phase uracil, methylated uracils, and methylated adenines have been reported in the C=O and NH stretching regions [3]. The infrared spectra of uracil [3] and deuterated uracil [3], thymine [3], and adenine [3] have also been reported in rare gas matrices. As for many polyatomic molecules, the thorough assignment of NA infrared spectra requires an interplay between theoretical predictions and experimental results. Some theoretical treatments of the infrared spectrum of uracil include calculations at the Hartree-Fock level using a 6-31G** basis set [3] as well as calculations based on density functional methods [3]. For thymine, similar predictions of the vibrational spectra have been carried out at the SCF level using 6-31G** [3] and 6-31G(d) [3] basis sets.

The structural, vibrational, electronic, and optical properties of DNA bases have been calculated from first-principles using a DFT-GGA implementation based on ultrasoft pseudopotentials and a plane-wave basis set [4]. The accuracy of the calculated bond lengths, vibrational frequencies, molecule dipoles, and ionization energies is comparable to *ab initio* quantum chemical methods. The results showed weak amino group pyramidalization for adenine, cytosine, and guanine. Pronounced differences between the optical absorption spectra of the DNA bases were observed, and large exciton binding energies between 3 and 4 eV were predicted for the HOMO-LUMO transitions [4]. The equilibrium geometries, APT charges, fundamental vibrational frequencies along with their corresponding intensities in IR spectrum, Raman activities and depolarization ratios of the Raman bands for the neutral and its radical species (G , G^+ , G^-) of the guanine molecule were computed by density functional B3LYP method [5]. The frequency calculations indicated that they were at energy minima. The G^+ species favoured the planar geometrical structure while the neutral G and G^- species is non-planar symmetric structure. Redistribution of the electrons on the G^+ species, the atomic charges of each atom were slightly increased. Both the cationic and anionic radicals of the G molecule were found to be stable. The stretching mode of C=O decreased for the G^- species and to be nearly equal in the G^+ species. For the anionic species of the G molecule, the magnitude of the calculated frequency was nearly same but the IR intensity and Raman activity increased by a large factor.

A semiempirical molecular dynamic for describing the vibrational properties of uracil with the spectra ranging from 126 to 3370 cm^{-1} given by the MD simulations was carried out [6]. These frequencies were assigned to their corresponding eigen modes by using the finite difference harmonic (FDH) method. The calculated frequencies were in good agreement with the experimental measurements. The authors also made up for the loss frequencies which have not been detected in experiments as yet. This was the first time to report the uracil's eigen modes and vibrational frequencies calculated by MD method in a complete way.

The study of vibrational spectra of nucleobases by [7] showed that in most of the cases, the spectra exhibit well resolved vibrational structures, with broad bands associated with very short excited state lifetimes. The similarity between the electronic properties e.g. excitation energy and very short excited state lifetimes for the canonical tautomers of protonated and neutral DNA bases, suggested that the former could also play an important role in the photostability mechanism of DNA.

It is the purpose of this work to perform DFT calculations by employing LDA and GGA exchange correlations to determine vibrational frequencies, zero point vibrational energy, HOMO-LUMO gap and infrared spectra of the five nucleobases : adenine, cytosine, guanine, thymine and uracil and compare. The ultimate goal is to compare the performance of the two exchange correlations; LDA and GGA and to show how they relate to previously reported experimental and theoretical work. Details of the energetics and structures of these molecules can be found in [8].

2.0 Theoretical Background

Density Functional Theory (DFT)

Density Functional Theory (DFT) is a computational method that derives properties of the molecules base on a determination of their electron density [9]. DFT methods have become the most widely-spread *ab-initio* methods in Computational Material Science (CMS) and Solid state Physics, due to their high computational efficiency and very good accuracy for the structure of molecules, crystals, surfaces and their interactions. In DFT methods, the energy of the molecule is a functional of the electron density [10,11]. Further description of DFT can be found in [12-15]

Vibrational Frequency

The vibrational frequencies are calculated with the following equations [16].

$$V_{ij} = \frac{1}{\sqrt{m_i m_j}} \left(\frac{\partial^2 V}{\partial q_i \partial q_j} \right) \tag{1}$$

where

V_{ij} is the Hessian matrix, m_i refers to the mass of atom i , and ∂_{q_i} refers to a displacement of atom i in the x-, y-, or z-direction,

$$VU = \lambda U \tag{2}$$

where U is a matrix of eigenvectors and λ is a vector of eigenvalues, and

$$\lambda_k = (2\pi\nu_k)^2 \quad (3)$$

where λ_k is the k th eigenvalue and ν_k is the k th vibrational frequency.

The infrared intensities can be computed with the equation [16]

$$\frac{\partial E_{SCF}}{\partial f \partial a} = 2 \sum_i^{d.o} h_{ij}^{fa} + 4 \sum_i^{d.o} \sum_j^{all} U_{ji}^a h_{ij}^f \quad (4)$$

where $h_{ij}^{fa} = \sum_{\mu\nu}^{AO} C_{\mu}^{i0} C_{\nu}^{j0} \left(\frac{\partial^2 h_{\mu\nu}}{\partial f \partial a} \right)$ (5)

E_{SCF} is the self-consistent field energy, f is the electric field, a is a nuclear coordinate, $h_{\mu\nu}$ is the one-electron atomic orbital integral, U^a is related to the derivative of the molecular orbital coefficients with respect to a by

$$\frac{\partial C_{\mu}^i}{\partial a} = \sum_m^{all} U_{mi}^a C_{\mu}^{m0} \quad (6)$$

The term “all” in the above summations refers to all occupied and virtual molecular orbitals and .d.o.. refers to doubly occupied orbitals such as those found in the ground state of a closed-shell system. Terms such as C_{μ}^{i0} refers to the coefficients of the atomic orbital m in the i th unperturbed molecular orbital.

3.0 Homo-Lumo Energy

The Highest occupied molecular orbital energy (HOMO) and lowest unoccupied molecular orbital energy (LUMO) are very popular quantum chemical parameters. These orbitals, also called the frontier orbitals, determine the way the molecule interacts with other species [17]. The HOMO is the orbital that could act as an electron donor, since it is the outermost (highest energy) orbital containing electrons. The LUMO is the orbital that could act as the electron acceptor, since it is the innermost (lowest energy) orbital that has room to accept electrons. According to the frontier molecular orbital theory, the formation of a transition state is due to an interaction between the frontier orbitals (HOMO and LUMO) of reactants. The energy of the HOMO is directly related to the ionization potential and the energy of the LUMO is directly related to the electron affinity. The HOMO–LUMO gap, that is the difference in energy between the HOMO and LUMO, is an important stability index. A large HOMO–LUMO gap implies high stability for the molecule in chemical reactions. The concept of “activation hardness” has been also defined on the basis of the HOMO–LUMO energy gap. The qualitative definition of hardness is closely related to the polarizability, since a decrease of the energy gap usually leads to easier polarization of the molecule. The HOMO–LUMO gap is defined as [18]

$$\Delta E = E_{LUMO} - E_{HOMO}, \quad (7)$$

where

ΔE = is the HOMO-LUMO gap energy

E_{HOMO} = is the HOMO energy

E_{LUMO} = is the LUMO energy

3.0 Methodology

FHI-aims Code

The acronym FHI stands for Fritz Haber Institute while *aims* stand for ab initio molecular simulations. The code FHI-aims is developed by the theory department of FHI, Germany. It is an efficient computer program package that is used to calculate physical and chemical properties of condensed matter and materials (such as molecules, clusters, solids, liquids) based only on quantum-mechanical first principles. The primary production method is density functional theory (DFT). The package is also a flexible framework for advanced approaches to calculate ground- and excited-state properties. FHI-aims uses numeric atom-centered orbitals as the quantum-mechanical basis set. This enables accurate all-electron/ full-potential calculations at a computational cost which is competitive with, for instance, plane wave methods, without invoking a priori approximations to the potential (such as pseudopotentials, frozen cores) [19].

FHI-aims requires exactly two input files, located in the same directory where a calculation is started: *control.in* and *geometry.in*. The *geometry.in* file contains all information concerning the atomic structure of the system. This includes the nuclear coordinates, which are specified by the keyword *atom*, followed by cartesian coordinates (in units of Å) and the descriptor of the species. This obviously includes atomic positions, with a description of the particulars of each element (or *species*) expected in *control.in*.

The *control.in* file contains all other settings for the calculation. In particular, it specifies the physical and technical settings for the equations to be solved. The *control.in* contains all necessary computational information regarding the desired run.

Relaxation and Vibrational Runs

The molecular geometry of the five nucleobases with lowest conformational energy were obtained using CONFLEX

VER.7.A.0910 software [20].Open Babel 2.2.1 [21] was used to convert the geometries of the molecules from CONFLEX acceptable format to FHI-aims acceptable format.All the species were initially optimized with MMFF method and then the optimized structures were again relaxed with density functional theory using LDA and GGA exchange functionals. All the parameters were allowed to relax and all the calculations converged to an optimized geometry which corresponds to a true minimum, as revealed by lack of imaginary values in the wavenumber calculations.

Density Functional Theory (DFT) calculations were performed using FHI-aims code for both the relaxation and vibrational analysis of the nucleobases. For the relaxation runs, in the control.in file, tier 1 basis set of light species_ default was used to ensure fast and converge results..This process was repeated for each molecule using LDA(pw-lda) and GGA(pbe) exchange functionals. The final atomic geometry obtained from relaxation calculations were used as initial geometry.in for the vibrational calculations. The control.in used for the vibration was the same as that used for the relaxation except that for the vibration, tier 2 basis set of tight species_defaults was used. The tight settings prescribed denser integration grids than light settings and this lead to more accurate forces. The vibrational analysis was performed by computing the Hessian matrix and the force constants for all normal modes of each nucleobase.

4.0 Results and Discussion

Table 1 shows the values obtained for zero point vibrational energy and HOMO-LUMO gap using both lda and pbe exchange correlations. The results found are in agreement with those reported in [22,23]. Guanine has the largest HOMO-LUMO gap implying that it is the most stable in chemical reactions. This follows by adenine, uracil, thymine and cytosine being the least stable.

Adeninehas39 vibrational modes and it belongs to the symmetry group C_s. Due to the low symmetry, the IR modes are active.

The vibrational frequencies of a single adenine molecule were calculated based on the optimized geometry using using lda and pbe exchange correlations. Table 2shows the vibrational frequencies of adenine compared with those reported in the literature [26]. Cytosine exhibits 33 normal modes. The molecule has a very low symmetry and belongs to the symmetry group C_s. The IR type of vibrations are active.The vibrational frequencies of cytosine were calculated based on the optimized

geometry using lda and pbe exchange correlations.The vibrational frequencies in comparison with those reported by [25] are shown in Table 3. Guaninehas 42 normal modes. The vibrational frequencies of a single guanine molecule were calculated based on the optimized geometry usinglda and pbe exchange correlations.Table 4 shows the vibrational frequencies in comparison to those of [26]. Thymine gives rise to 39 vibrational modes. The molecule belongs to the C_s symmetry group

with the lowest symmetry. Therefore, the vibrational modes are expected to be active. Starting from the ground state an optimized geometry of the thymine molecule and the vibrational frequencies are calculated using lda and pbe exchange correlations. The calculated values are shown in Table 5 in comparison to the calculations reported in[27, 28] . Uracil has 30 normal modes. The vibrational frequencies are calculated using lda and pbe exchange correlations. The calculated values are shown below in Table 6 in comparison to the calculations reported in[29].

Figures 1-10 show the IR-spectra of the five molecules. For adenine in Figures 1 and 2, the most intense peaks were observed at frequencies of about 1651 and 1613 cm⁻¹ respectively. For cytosine in Figures 3 and 4, the most intense peaks were observed at frequencies of about 1776 and 1731 cm⁻¹ respectively while in Figures 5 and 6 for guanine , the most intense peaks were found at frequencies around 1796 and1752 cm⁻¹ respectively. At the most intense peaks, the frequencies of about 1805 and 1706 cm⁻¹ were noted as shown in Figures 7 and 8 respectively for thymine. Similarly for uracil in Figures 9 and 10 the most intense peaks were observed at frequencies of1766 and 1724 cm⁻¹ respectively.

Table 1: Zero Point Vibrational Energy and HOMO-LUMO GAP

Nucleobase	Exchange corr.	Zero point Vibrational Energy (eV)		HOMO-LUMO GAP (eV)	
		This work	Ref.[22]	This work	Ref.[23]
Adenine	LDA	2.98	3.06	3.90	3.81
	PBE	2.96		3.87	
Cytosine	LDA	2.60	2.69	3.46	3.52
	PBE	2.59		3.41	
Guanine	LDA	3.11	3.19	3.98	3.83
	PBE	3.08		3.93	
Thymine	LDA	3.04	3.82	3.74
	PBE	3.03		3.82	
Uracil	LDA	2.31	3.84
	PBE	2.30		3.86	

Table 2: Calculated Vibrational Frequencies (in cm⁻¹) of Adenine

mode	PW-LDA This work	PBE This work	Ref. [24]	Ref. [24]	mode	PW-LDA This work	PBE This work	Ref. [24]	Ref. [24]
1	122.6	155.4	138.4	144.4	21	1057.1	1049.4	1091.5	1058.1
2	160.1	204.8	167.2	162.3	22	1132.8	1111.4	1152.6	1118.2
3	217.2	264.2	219.8	220.5	23	1222.5	1212.0	1251.9	1214.7
4	258.5	277.2	273.5	265.5	24	1246.7	1227.9	1277.0	1246.5
5	293.3	288.7	303.0	288.7	25	1321.2	1301.3	1345.4	1312.5
6	505.0	485.3	514.4	501.1	26	1357.6	1322.2	1371.9	1330.7
7	519.4	497.8	519.4	506.8	27	1370.2	1336.2	1380.4	1348.7
8	520.1	513.6	531.0	517.2	28	1403.0	1372.4	1432.7	1383.7
9	547.9	520.8	548.5	525.2	29	1423.1	1391.6	1448.4	1401.0
10	569.0	559.0	578.6	562.2	30	1473.4	1455.7	1523.0	1465.0
11	607.8	600.6	618.1	599.1	31	1488.8	1466.3	1534.3	1482.0
12	660.1	648.3	671.1	656.8	32	1555.6	1556.3	1625.7	1563.1
13	671.4	658.9	687.5	665.2	33	1625.3	1584.3	1650.1	1592.3
14	724.0	707.8	727.8	710.7	34	1651.9	1613.2	1681.4	1620.5
15	791.5	778.0	809.1	786.3	35	3076.3	3097.8	3188.8	3144.4
16	817.4	805.5	842.8	870.6	36	3163.0	3184.0	3266.4	3226.3
17	881.1	869.6	900.8	875.7	37	3513.9	3528.8	3615.9	3532.3
18	929.0	915.4	944.4	920.5	38	3549.8	3573.0	3651.1	3569.5
19	931.0	927.2	973.2	924.8	39	3652.1	3662.8	3743.5	3673.0
20	980.0	990.4	1014.8	983.5					

Table 3: Calculated Vibrational Frequencies (in cm⁻¹) of Cytosine

mode	PW-LDA This work	PBE This work	Ref. [25]	mode	PW-LDA This work	PBE This work	Ref. [25]
1	120.8	118.4	124	19	1061.8	1064.1	1031
2	190.4	187.1	192	20	1132.2	1105.6	1165
3	294.8	317.5	289	21	1275.7	1271.1	1199
4	332.2	331.3	332	22	1328.2	1330.0	1297
5	383.1	424.7	361	23	1390.2	1377.3	1370
6	428.0	477.2	420	24	1487.1	1456.7	1419
7	503.1	499.9	496	25	1562.7	1561.2	1564
8	530.1	525.2	506	26	1614.7	1598.0	1609
9	587.4	574.7	526	27	1641.0	1621.0	1733
10	603.6	584.7	571	28	1775.8	1730.6	1825
11	681.7	678.5	675	29	3034.6	3057.2	2646
12	727.9	723.3	725	30	3149.1	3166.3	2713
13	778.2	757.4	739	31	3476.3	3503.1	2814
14	790.9	773.7	768	32	3512.8	3513.9	3286
15	917.2	894.5	838	33	3630.0	3626.6	3316
16	950.6	952.7	920				
17	1008.5	997.4	938				
18	1049.1	1043.0	982				

Table 4: Calculated Vibrational Frequencies (in cm⁻¹) of Guanine

mode	PW-LDA This work	PBE This work	Ref. [26]
1	134.3	132.5	136
2	152.3	148.2	156
3	195.0	193.2	196
4	310.9	308.9	318
5	322.5	320.9	328
6	328.3	325.5	335
7	353.6	346.1	356
8	479.7	473.6	488
9	514.2	495.1	526
10	520.1	508.8	534
11	532.4	569.2	544
12	584.8	575.4	594
13	623.4	610.3	624
14	650.3	641.8	660
15	653.9	646.9	668
16	689.3	673.8	696
17	720.3	709.3	734
18	768.1	751.8	777
19	792.5	782.1	819
20	825.6	811.2	835
21	929.2	916.6	948

mode	PW-LDA This work	PBE This work	Ref. [26]
22	1022.0	1012.3	1044
23	1044.7	1033.9	1064
24	1061.7	1040.2	1069
25	1124.5	1110.2	1136
26	1153.5	1135.5	1169
27	1269.7	1263.2	1304
28	1298.0	1292.0	1332
29	1354.0	1325.7	1355
30	1376.3	1340.3	1382
31	1432.2	1396.8	1434
32	1495.3	1463.1	1508
33	1526.6	1509.7	1554
34	1564.5	1555.5	1603
35	1598.9	1565.2	1614
36	1635.2	1608.9	1661
37	1795.6	1752.4	1792
38	3165.2	3189.3	3242
39	3479.0	3500.3	3577
40	3499.1	3508.8	3589
41	3545.6	3566.3	3645
42	3616.8	3612.2	3686

Table 5: Calculated Vibrational Frequencies (in cm⁻¹) of Thymine

mode	PW-LDA This work	PBE This work	Ref.[27]	Ref. [28]
1	110.5	107.0	78	106
2	123.8	131.3	114	133
3	150.3	141.2	172	147
4	267.6	270.5	276	262
5	294.4	289.7	456	284
6	378.2	373.3	588	373
7	390.2	381.3	801	380
8	453.9	448.4	910	443
9	534.8	527.3	903	526
10	555.0	539.1	660	542
11	591.8	586.8	705	581
12	664.2	656.6	306	654
13	740.0	719.4	368	713
14	740.6	719.8	455	716
15	761.4	743.9	542	734
16	795.4	781.6	584	776
17	857.9	866.5	715	872
18	939.4	934.0	719	935
19	985.9	990.4	856	982
20	1015.7	1026.2	903	1021

mode	PW-LDA This work	PBE This work	Ref.[27]	Ref. [28]
21	1141.9	1112.5	1099	1122
22	1170.8	1158.4	1143	1166
23	1233.8	1198.8	1269	1201
24	1321.6	1320.9	1369	1325
25	1343.7	1351.3	1302	1351
26	1352.9	1372.0	1385	1366
27	1384.2	1376.5	1386	1380
28	1400.7	1419.4	1413	1412
29	1414.7	1440.7	1540	1433
30	1472.6	1452.3	1611	1454
31	1680.8	1647.3	1835	1650
32	1750.9	1705.9	1679	1712
33	1805.4	1761.1	1741	1756
34	2965.6	2983.2	2827	2938
35	3032.7	3041.6	2940	3005
36	3069.5	3072.8	2943	3026
37	3114.9	3136.8	2954	3098
38	3490.8	3520.1	3037	3491
39	3540.5	3568.7	3310	3532

Table 6: Calculated Vibrational Frequencies (in cm^{-1}) of Uracil

mode	PW-LDA This work	PBE Thiswork	REF [29]
1	143.1	134.8	150
2	166.1	160.5	170
3	376.1	371.4	385
4	387.3	377.9	396
5	509.8	505.4	519
6	529.9	523.3	541
7	547.4	539.6	558
8	560.5	541.0	563
9	669.3	655.0	687
10	707.0	704.3	729
11	747.9	723.6	752
12	769.5	750.1	772
13	794.0	786.5	813
14	925.1	924.6	965
15	947.5	933.0	970

mode	PW-LDA This work	PBE Thiswork	REF [29]
16	976.9	963.6	990
17	1063.5	1056.5	1091
18	1164.3	1147.3	1198
19	1205.0	1189.1	1231
20	1325.5	1331.0	1382
21	1362.5	1354.5	1407
22	1387.6	1374.3	1422
23	1472.0	1452.6	1506
24	1653.7	1625.9	1690
25	1765.9	1723.2	1808
26	1808.5	1763.5	1845
27	3127.4	3147.0	3221
28	3177.6	3198.0	3264
29	3490.1	3517.5	3620
30	3538.7	3567.4	3658

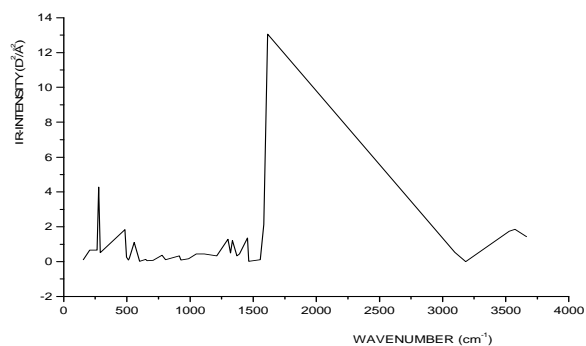


Fig. 1 IR-Spectrum for Adeninine (LDA)

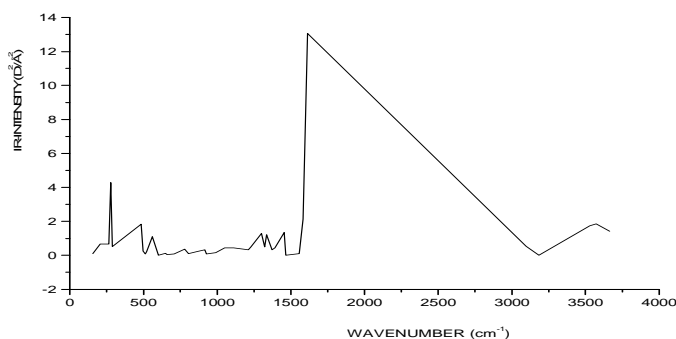


Fig. 2 IR-Spectrum for Adeninine (GGA-PBE)

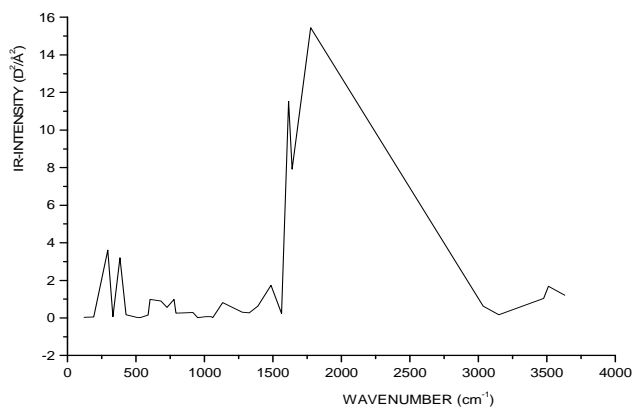


Fig. 3 IR-Spectrum for Cytosine (LDA)

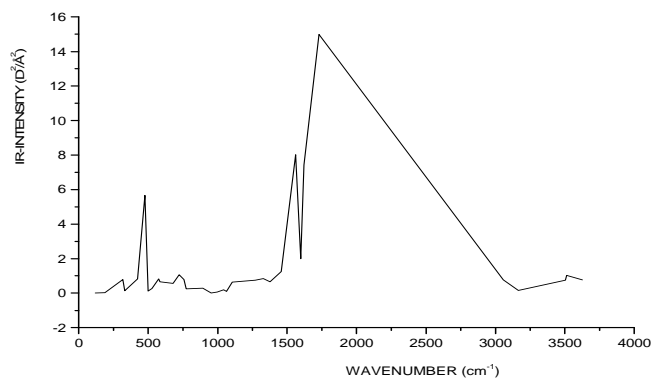


Fig. 4 IR-Spectrum for Cytosine (GGA-PBE)

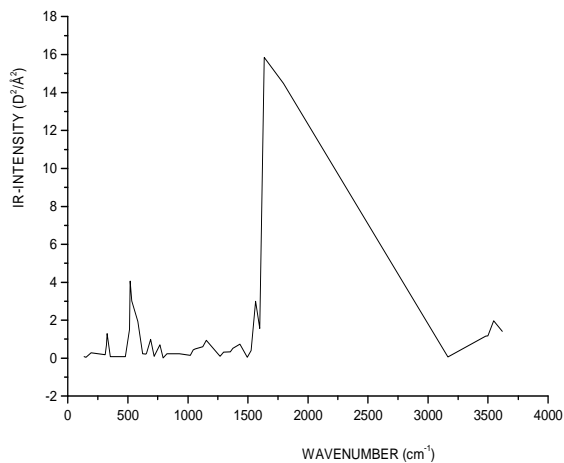


Fig. 5 IR-Spectrum for Guanine (LDA)

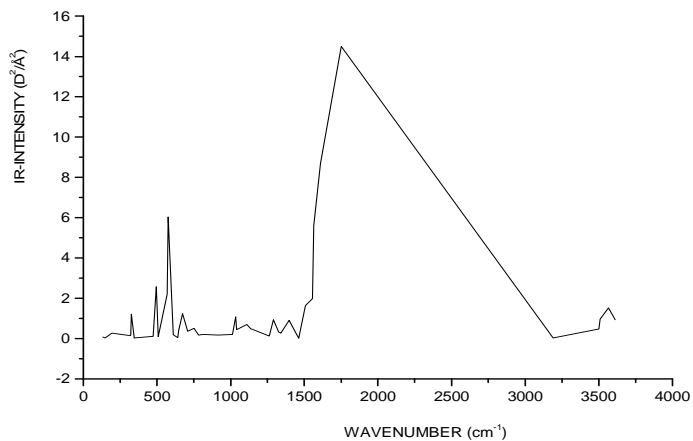


Fig. 6 IR-Spectrum for Guanine (GGA-PBE)

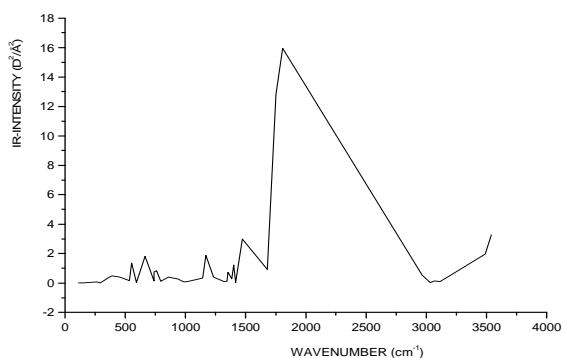


Fig. 7 IR-Spectrum for Thymine (LDA)

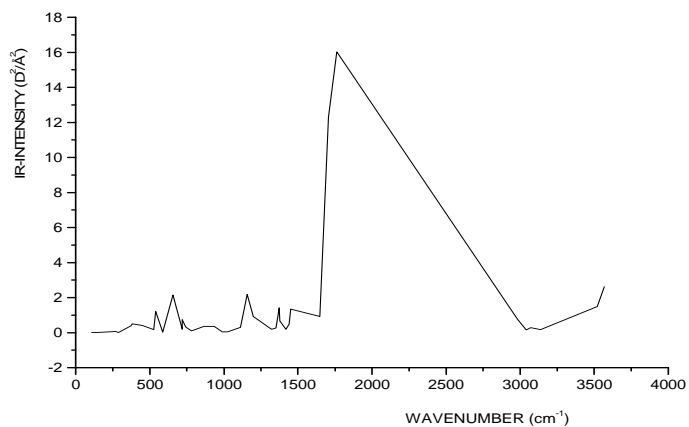


Fig. 8 IR-Spectrum for Thymine (GGA-PBE)

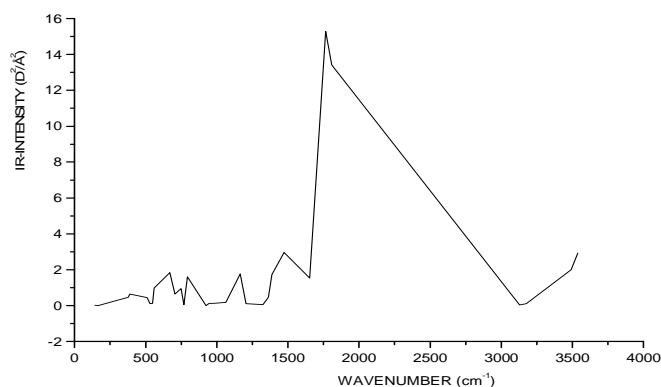


Fig. 9 IR-Spectrum for Uracil (LDA)

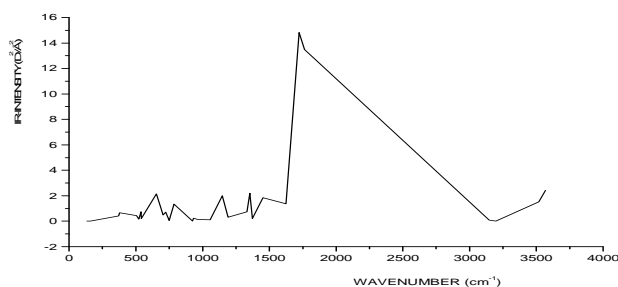


Fig. 10 IR-Spectrum for Uracil (GGA-PBE)

4.0 Conclusion

In the present work, vibrational frequencies, infrared spectra, zero point vibrational energy and HOMO-LUMO gap of the five nucleobases: adenine, cytosine, guanine, thymine and uracil were calculated in the light of DFT calculations employing both LDA and GGA exchange correlations. The performance of the two exchange correlations; GGA and LDA have been reported and compared with previously reported works. The results obtained have found to be in agreement with some previously reported works. The vibrational bands of the isolated molecules may be used as marker bands for studies carried out in interacting environments. In particular, the lower frequency bands, corresponding to the ring torsions and functional group wags, may be suitable for identifying the NA bases in more complex systems. Guanine has the largest HOMO-LUMO gap implying that it is the most stable in chemical reactions. This is followed by adenine, uracil, thymine and cytosine being the least stable.

5.0 References

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