Study of the Electronic and Spectrum Properties for a Medication Hydroxychloroquine

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Study of the Electronic and Spectrum Properties for a Medication Hydroxychloroquine

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Abstract. Calculated the electronics and vibrational properties of the medicine hydroxy-chloroquine nanoparticles based on the fitting of their UV−vis spectra, transmittable, IR, Raman spectrum, Electronic circular dichroism (ECD) and HOMO and LUMO, These properties were theoretically studied using Gaussian 09 program. The result shows the stability of hydroxy-chloroquine. The longer wavelength that (500 nm) means high absorbance and less energy. Transmittable, the highest transmittable value in the region is (0 - 3000cm^{-1}) and (2600 -1250 cm^{-1}) is offset by the lowest absorption here, the sample has good transparency characteristics at this region. Infrared spectrum, the area (2900 cm^{-1}) it is for the carbon and hydrogen Single bond C-H, and hybridization type sp3. Raman scattering, electronic effect on bond C-H in the area (2800 cm^{-1}) is very large and this bond type stretch. Electronic circular dichroism (ECD), when finding the sign of one or more bands can be an AC limitation. A positive skew angle is foretelling to become connected CD of the low-lying p–p* move at about 600 nm; certainly, for a negative CD, can find a negative angle is expected.

Keywords: Hydroxychloroquine, density functional theory, Lee-Yang–Parr, COVID-19.

1. Introduction

At the end of December, In China, in the city of Wuhan, some people were found infected with cases of pneumonia of unknown cause, and that this disease is related to the virus, which was called the 2019 virus (COVID -19) or the new coronavirus [1]. COVID-19 includes four genera: the alpha, beta, gamma, and delta, is RNA virus, [2]. Coronavirus is rapidly spreading worldwide in the current situation. The speed transmission of Coronavirus within the community can cause epidemics [3]. After the disease spread too many countries, some medications were taken to treat it Hydroxychloroquine. The brand name for Hydroxychloroquine is Plaquenil, and this medication is used to prevent malaria and can also be used to treat arthritis. It can be obtained by prescription only [4-5]. To minimize any possible side effects for Hydroxychloroquine While taking hydroxychloroquine you should see your doctor regularly to make sure the treatment is working [6]. However, in some people, hydroxychloroquine can cause: feeling sick (nausea), headaches [7]. Mild hair loss, ringing in the ears (tinnitus), blurred vision. The experimental treatment has been studied for coronavirus [8]. In this study, we will study some of the electronic and vibrational properties of the medicine hydroxychloroquine nanoparticles using the Gaussian program.

2. Theory

In the long term (after 2020), and with the development of nanotechnology, greatly helped in the development of nanomedicine. Specialists in nanoscale molecular parts focus on nanotechnology as the gears, bearings, and ratchets. Each nanoparticle can contain a few thousand neatly positioned atoms. These nano-mechanical parts will then be assembled into bigger working machines like nanosensors, and nanocomputers, nanoprocessors, and nanopumps. Nanomedicine has made clinicians

able to treat most diseases that kill people today, and quickly fix the most physical disease [9]. In this paper can be used Existing computer programs and methodologies have been used to solve some specific issues in chemistry within the framework of computational chemistry. To obtain the physical and chemical properties of molecules, solids and liquids this is done by practicing computer calculations [10]. The geometrically optimized hydroxychloroquine with the chemical formula (C18H26ClN3O), using density functional theory (DFT) with the Becke-3parameter exchange and the Lee-Yang–Parr correlation functional (B3LYP) /6-31g (d, P) basis set which included polarization functions. This was created using Gaussian 09 programs auxiliary by Gaussian view 6.0. Fig. (1) Shows the geometrically optimized structure of hydroxychloroquine.

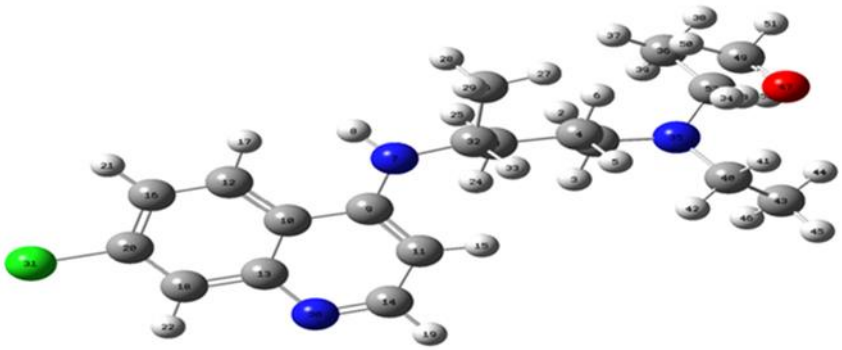

Figure 1. Shows the geometrically optimized of structure hydroxychloroquine.

3. Result and discussion

(Fig. 2) shows UV- visible to hydroxychloroquine between epsilon means constant (ε) called malar absorptivity and wavelength. To determine the concentrations of materials, a UV-visible spectroscopy technique is used, scientists were able to study reaction rates, and determine rate equations for interactions, and this technique is widely used in teaching and research institutes and in quantitative analysis of all molecules that absorb ultraviolet and visible electromagnetic radiation. The UV area ranged from 190 to 400 nm and the visible area was from 400 to 800 nm. This technicality can be used both quantitatively and qualitatively [11]. This fig. shows a longer wavelength that (500nm) means high absorbency and less energy. However, if it is extended further, the absorbed wavelength will eventually be long enough to be in the visible region of the spectrum [12].

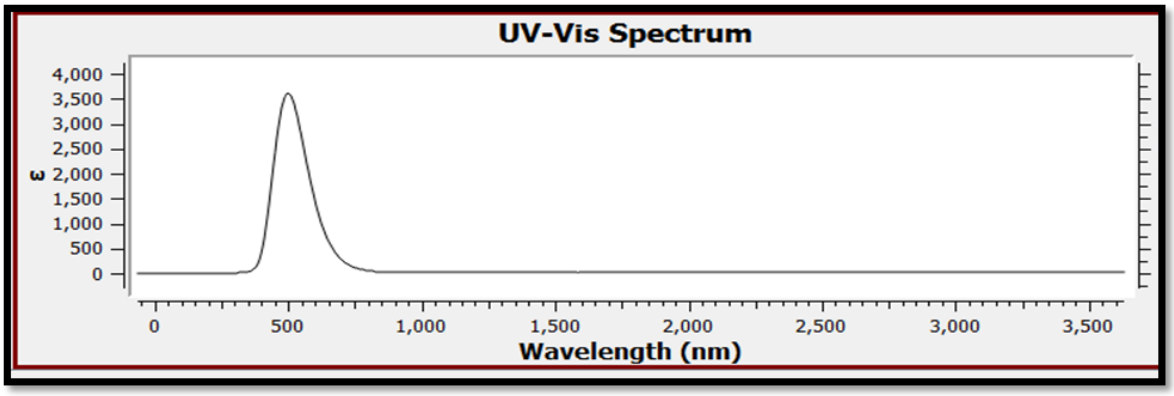

Figure 2. Ultraviolet–visible spectrum of hydroxychloroquine.

3.1. Transmittance

The transmittance (T) is the rate of the light power (I^0) falling on a body to that transmitted through it (I) [13].

$$T = \frac{I^{\circ}}{I} \ldots\ldots (1)$$

To calculate the percentage of transmittance (% T), the number is multiplied by 100, which is the rate of light transmitted in the material to the amount of light in the vacuum

$$\%T = \frac{I^{\circ}}{I} * 100 \ldots\ldots (2)$$

Fig. (3) Shows transmittance, the highest transmittance value in the region is (0 - 3000cm^{-1}) and (2600 -1250 cm^{-1}) is offset by the lowest absorption here, the sample has good transparency characteristics at this region [14]. In a region (1450 cm^{-1}) the highest absorbency and transmittance is almost zero.

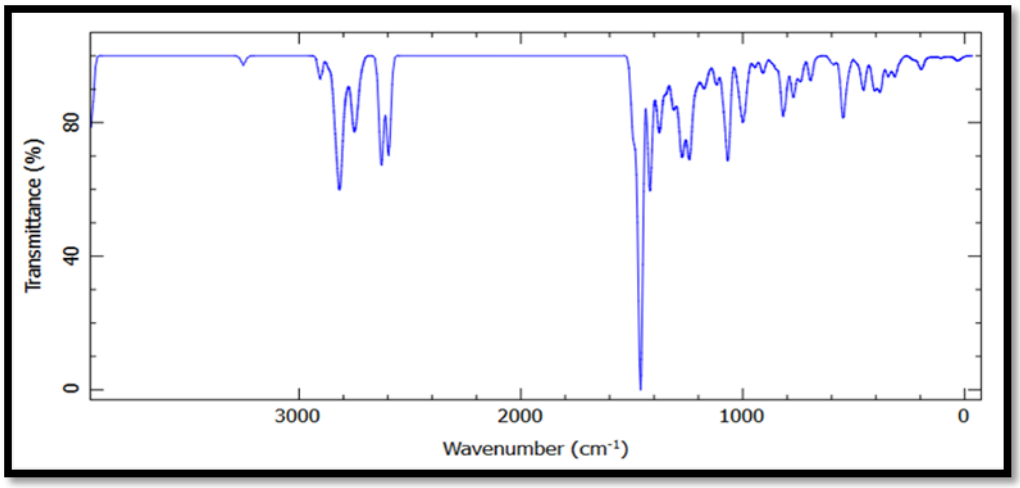

Figure 3. Transmittance spectrum of hydroxychloroquine.

3.2. Infrared Spectroscopy

Spectroscopy using infrared. Infrared is a branch of spectroscopy and deals with the infrared region (IR) of the electromagnetic spectrum [15]. At the region (1500cm^{-1}), the spectrum is divided into two parts. The first (0 – 1500cm^{-1}) this region is called the fingerprint area similar to the fingerprint of the human being, meaning that each compound has a fingerprint that differs from the other, and this region is difficult to explain, due to the difficulty in distinguishing the signs and the difference of values in them due to their convergence. This region indicates the identity of the molecule. As for the region after (1500cm^{-1}), it is the area of the functional group, and here we learn about the types of bonds. The area (2900 cm^{-1}) is for the carbon and hydrogen Single bond C-H, and hybridization type sp3 [16].

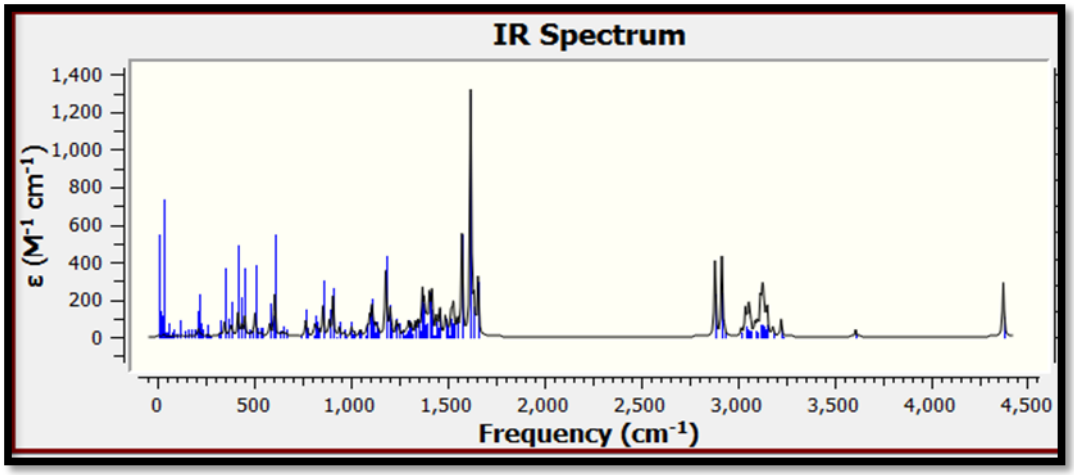

Figure 4. Infrared spectrum of hydroxychloroquine.

3.3. Raman scattering

When light scatters off from molecules, it causes changes in the energy of a photon equal to the energy of a molecule's vibrational transition. This dispersion is known as the Raman scattering and it is a type of inelastic scattering [17]. Fig. (5) Can be seen Raman scattering of hydroxychloroquine, electronic effect on bond C-H in the area (2800 cm^{-1}) is very large and this bond type stretch [18].

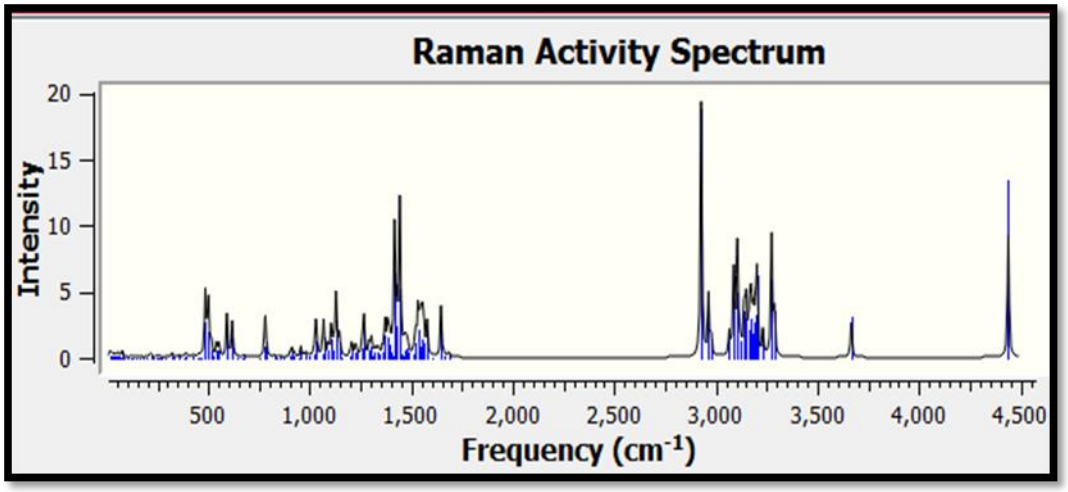

Figure 5: Raman scattering of hydroxychloroquine.

3.4. Electronic circular dichroism

Fig. (6) Shows Electronic circular dichroism (ECD), Determining the absolute combination (AC) is often a difficult aspect of elucidating the composition of hydroxychloroquine. Where chiral compounds possess suitable hydroxychloroquine, (ECD) may supply a robust path to determine that absolute combination. Recently, the use of ECD calculations by y (DFT) has become more and more widespread. AC limitation by foretelling the sign of one or more bands. The diastereomeric When interactions the right and left circularly polarized light beams with any non-racemic sample this is like two chiral physical entities, one of which is the mirror image of the other [19]. As a result, the difference is defined as circular dichroism (CD).

$$CD = A^L - A^R \dots\dots\dots (3)$$

Where AL and AR stand for right and left circularly polarized light, respectively, it is absorbed. Rotatory force and electronic transfer although it is beyond our capacity to describe the interactions of light with the molecule, it is useful to recall that the electric and magnetic dipoles can be identified for each electronic transition. The flexibility of CD tools is mainly measured. A molar quantity can be calculated using Lambert and Beer's law as an analogy:

$$\Delta\varepsilon = \varepsilon^L - \varepsilon^R \dots\dots.. (4)$$

Because a positive skew angle is believed to be correlating with a positive CD of the low lying p–p* transition at nearly 600 nm, this figure has a positive peak; of course, a negative angle is expected to have a negative CDThe move between (HOMO) and (LUMO) result in both non-vanishing electric and magnetic transition dipole moments, which are not orthogonal and give rise to a non-vanishing rotational strength [20]. This means that the polarization of the drug hydroxychloroquine is horizontal.

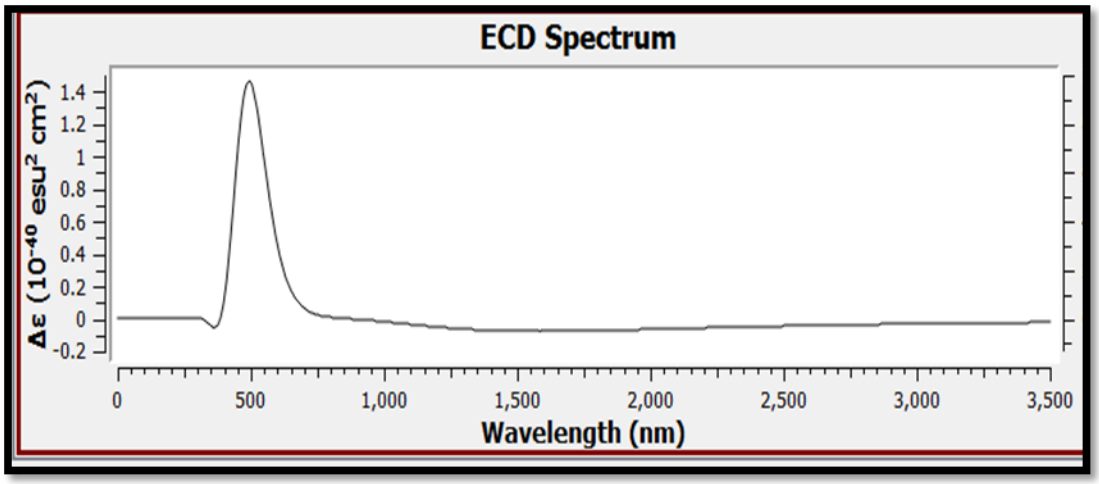

Figure 6. Electronic circular dichroism (ECD) of hydroxychloroquine.

3.5. HOMO and LUMO

The stability of hydroxychloroquine can be seen in the fig. (7). Molecular orbitals and their characteristics like energy are utilized to demonstrate numerous types of interactions and to forecast the most reactive site in conjugate systems [21]. The maximum significant orbitals in the molecule are

(HOMO) and (LUMO). A tiny gap in the border electron shells is more polarizable when the molecule has a high chemical reactivity and low kinetic stability. The HOMO and LUMO Eigenvalues, as well as their energy gaps, represent the molecule's biological activity. HOMO tends to give these electrons as an electron donor, and so the ionization potential is proportional to the energy of the HOMO. On the other hand, LUMO may receive electrons, and its energy is proportional to its electron affinity [22-24]. We looked at two important chemical orbitals, for the hydroxychloroquine, HOMO is equal to (-0.21016 a.u.), and LUMO is equal to (-0.11282 a.u.) which are given in Fig. (7). The energy gap is equal to (2.6 eV).

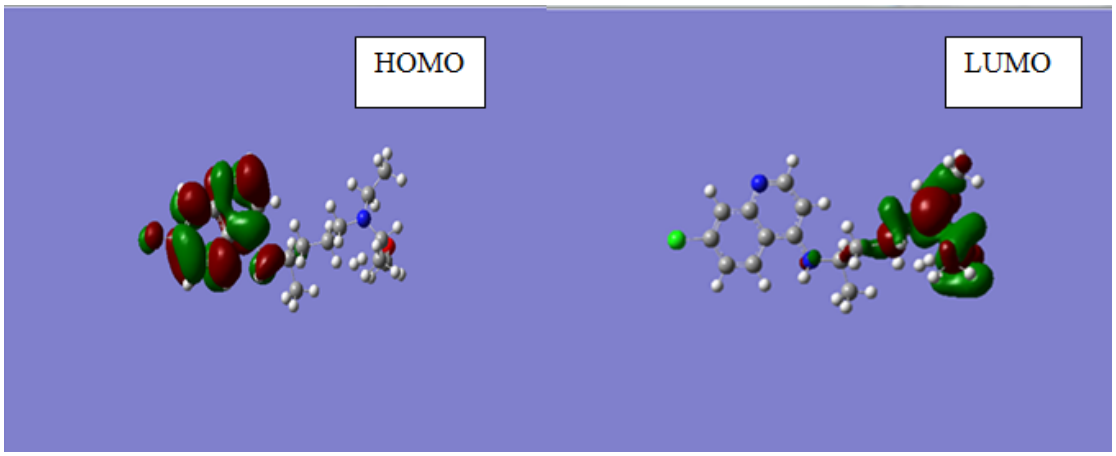

Figure 7. HOMO and LUMO of hydroxychloroquine.

4. Conclusions

Stability of hydroxychloroquine, and less energy. The sample has good transparency characteristics at region (0 – 3000 cm^{-1}) and (2600 -1250 cm^{-1}). A region (1450 cm^{-1}) transmittance is almost zero. (ECD) this means that the polarization of the drug hydroxychloroquine is horizontal. HOMO equal to (-0.21016 a.u.), and LUMO equal to (-0.11282 a.u.) which are given in Fig. (7). Energy gap equal to (2.6 eV). Raman scattering of hydroxychloroquine, electronic effect on bond C-H in the area (2800 cm^{-1}) is very large and this bond type stretch. The infrared region (IR) of the electromagnetic spectrum, as for the region after (1500cm^{-1}), it is the area of the functional group, and here we learn about the types of bonds. The area (2900 cm^{-1}) is for the carbon and hydrogen Single bond C-H, and hybridization type sp3.

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