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Study of The Optoelectronic Potential of Carbazole, Quinoline, Xanthone Compounds and Their Derivatives

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Abstract

Organic compounds and polymers have been intensively studied in the field of optoelectronics because they have chromophores associated with conjugated double bonds, which are responsible for light absorption. This study examines the optoelectronic properties of organic compounds or polymers such as carbazole, quinoline, xanthone, and their derivatives in silico. The study was conducted using the TDDFT electronic structure method, B3LYP 6-31G* basis set, using ORCA software. The study examined carbazole, benzo a-carbazole, benzo b-carbazole, benzo c-carbazole, benzo d-carbazole, quinoline, benzo b-quinoline, benzo c-quinoline, xanthene, benzo b-xanthene, benzo c-xanthene, and benzo kl-xanthene, which produced band gaps of 4.730; 4.228; 3.676; 4.101; 2.703; 4.583; 3.320; 4.453; 4.536; 4.206; 3.796; and 4.206, absorption wavelengths in the range of 148.9 to 542.9 nm, excitation energies of 7.311; 6.704; 5,871; 5,290; 5,992; 6,450; 5,834; 6,284; 5,517; 6,199, 6,802; and 6,159, oscillator strength of 0.483; 0.474; 0.890; 0.746; 0.161; 0.707; 2.780; 0.534; 0.632; 1.219; 0.572; and 0.646, and LHE values of 0.671; 0.664; 0.871; 0.820; 0.309; 0.803; 0.998; 0.707; 0.766; 0.939; and 0.999, indicating that these compounds have great potential for optoelectronic applications.

Keywords: Carbazole, Quinoline, Xanthone, TDDFT

INTRODUCTION

With the development of technology, the field of optoelectronics has attracted significant attention. This is supported by research developments in renewable energy to reduce the use of non-renewable energy (Ang et al., 2022). In this context, optoelectronics plays an important role in the development of renewable energy. Optoelectronics is a field studied in the development of renewable energy. This field studies the interaction between light and the electronic properties of a material. In everyday life, optoelectronic applications are present in various forms such as solar cells, cameras, sensors, LEDs, OLEDs, and others [1]

Chemical compounds as raw materials are in high demand in research for optoelectronic applications. In the early days of optoelectronics, inorganic compounds were one of the most popular materials due to their advantages of good conductivity, high thermal and chemical stability, and relatively long service life. One of the inorganic compounds that was popular in the early development of optoelectronics was gallium arsenide for infrared applications. The use of gallium arsenide is supported by its crystal structure, which plays a role in the formation of valence bands and conduction bands. The distance between these two energy bands is known as the band gap, which determines the type of light that can be absorbed or emitted by a material [2]. If the band gap is wide, it is suitable for UV applications, while if the band gap is small, it is suitable for infrared or visible light applications [3]. Despite their promising optical characteristics, the use of inorganic compounds is not without limitations, such as structural flexibility, production processes, device design, and toxicity due to the waste produced [4]. These limitations have prompted scientists to turn to other alternatives, one of which is organic compounds or polymers.

Organic compounds and polymers have been intensively studied in the field of optoelectronics because they have chromophores associated with conjugated double bonds, which are responsible for light absorption. In addition, organic compounds have advantages in terms of flexibility, light weight, and low cost compared to inorganic compounds [5]. Despite their physical advantages, the optoelectronic properties of molecules still depend on their chemical structure, which is reflected in parameters such as HOMO and LUMO, band gap values, electron transitions, and oscillator strength [6], [7]. Therefore, the selection of chemical compound structures needs to be considered when designing materials for optoelectronic applications. Although many organic compounds have been reported to have good optical and electronic properties, the relationship between several basic chemical structures and changes in optoelectronic properties is not yet fully understood, so further research is still needed.

This study used the chemical compounds carbazole, quinoline, xanthone, and simple derivatives, namely benzo a-carbazole, benzo b-carbazole, benzo c-carbazole, benzo d-carbazole, benzo b-quinoline, benzo c-quinoline, benzo b-xanthene, benzo c-xanthene, and benzo kl-xanthene. Several carbazole and quinoline derivatives have been used for applications in DSSC (Dye Sensitized Solar-Cell) solar cells, while xanthone derivatives dominate in the field of medicine [8], [9], [10]. However, the structures of carbazole, quinoline, and xanthone compounds have broader potential in various fields, including optoelectronics, thus requiring further research. Due to the limitations of experimental approaches in exploring molecular structures and electronic mechanisms, as well as low efficiency, this study uses theoretical and computational approaches to maximize the exploration of the structures and optoelectronic properties of compounds.

A theoretical and computational approach is highly suitable for this research because it allows direct observation of electronic and optical properties through quantum calculations, such as electron density distribution, molecular orbital shape and character, and electronic transitions. The computational method used is TDDFT (Time-Dependent Density Functional Theory, an extension of DFT (Density Functional Theory)[11], which accurately calculates excitation energy, absorption wavelength, oscillator strength, and electronic transition characteristics, making it relevant for the study of optical and optoelectronic properties. The calculations were performed using the B3LYP function with a 6-31G* basis set, which offers an optimal balance between accuracy and efficiency in describing the structure and distribution of electrons in molecules [12]. In computational chemistry, several software programs support the TDDFT method, such as Orca, Gaussian, and NWChem. This study used Orca because of its advantages in terms of computational speed, low cost, ease of use, and accuracy that is almost the same as other major software [13].

COMPUTATIONAL SECTION

Material and Methods

In this study, the following compound structures were used: carbazole, benzo a-carbazole, benzo b-carbazole, benzo c-carbazole, benzo c-carbazole, quinoline, benzo b-quinoline, benzo c-quinoline, xanthone, benzo b-xanthone, benzo c-xanthene, and benzo kl-xanthene, abbreviated as carb, a-car, b-car, c-car, d-car, quin, b-quin, c-quin, xan, b-xan, c-xan, and kl-xan in 3D form obtained from PubChem data. The method used was TD-DFT with the B3LYP 6-31G* basis function using ORCA software for computation, Avogadro for molecule visualization, and Command Prompt and Notepad for input and output data management.

Structure Modeling

Compound structures were obtained from the PubChem database and drawn in 2D using ChemDraw, then saved in MDL Molfiles format. The 2D structures were converted into 3D using Avogadro to proceed to the Geometry Optimization stage, to produce the most stable molecular configuration.

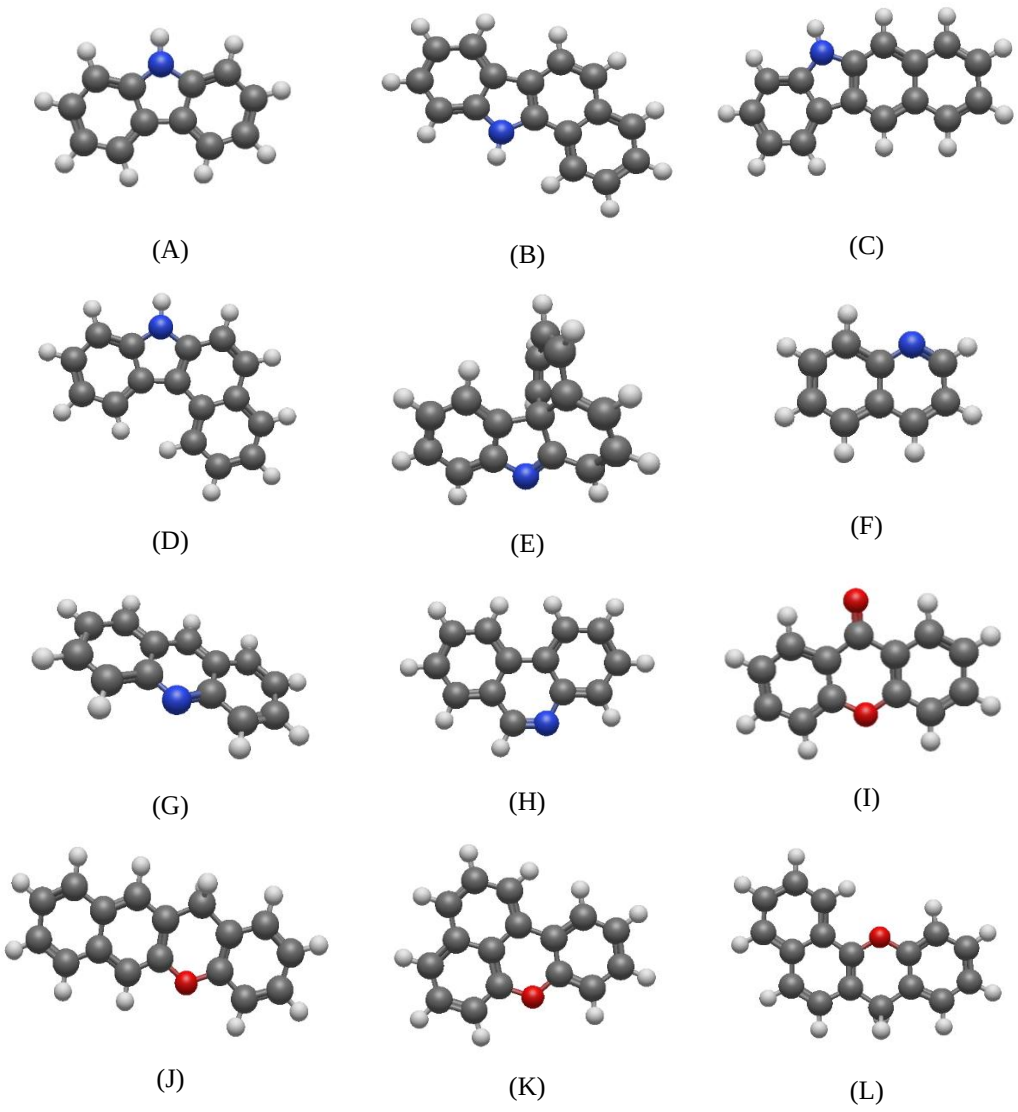


Figure 1. 3D visualization of the structures of carb, a-car, b-car, c-car, d-car, quin, b-quin, c-quin, xan, b-xan, c-xan, and kl-xan compounds.

Geometry Optimization and Single Point Energy Determination

The molecular structure was entered into Avogadro and the structure file was input into TDDFT with the B3LYP 6-31G* basis function and saved in INP format. The calculation was run using ORCA via Command Prompt and the result was an OUT file, which was visualized using Avogadro. This output file was used for single point energy calculation with the same TDDFT configuration, saved in INP format and run using ORCA. The OUT file result was visualized using Avogadro for further analysis.

RESULTS AND DISCUSSION

Electronic Properties

The optoelectronic properties of a compound molecule can be determined through its electron density and HOMO-LUMO energy. Electron density can be observed through the colors emitted in the following image.

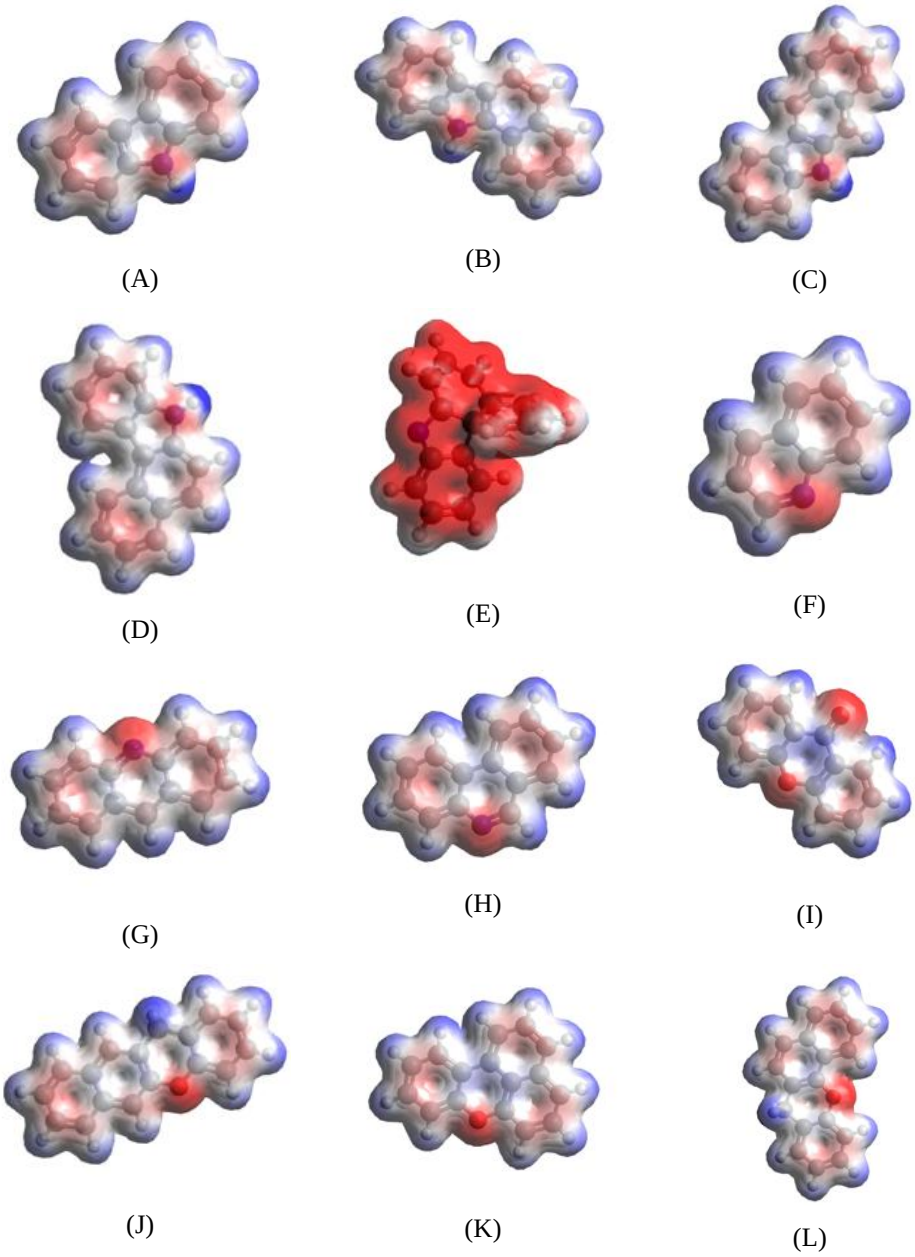


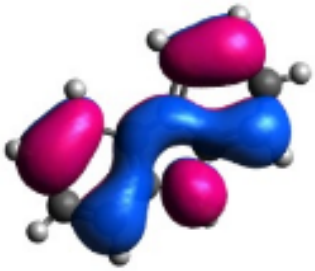
Figure 2. Visualization of electron density in carb, a-car, b-car, c-car, d-car, quino, b-quin, c-quin, xan, b-xan, c-xan, and kl-xan compounds.

Based on the image, d-car shows high electron density, which is indicated by the dominance of red colors. The dark red areas indicate areas with dense or numerous electrons, while the dark blue areas indicate areas with few electrons. This indicates that d-car has strong delocalization, but the charge distribution is unbalanced because most areas are negatively charged and only a small portion of areas are positively charged.

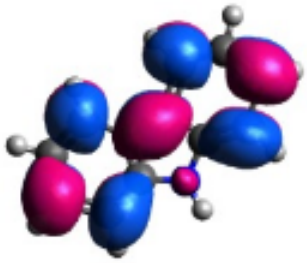
In contrast, the other nine compounds show an even charge distribution and good delocalization, with no intense red or blue colors and a uniform white or light blue color throughout the molecular ring chain. Thus, d-car has high electron density but poor delocalization, while the other 9 compounds have good delocalization with evenly distributed electron density.

Each compound has varying HOMO and LUMO energies depending on its structure. HOMO and LUMO are crucial factors in determining the optoelectronic properties of a compound molecule because they provide an overview or possibility of electron transfer (Jeong et al., 2022). HOMO is related to the ability to donate electrons, while LUMO is related to the ability to accept electrons [14]. This makes HOMO and LUMO one of the main points observed by scientists when researching new compounds.

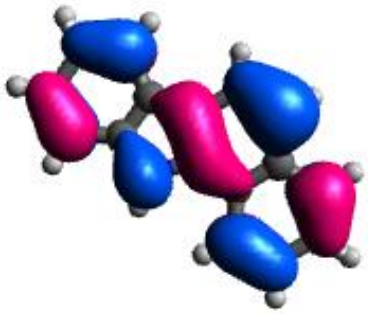
The HOMO energy levels obtained from the vacuum (gas) phase for carb, a-car, b-car, c-car, d-car, quin, b-quin, c-quin, xan, b-xan, c-xan, and kl-xan are -5.330; -5.055; -4.896; -5.136; -4.949; -6.032; -5.394; -5.941; -6.198; -5.302; -4.910; and -5.159. For the LUMO energy of the same compound, the values are -0.600; -0.827; -1.220; -1.035; -2.245; -1.449; -1.488; -1.096; -1.662; -1.204; and -0.953. High HOMO energy indicates that electrons are more easily excited, meaning that molecules are more easily oxidized (release electrons). Conversely, low LUMO energy indicates that molecules are more easily accept electrons because the distance between HOMO and LUMO is relatively close, resulting in low excitation energy [15]. Based on the calculation results, the highest HOMO value is c-xan, while the lowest LUMO value is xanton.



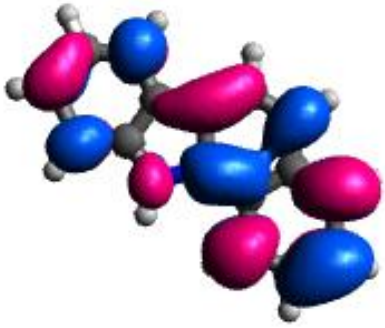
Carb (HOMO)



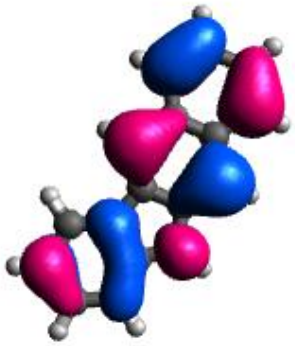
Carb (LUMO)



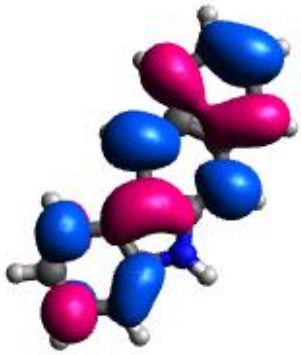
A-car (HOMO)



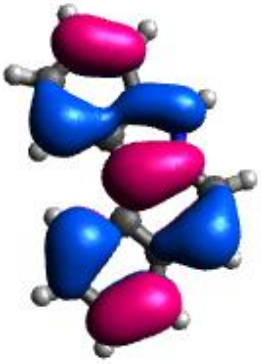
A-car (LUMO)



B-car (HOMO)

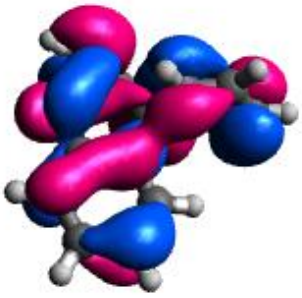


B-car (LUMO)

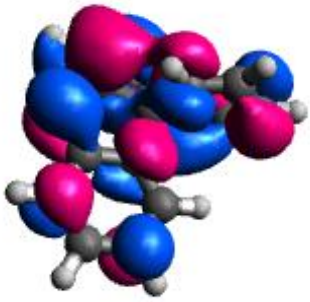


C-car (HOMO)

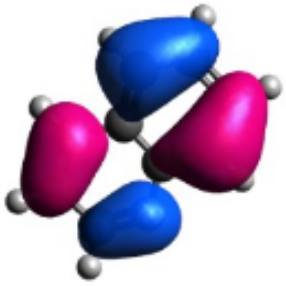
C-car (LUMO)



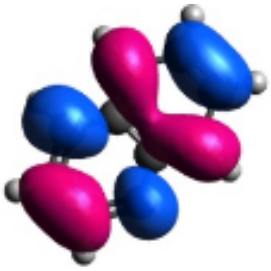
D-car (HOMO)



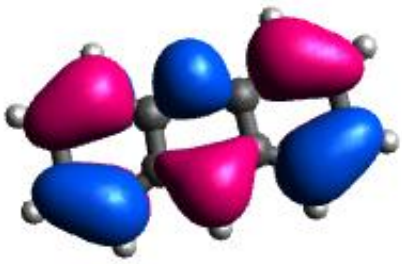
D-car (LUMO)



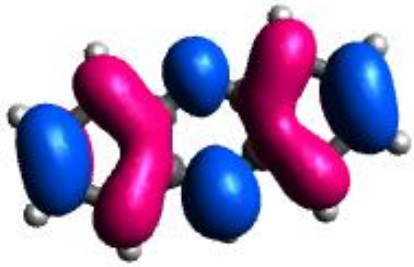
Quin (HOMO)



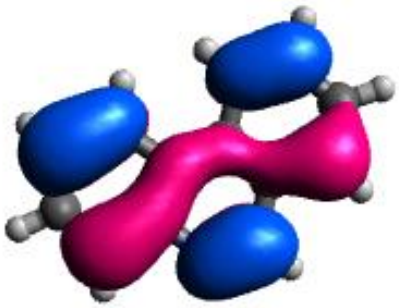
Quin (LUMO)



B-quin (HOMO)

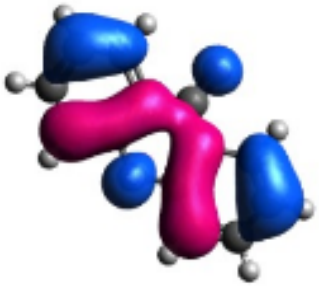


B-quin (LUMO)

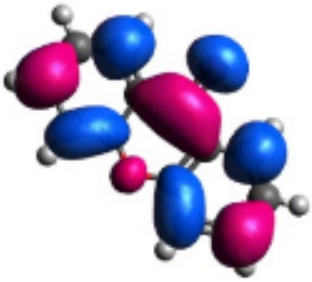


C-quin (HOMO)

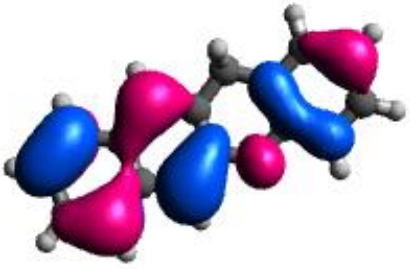
C-quin (LUMO)



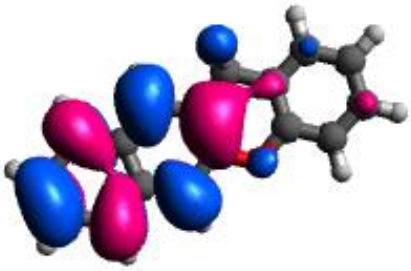
Xan (HOMO)



Xan (LUMO)



B-xan (HOMO)



B-xan (LUMO)

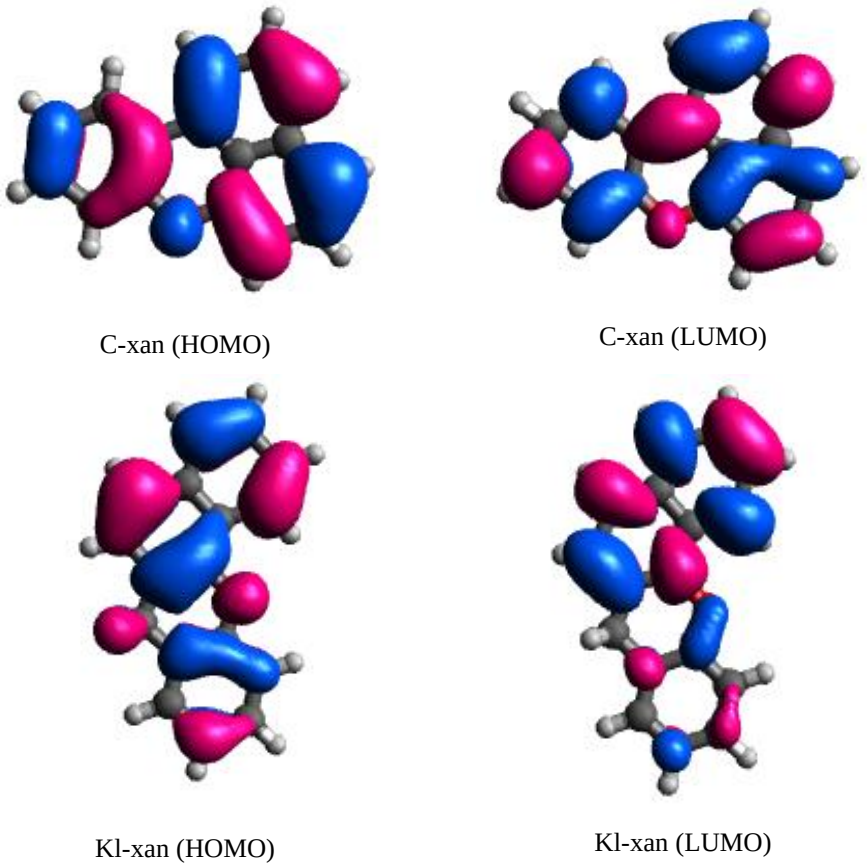


Figure 3. Visualization of HOMO LUMO of carb, a-car, b-car, c-car, d-car, quin, b-quin, c-quin, xan, b-xan, c-xan, and kl-xan compounds.

Based on the visualization results, the dominant LUMO energy undergoes delocalization so that it overlaps with HOMO. This affects the optoelectronic properties of these compounds. This is in line with the general principle in quantum chemistry, where the overlap of HOMO and LUMO determines the strength of electron interactions [16]. This occurs because the overlap between HOMO and LUMO reduces the energy difference between the two, allowing the compound to more easily absorb or emit light at the relevant wavelength [17].

Band gap refers to the distance or energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) [18]. The band gap determines the possibility of electron transfer, thereby directly affecting the optoelectronic properties of the compound. The band gap values obtained from carb, a-car, b-car, c-car, d-car, quin, b-quin, c-quin, b-xan, c-xan, and kl-xan are 4.730; 4.228; 3.676; 4.101; 2.703; 4.583; 3.320; 4.453; 4.536; 4.206; 3.796; and 4.206. Based on the results obtained, it is known that a high band gap causes the compound to only absorb UV and blue light. This is because the large distance requires greater energy for electron excitation, where the absorbed light tends to be high energy, namely light with short wavelengths such as blue light or UV [19].

Absorbation Properties

Excitation energy refers to the energy used to cause electrons to move from a lower energy state to a higher energy state [20]. In addition, excitation energy is related to the absorption wavelength, which determines the color or wavelength of light that can be absorbed by a molecule. The intensity of absorption is determined by the oscillator strength (f), which is a quantitative measure of how much light a molecule absorbs,

which can then be used to observe the efficiency of light absorption. Table 1 lists the excitation energy, absorption wavelength, oscillator strength, and light absorption efficiency.

Table 1. Absorption parameters of compounds

Compound name	Excitation energy (eV)	Absorption wavelength (nm)	Oscillator strength	LHE
carb	7,311	161,7 – 296,5	0,483	0,671
a-car	6,704	177,9 – 323,6	0,474	0,664
b-car	5,871	182,3 – 362,5	0,890	0,871
c-carb	5,290	181,1 – 328,0	0,746	0,820
d-carb	5,992	205,0 – 542,9	0,161	0,309
quin	6,450	148,9 – 299,8	0,707	0,803
b-quin	5,834	164,0 – 378,2	2,780	0,998
c-quin	6,284	174,2 – 319,6	0,534	0,707
xan	5,517	174,1 – 347,6	0,632	0,766
b-xan	6,199	180,8 – 317,4	1,219	0,939
c-xan	6,802	182,2 – 357,6	0,572	0,999
kl-xan	6,159	179,3 - 318,2	0,646	0,999

Based on the data in Table 1, it is known that the excitation energy obtained is quite high. This indicates that the energy required for an electron to move from its ground state to an excited state is large, resulting in a small absorption wavelength, which means that these compounds only absorb light in the blue light and UV ranges. The longest absorption wavelength of several of these chemical compounds is d-car.

The strength of the oscillator (f) describes the probability of an electronic transition occurring when a molecule absorbs light at a specific excitation energy. While the excitation energy determines the position of the absorption spectrum, the strength of the oscillator determines how strong the absorption is. The highest order of oscillator strength for these compounds is b-quin > b-xan > b-car > c-car > quin > kl-xan > xan > c-xan > c-quin > carb > a-car > d-car. From the data obtained, a sufficiently high oscillator strength value indicates a faster electron transition rate, so that electron transitions occur easily and are clearly visible in the absorption wavelength spectrum. Based on these results, the compound with the highest oscillator strength is b-quin.

Light absorption efficiency (LHE) is an important parameter for indicating the ability of a compound to capture light and convert it into an excited state. The LHE value is consistent with the oscillator strength because the LHE value is calculated directly from the oscillator strength value. The greater the oscillator strength of an electron transition, the greater the fraction of light that can be absorbed, thereby increasing the LHE value. This is what makes a high LHE value indicative of good absorption ability. Based on the data obtained, the order of LHE values from highest to lowest includes c-xan = kl-xan > b-quin > b-xan > b-car >

c-car < quin > xan > c-quin > carb > a-car > d-car. LHE values around 0.7-0.9 are considered close to ideal, and 9 compounds except a-car have strong potential for optoelectronic applications.

CONCLUSION

Based on the results obtained, the band gaps are 4.730, 4.228, 3.676, 4.101, 2.703, 4.583, 3.320, 4.453, 4.536, 4.206, 3.796, and 4.206, absorption wavelengths ranging from 148.9 to 542.9 nm, excitation energies of 7.311; 6.704; 5.871; 5.290; 5.992; 6.450; 5.834; 6.284; 5.517; 6.199, 6.802; and 6.159, oscillator strength of 0.483; 0.474; 0.890; 0.746; 0.161; 0.707; 2.780; 0.534; 0.632; 1.219; 0.572; and 0.646, as well as LHE values of 0.671; 0.664; 0.871; 0.820; 0.309; 0.803; 0.998; 0.707; 0.766; 0.939; and 0.999. This indicates that these compounds have the potential to be applied in UV optoelectronics.

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