



Original Research Article

A computational study of thermophysical, HOMO, LUMO, vibrational spectrum and UV-visible spectrum of cannabicyclol (CBL), and cannabigerol (CBG) using DFT

Md Nuruzzaman Sarker^a , Ajoy Kumer^{b*} , Mohammad Jahidul Islam^a , Sunanda Paul^c

^a Department of Physics, European University of Bangladesh, Dhaka-1216, Bangladesh

^b Department of Chemistry, European University of Bangladesh, Dhaka-1216, Bangladesh

^c Department of Biochemistry and Molecular Biology, University of Chittagong, Chittagong, Hathazari-4334, Bangladesh

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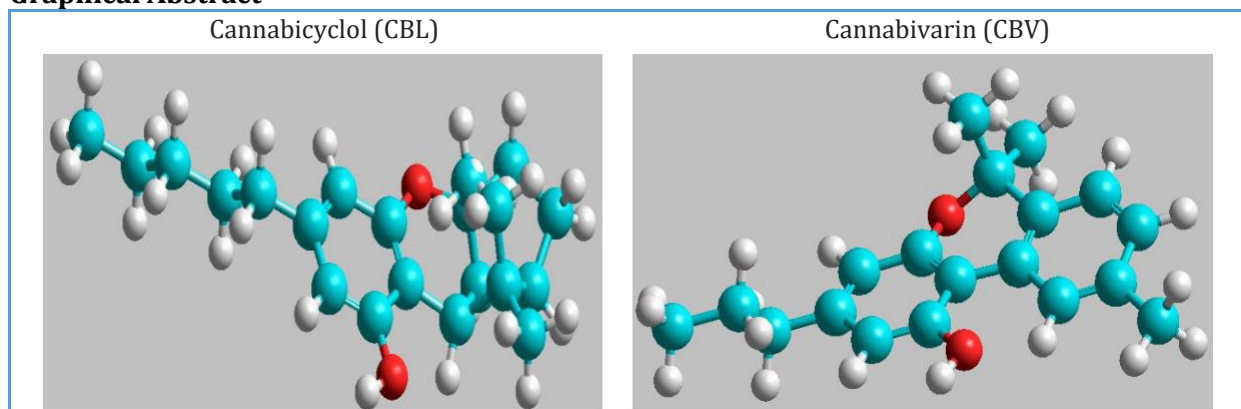
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ABSTRACT

Cannabicyclol, also called CBL, is one of the least known and studied isomer of cannabinoids in the cannabis plant, and it is the precursor of the different cannabinoids found in marijuana plant having with widespread medicinal use. In this work, the thermophysical properties of CBL such as, free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, and heat of formation were estimated using density functional theory for developing use as pharmaceutical pursues. In addition, the chemical reactivity properties including highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), HOMO-LUMO gap, ionization potential, electronegativity, hardness, softness, and electron affinity were evaluated. It was found that, the magnitude of HOMO was -8.98 and -8.53, LUMO was 0.19, -0.31 and HOMO -LUMO gap was -9.17 and -8.22 eV of CBL and CBG, respectively. The vibrational spectrum and electronics spectrum were simulated for identification and characterization. These studies provided a proper and predictable data for further use in any chemical and pharmaceutical purpose.

Graphical Abstract



Introduction

Cannabis sativa is the world's most recognizable plant for some medical useable chemicals. There are two types of cannabis plants of flowers, male or female. Male flowers grow in stretched out clusters along the leaves and turn yellow and die after blossoming. Female flowers grow in spike-like clusters and remain dark green for a month after blossoming, until the seed ripens [1]. Marijuana refers to absorbed leaf, flowers, stalks, and seeds from *cannabis sativa* or *cannabis indica* plant [2, 3]. The plant contains the mind-altering chemical THC and other similar compounds [4]. Tetrahydrocannabinol (THC), and Cannabinoids (CBD) are the main psychoactive chemical in marijuana and other drugs. Some people may smoke marijuana in hand-rolled cigarettes (joints) or in pipes or water pipes (bongs) [5]. The THCs can supply very large amount of tea to the body, and their use has sent some people to the emergency room. Another danger is to prepare this exhaust, which usually involves the boutine (light fluid). Many people burn in the fire and they are severely burned using a booting for tea at home.

Marijuana over activates parts of the brain that contain the highest number of these receptors. This causes the "high" that people

feel. Other effects include altered senses, altered sense of time, changes in mood, impaired body movement, difficulty with thinking and problem-solving, impaired memory, hallucinations (when taken in high doses), delusions (when taken in high doses), psychosis (when taken in high doses) [6, 7].

Cannabis has a psychoactive and physical effect when someone accepts it more than a limited dose [8]. Consumption of immediate effects from eating cancer includes entertainment, increased Cummins, body pictures, hearing, visual illusion, and ataxia. Recently, more than 100 natural species of cannabis have been detected from the cannabis sativa plant, which are active in the two-most active pharmacology in the region. Some immediate unexpected side effects include reduction in short-term memory, dry mouth, impaired motor skills and eye reddening [9]. In addition to a personal change between perception and mood, increased heart rate among the most common short-term physical and nervous effects, hunger and food costs, reducing blood pressure, short-term and memory loss of work cannabis impeded the ability of driving a person.

CBG cannabis strains are used therapeutically as an antidepressant, and as a functioning painkiller, killer to bacterial growth, reduce inflammation, inhibit cell

growth in tumour and cancer cells, promote bone growth, and low-affinity antagonist. It is also beneficial for the treatment of psoriasis, glaucoma, multiple sclerosis and skin diseases. On the other hand, the similar cannabis is CBL in basis of structure which is famous for the use of poisonous effect. If anybody takes the dose of 8mg per kilo of bodyweight, very few minute he/she is death. The main limitation of CBG, CBL has no vast research. In our study, a theoretical investigation was estimated for physiochemical and chemical reactivity using DFT of computational overview. This theoretical investigation of physical, chemical, thermochemical and HOMO, LUMO profile was established using computational tools. To estimate the chemical reactivity, the electrophilicity (ω), the chemical potential (μ), electronegativity (χ), hardness (η) and softness (S) be put into a molecular orbital's framework parameter were calculated and compared our previous work [10–13]. It was found for simulating of different organic acid, ionic liquids, cannabis and other molecule from A. Kumer et al., that the HOMO LUMO gap is about 2.0 to 5.0 eV and has a temperature activity on entropy and heat capacity [14–17] which is use full theoretical parameter for further any uses in both of chemical industries and pharmaceutical industries [14, 18–20]. In this work, using DFT method, we calculate the electrophilicity (ω), the chemical potential (μ), electronegativity (χ), hardness (η) and softness (S) be put into a molecular orbital's framework, thermophysical and spectroscopy study.

The HOMO and LUMO energies are used for the determination of global reactivity descriptors. It is important that electrophilicity (ω), the chemical potential (μ), electronegativity (χ), hardness (η) and softness (S) be put into a molecular orbital's framework. We focus on the HOMO and LUMO

energies in order to determine the interesting molecular properties and chemical quantities are calculated as the following equation

$$\omega = \frac{I - A}{2} \quad (1)$$

$$\mu = \frac{I + A}{2} \quad (2)$$

$$\chi = \frac{I + A}{2} \quad (3)$$

$$\eta = \frac{I - A}{2} \quad (4)$$

$$S = \frac{1}{\eta} \quad (5)$$

Materials and methods

Computing methods for simulation

The molecular modeling program permits to build and analyze different molecular structures and determine the molecular, electronic, and biological properties. To create the spatial chemical structure of each calculated molecule, the two-dimensional structure of the molecule shall be built step-by-step by drawing. Then hydrogen atoms are automatically added from building option and chemical structure is converted into a 3D structure. The first step in getting the main characteristic parameters of molecules is to optimize the molecular structure to obtain a configuration characterized by minimum free energy. In sitting the DFT was fixed via 6G-31G*, and B3-LYP [21]. After completing optimization, the theoretical properties of the studied compound such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat of formation, the HOMO, LUMO are recorded. The QSAR properties of molecules like charge density, surface area grid, volume, LogP, polarizability, refractivity, molecular mass, were calculated. Using the computing in vibrational optimization, the UV-visible spectroscopy and IR spectroscopy were determined.

Result and discussion

Optimized structure

The optimized molecular structure provides some information about the molecular properties including, bond length,

bond angle, partial charge, and bond torsion. In Figure 1, the molecular orbital diagrams are presented having both of molecular symmetry and asymmetry properties. In the Figure 1, red color is oxygen atom, white color is hydrogen, and cyan is carbon.

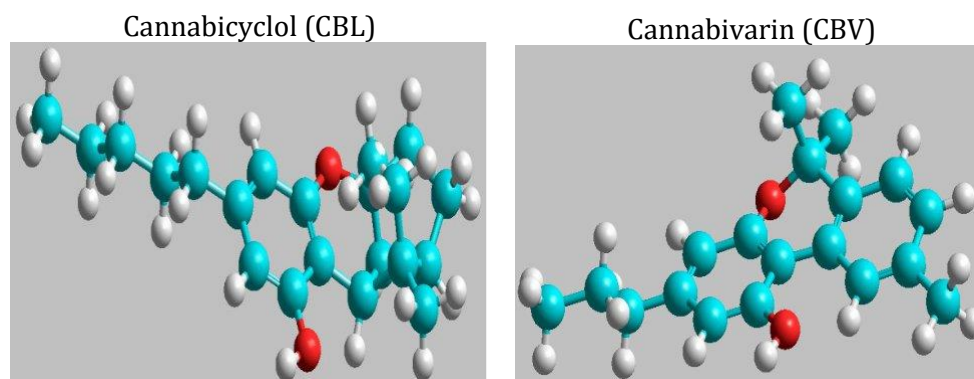


Figure 1. Optimized structure in the cylinder shape

Thermophysical and thermo-dynamical properties

The binding free energy of the optimized molecules is calculated by performing molecular simulation by DFT method. The molecule with minimum binding energy will have the maximum binding affinity and higher biological active. According to this more negative value, we can consider a more effective drug. In this case CBV is less biological active than CBL.

The bond dipole moment is the idea of an electric dipole moment to measure the polarity of a chemical bond within a molecule. In view of pharmaceutical industries, the dipole moment was a parameter for the drug by which a drug is to be used open or close packet. If any drug has a dipole moment, it can be able to absorb the ultraviolet light and have a possibility of properties. From Table 1, it was found that CBL, and CBL have 1.34 and 1.25 D.

Table 1. Thermophysical properties

Properties	CBL	CBV
Total energy, (kcal/mol)	-81584.1	-73293.88
Free energy, (kcal/mol)	-81584.1	-73293.88
Dipole moment, (D)	1.34	1.25
RMS gradient, (kcal/mol)	0.09	0.01
Binding energy, (kcal/mol)	-5328.21	-4579.94
Heat of formation, (kcal/mol)	-57.34	-67.67
Electronic energy, (kcal/mol)	-697039.42	-561522.88
Nuclear energy, (kcal/mol)	615455.31	488228.99

Temperature effect on entropy and heat capacity

In case of thermo chemistry, the entropy and heat capacity are the key factor for

determining the reaction environment. In case of drug design, entropy, which Sharp focuses on in a biomedical system, obliges the direction of all chemical reactions towards disorder. Therefore, it is this phenomenon that determines how tightly a drug binds to its target protein or molecules. When a drug binds to its target, its entropy decreases, so disorder must increase somewhere else in the cell, usually in the abundant water molecules found

in a cell, sharp suggests. That increase in disorder can be detected as heat flowing into the water surrounding the drug-target bond. Here, it is found that temperature has activity in any single system for bioactive molecule. From the Table 2, we can see that with increasing the temperature of any molecular system, the entropy and heat capacity well poorly increased means that disorder decreases.

Table 2. Data for entropy and heat capacity

	273 K		298 K		323 K	
	Entropy	Heat capacity, (kcal/mol-deg)	Entropy	Heat capacity, (kcal/mol-deg)	Entropy	Heat capacity, (kcal/mol-deg)
CBL	0.14	0.07	0.15	0.08	0.16	0.09
CBV	0.13	0.07	0.14	0.08	0.15	0.09

Chemical reactivity parameters

HOMO LUMO in different levels

The terms of HOMO and LUMO are also considered as *frontier orbitals* on basis of frontier molecular orbital theory. The energy levels of the molecular orbitals order

HOMO and LUMO give information on the possible electronic transition, chemical stability, and chemical strength. The HOMO and LUMO also indicate the electrophilic and nucleophilic attraction region in molecule. In Table 3, includes the magnitude of HOMO, LUMO in different levels.

Table 3. Data for HOMO LUMO

	CBL	CBV
HOMO(0), eV	-8.98	-8.53
HOMO(-1), eV	0.19	-0.31
LUMO, (0), eV	0.19	-0.31
LUMO, (-1), eV	-8.98	-8.53

HOMO, and LUMO picture in zero level

In the molecular orbital diagram, it is found that where region is to be attracted the nucleophilic or electrophilic reagent. From the Figure 2, the blue color mentions the negative charge region where only

nucleophilic can be attracted. On the other hand, green color indicates the positive charge area where the electrophilic groups are attached. In CBL is less reactive in both of the nucleophilic or electrophilic reaction than CBV.

CBL

CBV

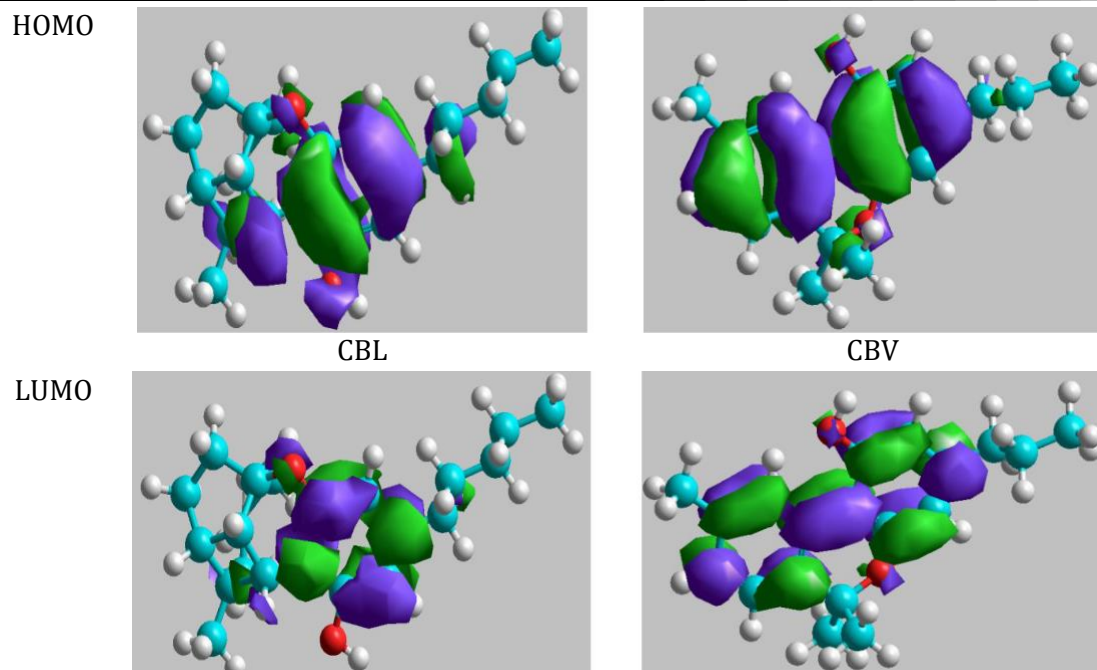


Figure 2. The frontier orbitals: a) HOMO and b) LUMO

HOMO LUMO gap, ionization potential, and electron affinity

The LUMO-HOMO gap is the most important parameter for the chemical reactivity. A LUMO-HOMO gap is considered as the high reactivity, as given Table 3. A. Kumer et. al. (2019) published some series of papers where the HOMO, LUMO gap was almost 8.0 to

11.0 eV and In CBL and CBV have -9.17 and -8.22 eV LUMO –HOMO gap. The energy gap is used to determine the molecular electrical transport properties. In addition, according to Koopmans' theorem, the energy gap, E_{gap} , defined as the difference between HOMO and LUMO energy [22].

$$E_{gap} = (E_{LUMO} - E_{HOMO}) \approx IP - EA$$

$$-- \quad (6)$$

$$-- \quad (7)$$

The ionization potential (I) and electron affinity (A) can be estimated from the HOMO and LUMO energy values as following and magnitude is listed in Table 4.

Table 4. Data for LUMO- HOMO gap (ΔE), IP, and EA

	CBL	CBV
HOMO, LUMO gap, eV	-9.17	-8.22
Ionization potential (I), eV	8.98	8.53
Electron affinity (A), eV	-0.19	0.31

Chemical potential, electronegativity, hardness, and softness

Chemical potential of the species is such that the particles given can be absorbed or released due to the change in the number of

particles. According to electrochemistry, ions, molecule or species do not always have a tendency to go from higher to lower chemical potential, but they do always go from higher to lower electrochemical potential. The electrochemical potential completely characterizes all of the influences on an ion's motion, while the chemical potential includes everything except the electric force. On the other hand, the electronegativity is a measure of how strongly an atom attracts the electrons in a bond which is completely equal and

opposite to the chemical potential. An atom with high electronegativity attracts electrons strongly, while an atom with low electronegativity attracts them weakly. Electronegativity values are used to predict how different atoms will behave when bonded to each other, making this an important skill in basic chemistry. The electronegativity of CBL and CBV was found from Table 5 about -4.39 eV and -4.42 eV and chemical potential is 4.39 eV and 4.42 eV respectively.

Table 5. Chemical reactivity and chemical kinetics

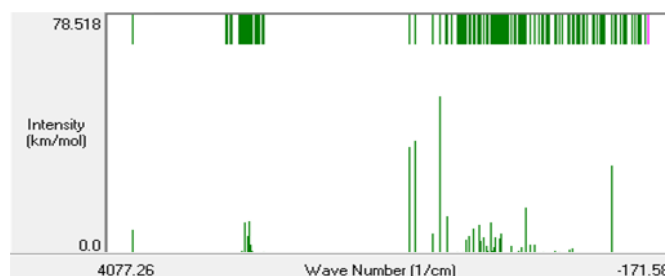
	CBL	CBV
Hardness, (η)	4.58	4.11
Softness (S)	0.21	0.24
Electrophilicity (ω)	2.10	2.20
Chemical potential (μ)	-4.39	-4.42
Electronegativity, (χ)	4.39	4.42

Vibrational spectra for FT-IR

The existence of the functional groups in the organic molecule can be identified through the vibrational spectroscopy in the principle. In the cannabis, a strong peak in 3400-3500

cm^{-1} is considered for the presence of OH group. In the other hand, the 2500-2200 cm^{-1} spectrum for C-H in benzene ring is identified which is given in Figure 3 and Table 6 included the data for optimized condition to calculate vibrational spectrum.

CBL



CBV

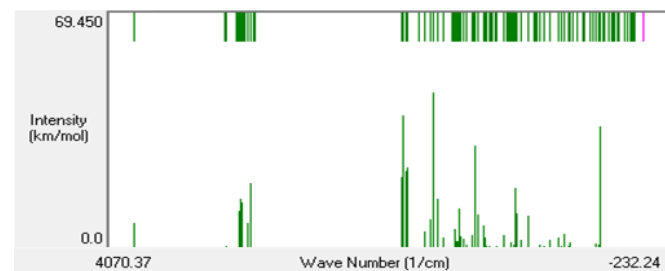


Figure 3. Vibrational spectrum for IR

Table 6. Data for optimized condition to calculate vibrational spectrum

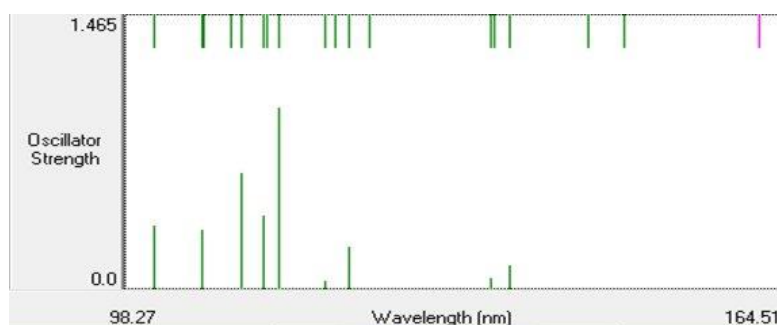
	Normal Mode	Degeneracy	Frequency	Intensity	Symmetry
CBL	1	1	21.55	0.043	1 A
CBV	1	1	-36.66	0.062	1 A

UV spectrum

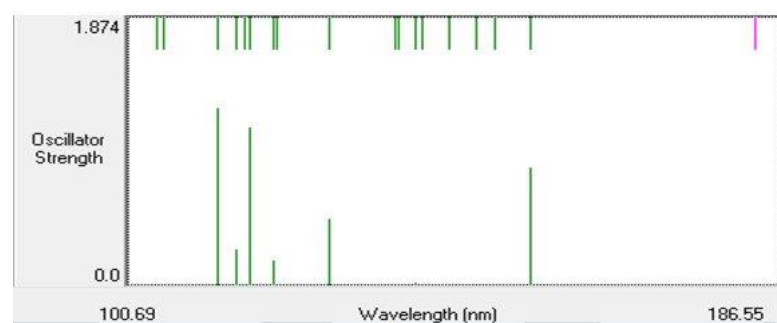
UV visible spectroscopy combines the angular concentration located inside an organic resin or compounds. In the case of cannabis, the conjugation of UV visible spectroscopy with their opposite conjugation,

vibration level conjugation and oxygen-based lone pair of electrons is determined by those of spectrum found in 120-30 nm as a broad peak shown in Figure 4 and Table 7 included the data for optimized condition to calculate electronics spectrum.

CBL



CBV

**Figure 4.** Vibrational spectrum for UV**Table 7.** Data for optimized condition to calculate electronic spectrum

	Transition	Degeneracy	Spin Multiplicity	Wavelength	Oscillator Strength
CBL	1	1	Triplet	161.49	0.0
CBV	1	1	Triplet	182.65	0.0

Conclusion

In this research study, it was found that, it is possible to see a change in the physical properties of cannabis molecules. However, the heat capacity and entropy may vary as

temperature is changed. The chemical reactivity was calculated using HOMO, LUMO. The best finding of this work in term of thermochemical and thermophysical and chemical reactivity in views of following properties such as

electrophilicity (ω), the chemical potential (μ), electronegativity (χ), hardness (η) and softness (S) are almost similar in the tested molecules.

Disclosure statement

No potential conflict of interest was reported by the authors.

Orcid

Md Nuruzzaman Sarker  0000-0003-2760-0113

Ajoy Kumer  0000-0001-5136-6166

Mohammad Jahidul Islam  0000-0002-4125-8222

Sunanda Paul  0000-0001-7739-4018

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