

## Research Article

# Absorption of Methylene, Hydrohalogenocarbenes and Dihalogenocarbenes in the Ultraviolet Visible Range: Ab Initio and Density Functional Theory (DFT) Approaches

Alao Latifatou Laye<sup>1,\*</sup> , Diomande Sekou<sup>2</sup> , Bede Affoue Lucie<sup>1</sup> ,  
Assoma Amon Benjamine<sup>1</sup>, Kone Soleymane<sup>1</sup>

<sup>1</sup>Department of Science, Structures of Matter and Technology (SSMT), University of Felix Houphouët-Boigny, Abidjan, Ivory Coast

<sup>2</sup>Department of Agro-Industrial Sciences and Technologies (AIST), University of San Pedro, San Pedro, Ivory Coast

## Abstract

Carbenes are unstable biradical molecules with a longer lifetime in space than on Earth. This theoretical study focused on analyzing the spectroscopic properties of methylene and monohalogenated and dihalogenated derivatives in the ultraviolet-visible range. Structures of these compounds can exist in two electronic states depending on the orbitals containing the non-bonding electrons: singlet  $S_0$  and triplet  $T_1$ . Three theoretical levels HF/6-311++G (d, p), MP2/6-311++G (d, p), and B3LYP/6-311++G (d, p) were used to perform this analysis. Absorption spectra were calculated for the optimized structures ( $S_0$  and  $T_1$ ) of methylene, three hydrohalogenocarbenes and two dihalogenocarbenes at each of the chosen theoretical levels. The calculations allowed us to study the behavior of these carbenes in ultraviolet-visible absorption. It was determined that, at maximum absorption, all of these carbenes in the singlet  $S_0$  state absorb in the visible range. However, in the  $T_1$  triplet state, they absorb in the ultraviolet range. Under maximum oscillation conditions, these carbenes absorb in the ultraviolet regardless of the electronic state of the structure. The calculated absorption wavelengths show that the transition from the ground state to their excited states of the studied carbenes is sometimes accompanied by a bathochromic effect and sometimes by a hypsochromic effect.

## Keywords

Carbene, Theory Level, Spectroscopy, Wavelength, Bathochrome, Hypsochrome

## 1. Introduction

To date, approximately 200 polyatomic chemical species (molecules, free radicals, or ions) have been detected in interstellar space using spectroscopy. The first molecule detected in interstellar space, in 1937 [1], was the CH radical (methylidene). Methylene [2] was detected in 1995. This species is

the simplest of the carbenes. It is the subject of this study.

The presence of methylene and free radicals in the interstellar medium shows that carbenes can be found in space. These molecular entities are very short-lived biradicals.

Carbene species are neutral organic species composed of a

\*Correspondence: Alao Latifatou Laye (latifaalao500@gmail.com)

Received: 12 May 2026; Accepted: 28 May 2026; Published: 10 June 2026



divalent carbon atom with six valence electrons: two electrons in each bond with neighboring atoms and two unbound electrons. They are produced by the photolysis of “Diazo” or “Diazirine” compounds. They are also characterized by two electrons not involved in bonds (Figure 1).

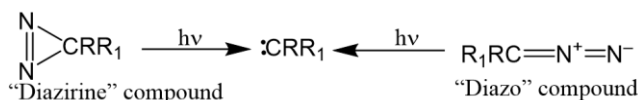


Figure 1. carbene production by photolysis.

Carbene molecules can exist in two different forms depending on the orbitals occupied by the non-bonding electrons: the singlet form ( $S_0$  and  $S_1$ ) and the triplet form ( $T_1$ ) [3-7] (Figure 2). In the singlet form, the two electrons are paired in one of the  $sp$  hybrid orbitals. However, the triplet form has two unpaired electrons. They are located, respectively, in one of the  $sp^2$  hybrid orbitals and in the vacant  $p_z$  orbital.

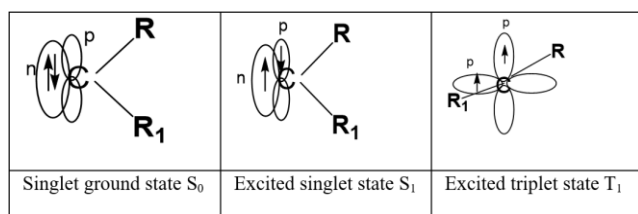


Figure 2. Different electronic states of carbenes.

These electrons, not involved in bonds, make carbenes unstable. They are considered highly reactive transient species that are difficult to isolate. However, these molecules can be found in space, where they have a longer lifetime, whereas in the terrestrial environment, direct access to them is difficult, even impossible. Hence the interest in studying them using theoretical chemistry. Adóti and al. [8] studied the stability and reactivity of carbenes using two semi-empirical methods, AM1 and MNDO. Their results showed low accuracy in analyzing the properties of carbenes and a recurring discrepancy between calculated and experimental values.

The aim of this work is to use absorption properties to identify carbenes (methylene and its analogs). This involves determining the ultraviolet absorption spectra and related properties of carbenes. Various theoretical approaches are used to perform these calculations, including ab initio methods and density functional theory.

## 2. Materials and Methods

### 2.1. Structures of the Molecules Studied

As well as methylene, three (03) hydrohalogenocarbenes

and two (02) dihalogenocarbenes were studied in this work. Table 1 shows these molecules.

Table 1. Structures of methylene and five studied carbene derivatives Absorption wavelengths.

Methylene	Hydrohalogenocarbenes	Dihalogenocarbenes
	X = F or Cl or Br	X1 = X2 = F or Cl

### 2.2. Computational Methods

The calculations for this study were performed in the gas phase using the Gaussian 09 [9] software. Three Ab Initio methods were used: the Hartree-Fock method [10, 11] (HF) and two post-HF methods [11]: MP2 and CIS [12]. the Density Functional Theory (DFT) method was also employed using the B3LYP functional [13, 14]. Each of these methods involved optimizing the geometry of all the structures.

A single-point calculation is then made on each optimized structure using the CIS method in the RHF framework for the singlet state  $S_0$  and in the UHF framework for the triplet state  $T_1$ . For each calculation, the 6-311++G (d, p) triple-zeta basis set is used in association with the chosen method. In particular, The CIS configuration interaction method was used to determine the absorption wavelength and the corresponding oscillation strength.

## 3. Results and Discussion

### Absorption Properties of the Studied

For each of the seven carbenes studied, the singlet  $S_0$  and triplet  $T_1$  states were submitted to the calculations described in Section I.2. Thus, we determined the maximum absorption wavelength ( $\lambda_{max}$ ) and the corresponding oscillator strength ( $f$ ). In addition, we considered the maximum value of this strength ( $f_{max}$ ) and the associated wavelength. For the analysis of the results, the difference  $\lambda_{max}(S_0) - \lambda_{max}(T_1)$  is denoted by  $\Delta\lambda_{max}$ . For the maximum values of the oscillation strength of states  $S_0$  and  $T_1$ , the difference between the corresponding wavelengths  $\lambda(S_0) - \lambda(T_1)$  is denoted by  $\Delta\lambda$ . When  $\Delta\lambda_{max}$  or  $\Delta\lambda$  is positive, this is referred to as a bathochromic effect; otherwise, it is referred to as a hypsochromic effect.

### 3.1. Absorption of the Methylene

Table 2 and Table 3 show the results obtained for methylene, which were used to calculate  $\Delta\lambda$  and  $\Delta\lambda_{max}$ , respectively. These values were calculated using different levels of theory.

**Table 2.** Absorption wavelengths  $\lambda$  (nm) and shifts  $\Delta\lambda$  (nm) associated with the maximum oscillation force  $f_{max}$  in the  $S_0$  and  $T_1$  electronic states of methylene; values calculated using the 6-311++G(d,p) basis set associated with different methods.

Calculation	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(S_0) - \lambda(T_1)$	$f(S_0) - f(T_1)$
method	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(S_0) - \lambda(T_1)$	$f(S_0) - f(T_1)$
HF	125	126	0.20	0.08	-1	0.12
B3LYP	125	129	0.20	0.08	-4	0.12
MP2	125	127	0.20	0.08	-2	0.12

The HF/6-311++G\*\*, MP2/6-311++G\*\*, and B3LYP/6-311++G\*\* theory levels used for the calculations yield consistent results for the same electronic state  $S_0$  or  $T_1$  at maximum oscillation ( $f_{max}$ ). These calculations identify the  $T_1$  state as the ground state of methylene [15]. The wavelengths associated with these electronic states all lie in the ultraviolet (UV) range. According to our calculations, the absorption wavelength of the singlet state ( $S_0$ ) of methylene is 125 nm. The values obtained clearly show that the wavelength  $\lambda$  (nm) is higher in the  $T_1$  state than in the  $S_0$  state. The difference between the absorption bands of the excited  $S_0$  state of methylene and its ground state  $T_1$  is negative. It ranges from -1 nm

to -4 nm. The transition of methylene from its ground state  $T_1$  to the  $S_0$  state is accompanied by a hypsochromic effect.

The calculation methods used estimate that the maximum oscillation force ( $f_{max}$ ) higher in the excited electronic state  $S_0$  than in the ground state  $T_1$ . For a given electronic state, the value of the oscillation force is constant. It is 0.20 for the  $S_0$  state and 0.08 for the  $T_1$  state. This force is higher in the singlet  $S_0$  state.

The values of the maximum absorption wavelengths and those of the corresponding oscillation forces, for these two electronic states of methylene are calculated and given in Table 3.

**Table 3.** Maximum absorption wavelengths ( $\lambda_{max}$  in nm) and corresponding oscillation forces  $f$  in the electronic states  $S_0$  and  $T_1$  of methylene calculated with the HF, MP2 and B3LYP methods with the 6-311++G\*\* function basis.

Calculation	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(S_0) - \lambda(T_1)$	$f(S_0) - f(T_1)$
method	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(S_0) - \lambda(T_1)$	$f(S_0) - f(T_1)$
HF	790	172	0.009	0.040	619	-0.031
B3LYP	742	173	0.009	0.037	569	-0.028
MP2	749	172	0.009	0.039	577	-0.030

Data in Table 3 clearly show that under conditions of maximum absorption, the wavelengths are very different from those at maximum oscillation. These increase very significantly when absorption is maximal in both the  $S_0$  and  $T_1$  electronic states of methylene. According to the three levels of theory used, the maximum absorption of methylene  $T_1$  (ground state) is observed in the UV range with an average wavelength  $\lambda_{max} = 172$  nm. However, methylene in the excited electronic state  $S_0$  absorbs most strongly in the visible range. The HF, B3LYP, and MP2 methods estimate  $\lambda_{max}$  to be 790 nm, 742 nm and 749 nm respectively. When absorption is at its maximum, the transition from the ground electronic state  $T_1$  to the excited state  $S_0$  of methylene is ac-

companied by a bathochromic effect. The gap between the absorption bands of the excited state  $S_0$  of methylene and its ground state  $T_1$  is positive and very large. It range from 569 nm to 619 nm.

When methylene absorption is at its maximum, the oscillation forces are higher in the triplet state  $T_1$ . This constant is opposite to that shown in Table 2, which was obtained when oscillation was at its maximum.

### 3.2. Absorption of Hydrohalogenocarbenes

The results of the calculations of the absorption wavelengths ( $\lambda$ ) and oscillation forces of the hydrohalogenocarbenes are reported in Tables 4 and 5.

**Table 4.** Absorption wavelengths  $\lambda$  (nm) and shifts  $\Delta\lambda$  (nm) associated with the maximum oscillation force  $f_{max}$  in the  $S_0$  and  $T_1$  electronic states of hydrohalogenocarbenes calculated with three methods.

Hydrohalo-genocarbenes	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f_{max}$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(T_1) - \lambda(S_0)$	$f(T_1) - f(S_0)$
HF/6-311++G(d,p)						
CHF	104	123	0.262	0.063	19	0.2
CHCl	151	158	0.219	0.051	7	0.2
CHBr	142	155	0.268	0.047	14	0.2
B3LYP /6-311++G(d,p)						
CHF	104	124	0.256	0.062	20	0.2
CHCl	152	157	0.208	0.051	6	0.2
CHBr	141	180	0.307	0.362	39	-0.1
MP2 /6-311++G(d,p)						
CHF	104	124	0.259	0.061	20	0.2
CHCl	149	157	0.229	0.052	8	0.2
CHBr	142	155	0.232	0.069	14	0.2

Data in Table 4 indicate that these hydrohalogenocarbenes in the  $S_0$  and  $T_1$  states, when the oscillation force is at its maximum, absorb in the ultraviolet range. Calculations estimate that, for a given hydrohalogenocarbene in the same electronic state, the values of the absorption wavelengths are very close. Only one value of  $\lambda$  deviates from this observation. This is the value obtained ( $\lambda = 180 \text{ nm}$ ) at the B3LYP/6-311++G(d,p) level for hydrohalogenocarbene in its triplet state  $T_1$ . For the three hydrohalogenocarbenes CHF, CHCl, and CHBr, calculations show that the absorption wavelength is shorter for CHF and longer for CHCl. Furthermore, for all three compounds, the wavelength is longer at state  $T_1$  than at state  $S_0$ .

The singlet state  $S_0$ , more stable than the triplet state  $T_1$  for hydrohalogenocarbenes, corresponds to the ground state of these compounds. For these compounds, the transition from the ground state to the excited state  $T_1$  occurs by absorption with a bathochromic effect.

Data in Table 4 shows that the maximum oscillation force ( $f_{max}$ ) is higher in the ground state ( $S_0$ ). Its value varies by the same amount (0.2) between the two electronic states  $S_0$  and  $T_1$  in the three hydrohalogenocarbenes.

The values of the maximum absorption wavelengths and those of the corresponding oscillation forces, for these two electronic states of the three hydrohalogenocarbenes, are also calculated and reported in Table 5.

**Table 5.** Maximum absorption wavelengths ( $\lambda_{max}$  in nm) and corresponding oscillation forces  $f$  in the electronic states  $S_0$  and  $T_1$  of hydrohalogenocarbenes calculated with three methods.

Hydrohalo-genocarbenes	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f_{max}$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(T_1) - \lambda(S_0)$	$f(T_1) - f(S_0)$
HF/6-311++G(d,p)						
CHF	479	174	0.017	0.032	-305	-0.01
CHCl	598	204	0.010	0.000	-394	0.01
CHBr	625	239	0.008	0.000	-386	0.01
B3LYP /6-311++G(d,p)						

Hydrohalo-genocarbenes	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f_{max}$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(T_1) - \lambda(S_0)$	$f(T_1) - f(S_0)$
CHF	470	172	0.016	0.030	-298	-0.01
CHCl	580	202	0.010	0.000	-377	0.01
CHBr	601	236	0.008	0.000	-365	0.01
MP2 /6-311++G(d,p)						
CHF	475	172	0.016	0.032	-303	-0.02
CHCl	593	201	0.009	0.001	-392	0.01
CHBr	613	234	0.008	0.000	-379	0.01

Data in this table clearly show that under maximum absorption conditions, the wavelengths are very different from those at maximum oscillation. They increase significantly when absorption is maximum in both the  $S_0$  and  $T_1$  electronic states of hydrohalogenocarbenes. Our calculations indicate that the absorption wavelength remains lower for the CHF compound and higher for the CHBr compound. Furthermore, for all three compounds, the wavelength is higher in the  $S_0$  state than in the  $T_1$  state. Between the ground states  $S_0$  of hydrohalogenocarbenes [15] and their excited states  $T_1$ , there is a significant decrease in the maximum absorption wavelength. This transition is accompanied by a significant hypsochromic effect.

The three levels of calculations consistently indicate that these molecules, in their  $T_1$  electronic states, absorb in the UV range. The maximum absorption lengths  $\lambda_{max}$  vary between

174 and 236 nm. In the  $S_0$  electronic state, the calculated maximum absorption lengths  $\lambda_{max}$  vary between 475 and 625 nm. These absorptions are all located in the visible range.

With the exception of the CHF compound, the oscillation force associated with  $\lambda_{max}$  is greater in the  $S_0$  state. It is zero for the hydrohalogenocarbenes CHCl and CHBr in the  $T_1$  state. In the CHX compounds (X = F, Cl, Br) in the  $S_0$  state, it decreases as the atomic number increases.

### 3.3. Absorption of Dihalogenocarbenes

The results of the calculations of the absorption wavelengths ( $\lambda$ ) and oscillation forces of the dihalogenocarbenes are reported in Tables 6 and 7.

**Table 6.** Absorption wavelengths  $\lambda$  (nm) and shifts  $\Delta\lambda$  (nm) associated with the maximum oscillation force  $f_{max}$  in the  $S_0$  and  $T_1$  electronic states of dihalogenocarbenes calculated with three methods.

Dihalo-geno-carbenes	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f_{max}$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(T_1) - \lambda(S_0)$	$f(T_1) - f(S_0)$
HF/6-311++G(d,p)						
CF2	115	108	0.212	0.034	-7	0.18
CCl2	167	153	0.058	0.047	-14	0.01
B3LYP /6-311++G(d,p)						
CF2	113	168	0.216	0.027	55	0.19
CCl2	138	153	0.120	0.045	15	0.07
MP2 /6-311++G(d,p)						
CF2	125	111	0.179	0.028	-15	0.15
CCl2	136	152	0.191	0.050	16	0.14

Results in Table 6 reveal no general trend in the absorption wavelength of one electronic state compared to another. It is sometimes longer for the  $S_0$  state and sometimes shorter for the  $S_0$  state. The DFT (B3LYP) and MP2 methods estimate that the absorption wavelength associated with  $f_{max}$  is longer when the  $CCl_2$  compound is in the  $T_1$  state, contrary to the HF method. For the  $CF_2$  compound, HF and MP2 calculations estimate that the absorption wavelength of the  $S_0$  state is greater than that of the  $T_1$  state. The DFT method predicts the opposite. All these results indicate that from the ground state  $S_0$  to the  $T_1$  state, the UV absorption of the  $CF_2$  and  $CCl_2$  compounds is sometimes accompanied by a bathochromic effect and some-

times by a hypsochromic effect. The results show that the dihalogenocarbenes  $CF_2$  and  $CCl_2$ , in the  $S_0$  or  $T_1$  electronic state, absorb in the ultraviolet. In the  $T_1$  state, the compound  $CCl_2$  absorbs at 253 nm according to the three calculation methods.

The maximum oscillation force constant is higher when the compound is in the  $S_0$  state. But for a given state, the maximum oscillation force decreases as the atomic number ( $Z$ ) of the halogen increases.

The values of the maximum absorption wavelengths and those of the corresponding oscillation forces, for the two electronic states of the dihalogenocarbenes studied are also calculated and reported in Table 7.

**Table 7.** Maximum absorption wavelengths ( $\lambda_{max}$  in nm) and corresponding oscillation forces  $f$  in the electronic states  $S_0$  and  $T_1$  of dihalogenocarbenes calculated with three methods.

Dihalogeno-carbenes	$\lambda$		$f_{max}$		$\Delta\lambda$	$\Delta f_{max}$
	$S_0$	$T_1$	$S_0$	$T_1$	$\lambda(T_1) - \lambda(S_0)$	$f(T_1) - f(S_0)$
HF/6-311++G(d,p)						
$CF_2$	232	170	0.075	0.028	-62	0.05
$CCl_2$	469	236	0.009	0.001	-233	0.00
B3LYP /6-311++G(d,p)						
$CF_2$	237	168	0.071	0.027	-69	0.04
$CCl_2$	462	240	0.009	0.001	-222	0.01
MP2 /6-311++G(d,p)						
$CF_2$	289	168	0.059	0.028	-121	0.03
$CCl_2$	469	235	0.009	0.001	-234	0.01

Results in Table 7 illustrate that the maximum wavelength ( $\lambda_{max}$ ) of the studied dihalogenocarbenes is greatest in the ground state  $S_0$  [15]. According to the results of the three calculation methods, the  $CF_2$  compound absorbs in the ultraviolet in both the ground state  $S_0$  and the excited state  $T_1$ . As for the dichlorocarbene, it absorbs in the visible in the  $S_0$  state and in the ultraviolet in the excited state  $T_1$ . For dihalogenocarbenes, the transition from the  $S_0$  state to the  $T_1$  state is accompanied by a decrease in the maximum absorption wavelength (hypsochromic effect). All calculations yield more consistent values for the maximum wavelength ( $\lambda_{max}$ ) for the  $T_1$  state compared to the  $S_0$  state.

Compared to hydrohalogenocarbenes, dihalogenocarbenes exhibit a significant decrease in the maximum absorption wavelengths of the  $S_0$  state. This decrease is even more pronounced for compound  $CF_2$ . In the  $T_1$  state, compounds CHF and  $CF_2$  have very similar maximum absorption wavelengths (168 nm to 172 nm). Comparison of the maximum absorption

wavelengths of  $CHCl$  and  $CCl_2$  compounds in the  $T_1$  state shows an increase from 32 nm to 38 nm for  $CCl_2$  according to the different calculation methods.

The oscillation force associated with  $\lambda_{max}$  is estimated to be very low, particularly for dichlorocarbene ( $CCl_2$ ). For difluorocarbene ( $CF_2$ ), the value of this force is always lower in the  $T_1$  electronic state.

## 4. Conclusion

This study demonstrated, using three levels of theory, that when the oscillation force of methylene is at its maximum ( $f_{max}$ ), both the electronic states  $T_1$  (ground) and  $S_0$  (excited) of methylene absorb in the ultraviolet. These calculations also reveal that the absorption accompanying the transition from the  $T_1$  to the  $S_0$  electronic state of methylene undergoes a wavelength decrease; hence, a hypsochromic effect. However,

under the conditions of maximum absorption ( $\lambda_{max}$ ), the two states  $T_1$  and  $S_0$  of methylene absorb in two distinct spectroscopic ranges. In its ground state ( $T_1$ ), methylene absorbs in the ultraviolet. When this carbene is in its excited state ( $S_0$ ), it absorbs in the visible, according to all the levels of theory used.

Extending the calculations to hydrohalogenocarbenes, we found that the  $S_0$  electronic state is the ground state of these carbenes. Both the  $S_0$  and  $T_1$  electronic states of the studied hydrohalogenocarbenes absorb in the ultraviolet when the oscillation forces are at their maximum. However, the absorption accompanying the transition from their  $S_0$  to  $T_1$  electronic states undergoes an increase in wavelength; hence, a bathochromic effect. When absorption is at its maximum, the studied hydrohalogenocarbenes, in their  $S_0$  ground electronic state, absorb in the visible spectrum. In their excited  $T_1$  state, they absorb in the ultraviolet.

Applied to the two dihalogenocarbenes  $CF_2$  and  $CCl_2$ , the theoretical levels used show that both the ground electronic state  $S_0$  and the excited electronic state  $T_1$  absorb in the ultraviolet. When the oscillation forces are at their maximum, the transition from the  $S_0$  to the  $T_1$  electronic state for these compounds is sometimes accompanied by a bathochromic effect and sometimes by a hypsochromic effect. When absorption is at its maximum, only the  $S_0$  electronic state of  $CCl_2$  absorbs in the visible region. In its excited state  $T_1$ , this compound absorbs in the ultraviolet. Both the  $S_0$  and  $T_1$  states of the carbene  $CF_2$  absorb in the ultraviolet.

## Abbreviations

UV	Ultraviolet
$S_0$ State	Singlet State
$T_1$ State	Triplet State

## Author Contributions

**Alao Latifatou Laye:** Conceptualization, Formal Analysis, Methodology, Resources, Software, Validation, Visualization, Writing – original draft, Writing – review & editing

**Diomande Sekou:** Data curation, Formal Analysis, Investigation, Validation, Visualization, Writing – review & editing

**Bede Affoue Lucie:** Data curation, Formal Analysis, Methodology, Writing – review & editing

**Assoma Amon Benjamine:** Data curation, Investigation, Writing – review & editing

**Kone Soleymane:** Conceptualization, Supervision, Visualization, Writing – review & editing

## Conflicts of Interest

The authors declare no conflicts of interest.

## References

- [1] P. Swings and L. Rosenfeld «Considerations Regarding Interstellar Molecules », *Astrophysical Journal*, 1937, vol. 86, p. 483-486, DOI 10.1086/143880. [Online]. Available: <https://ui.adsabs.harvard.edu/abs/1937ApJ....86..483S/abstract>
- [2] J. M. Hollis, P. R. Jewell and F. J. Lovas, «Confirmation of interstellar methylene », *Astrophysical Journal*, 1995, Part 1, vol. 438, P 259-264, <https://doi.org/10.1086/175070>
- [3] G. Herzberg, «Molecular Spectra and Molecular Structure. III. Electronic Spectra and Electronic Structure of Polyatomic Molecules », D Van Nostrand, Princeton, New-Jersey, 1966, page 336.
- [4] M. Krauss, « Triplet state of the carbene radical », *Journal of Research of the National Bureau of Standards (J. Res. NBS)*, 1964, 68A, p. 635.
- [5] Balci M. Reaksiyon mekanizmaları. 3th ed. Türkiye Bilimler Akademisi; 2012. 597 p.
- [6] Moss RA, Platz MS, Jones, Jr. M., «Reactive Intermediate Chemistry », Wiley-Interscience, 2004. 1067 p. ISBN: 0-471-23324-2.
- [7] Nemirowski A, Schreiner PR. « Electronic Stabilization of Ground State Triplet Carbenes », *J. Org. Chem.* 2007; 72 (25): 9533–9540. <https://doi.org/10.1021/jo701615x>
- [8] Maroufou Adeyemi Ad éoti, «Contribution to the study of the mechanism of action of carbenes on unsaturated bonds », Thesis, University of Cocody, 1998.
- [9] Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., and al. (2009) Gaussian 09, Revision A. 02. Gaussian, Inc.
- [10] MJ Frisch, M. Head-Gordon and JA Pople, « Semi-direct algorithms for the MP2 energy and gradient », *Chem. Phys. Lett.*, 1990, 166 281-89. [https://doi.org/10.1016/0009-2614\(90\)80030-H](https://doi.org/10.1016/0009-2614(90)80030-H)
- [11] M. Head-Gordon and T. Head-Gordon, « Analytic MP2 frequencies without fifth-order storage. Theory and application to bifurcated hydrogen bonds in the water hexamer », *Chem. Phys. Lett*, 1994, 220 (1–2), 122-128. [https://doi.org/10.1016/0009-2614\(94\)00116-2](https://doi.org/10.1016/0009-2614(94)00116-2)
- [12] S. Saebo and J. Almlöf, «Avoiding the integral storage bottleneck in LCAO calculations of electron correlation », *Chem. Phys. Lett*, 1989, 154 (1), 83-89. [https://doi.org/10.1016/0009-2614\(89\)87442-1](https://doi.org/10.1016/0009-2614(89)87442-1)
- [13] P. Hohenberg and W. Kohn, « Inhomogeneous Electron Gas. », *Phys. Rev*, 1964, 136, B864. <https://doi.org/10.1103/PhysRev.136.B864>
- [14] W. Kohn and L. J. Shan, «Self-Consistent Equations Including Exchange and Correlation Effects », *Phys. Rev*, 1965, 140, A 1133. <https://doi.org/10.1103/PhysRev.140.A113>
- [15] Alao Latifatou Laye, « Contribution to the study of carbene properties using Ab initio methods and Density Functional Theory (DFT) from quantum chemistry », Thesis, University of Félix Houphouët-Boigny, 2019.