TRƯỜNG ĐẠI HỌC SƯ PHẠM TP HỒ CHÍ MINH
TẠP CHÍ KHOA HỌC
KHOA HỌC TỰ NHIÊN VÀ CÔNG NGHỆ
Tập 16, Số 6 (2019): 62-71

ISSN: 1859-3100

HO CHI MINH CITY UNIVERSITY OF EDUCATION
JOURNAL OF SCIENCE
NATURAL SCIENCES AND TECHNOLOGY
Vol. 16, No. 6 (2019): 62-71

Email: tapchikhoahoc@hcmue.edu.vn; Website: http://tckh.hcmue.edu.vn

VIBRATIONAL EFFECT ON UNIDIRECTIONAL TIME-DEPENDENT ANGULAR MOMENTUM IN LOW-SYMMETRY AROMATIC RING MOLECULE INDUCED BY TWO LINEARLY POLARIZED UV LASER

***La Dung Kiet*[1*]*, Hirobumi Mineo*[2]**
[1] *Ho Chi Minh City University of Education*
[2] *Advanced Institute of Materials Science – Ton Duc Thang University*
[*] *Corresponding author: La Dung Kiet – Email: ladungkiet@gmail.com*

Received: 20/01/2019; Revised: 30/01/2019; Accepted: 24/5/2019

ABSTRACT

In this study, we present the results of a theoretical study of the time-dependent angular momentum equation for low-symmetry aromatic ring molecule combine with vibrational effect using two linearly polarized UV laser. We consider the vibrational effect on Toluene molecule and show how the vibrational effect to change of the oscillation periods of unidirectional angular momentum.

Keywords: vibrational effect, low-symmetry aromatic ring molecules, π-electron.

1. Introduction

Recent advances in laser science and technology have made it possible to generate ultrashort UV laser pulses. That is an effective way to study electronic dynamic (Yuan & Bandrauk, 2012). Aromatic ring is an overall concept in organic chemistry and it contains π-electron (Schleyer, 2001). Chemically, π-electron in aromatic ring molecules play an important role in chemical reactions because it makes chemical reactions take place faster due to the delocalizing of π-electron in aromatic ring molecules. Therefore, it plays a key role in chemistry. Likewise, research into rotation of π-electron in aromatic ring molecules which is expected to make an important contribution to organic nanoelectronics and optoelectronics such as the design of next-generation ultrafast switching devices (Anthony, 2006).

One of the important research directions on the interaction between laser and aromatic ring molecules, that is control of rotation of π-electron in aromatic ring molecules (π-electron was rotated when external fields excited it). Rotation of π-electron was presented by the angular momentum of π-electron. There have been several theoretical studies on the generation of rotation of π-electron in aromatic ring molecules excited by ultrafast UV pulsed lasers. Firstly, the results of quantum chemical simulations of π-electron rotations in high-symmetric ring molecules have been reported by Manz's group and others in 2006 by using ultrashort circularly polarized UV laser pulses on Mg-

Porphyrin molecule (Barth & Manz, 2006). In 2007, Nosubuda and Yabana presented photo-induced electric current of benzene with D_{6h} symmetry by circularly polarized laser pulses applying the time-dependent density functional approach (Nobusada & Yabana, 2007). Noted that Mg-Porphyrin and Benzene are two typical high-symmetry aromatic ring molecules. Highly symmetrical molecules having degenerate electronic states can produce stationary angular momentum, i.e. π-electron rotation along the aromatic ring molecular frame by using a circularly polarized laser. The direction of angular momentum can be determined by the laser polarization directions. In 2006, Kanno et al. have demonstrated that 2,5-dichloro[n](3,6) pyrazinophane (DCP) (Kanno, Kono, & Fujimura, 2006), which is a low-symmetry aromatic ring molecule as well as Toluene and the angular momentum of these molecules having non-degenerate excited states (space of two excited states is 0.1 eV); it can be generated by using ultrashort UV laser pulses. However, the generated angurlar momentum is not unidirectional. This means that the direction of the angular momentum in low-symmetry molecules changes with elapsed time. For this reason, the direction of the angular momentum cannot be controlled in low-symmetry aromatic ring molecules.

By 2016, H. Mineo et al. have found that unidirectional angular momentum can be produced even in low-symmetry molecules (Mineo et al., 2016). This control scenario utilizes a dynamic Stark shift of two non-degenerate excited states using two linearly polarized stationary lasers. Each laser is set to selectively interact with one of the two electronic states, the lower and higher excited states are shifted up and down with the same rate, respectively, and the two excited states become degenerate at their midpoint. This means that the unidirectional angular momentum in low-symmetry aromatic ring molecules has been made. However, Mineo's study was carried out without vibrational effect. In real molecules, molecular dynamic included electronic and nuclear dynamics; however, in order to simplify the calculation, we normally neglected vibrational effect in molecules. Practically, we need to combine with vibrational effect in study the direction of angular momentum in low-symmetry aromatic ring molecules. In this paper, we present the results of a theoretical study of the time-dependent angular momentum equation for low-symmetry aromatic ring molecule combine with vibrational effect using two linearly polarized UV laser. Moreover, we consider vibrational effect on Toluene molecule and show how the nuclear vibrational effect to change of the unidirectional angular momentum.

2. Theory

2.1. Time-dependent angular momentum equation of low-symmetry aromatic ring molecules

The rotation of π-electron in aromatic ring molecules takes place while exciting of the polarized lasers, is represented by the direction of angular momentum. For high-symmetry aromatic ring molecules, the clockwise or counterclockwise directions of angular momentum can be determined by the laser polarization directions (Barth & Manz, 2006). This means that we could control the direction of angular momentum in high-symmetry aromatic ring molecules. However, the direction of angular momentum in low-symmetry is not unidirectional when using ultrashort UV laser pulses (Kanno et al., 2006); it means that the direction of the angular momentum changes with elapse time. As a result, the direction of the angular momentum could not be controlled in low-symmetry aromatic ring molecules.

In 2016, H. Mineo et al. have found that unidirectional angular momentum can be produced even in low-symmetry aromatic ring molecules (Mineo et al., 2016). This control scenario utilizes a dynamic Stark shift of two non-degenerate excited states using two linearly polarized stationary lasers.

The time-dependent angular momentum for low-symmtry aromatic ring molecules (Mineo et al., 2016), which is defined as depending on the three electronic state (one ground electronic state and two excited electronic states) involved in initial conditions such as $c_0(0)=1$ and $c_1(0)=c_2(0)=0$, is expressed as

$$L(t)=\langle\phi(t)|\hat{l}_z|\phi(t)\rangle=-2\hbar\,\mathrm{Im}(l_{12})\,\mathrm{Im}\left[c_1^*(t)c_2(t)\exp(-i\omega_{21}t)\right] \tag{1}$$

here, l_{12} is pure imaginary of element of two excited electronic states in aromatic ring molecules, w_{21} º w_2- w_1 is frequency difference between the two excited states. The wavefunction in the total system including electric fields of the stationary laser is given in the semiclassical treatment of laser-electron interacsion as

$$\phi(t)=c_0(t)e^{-i\omega_0 t}\phi_0+c_1(t)e^{-i\omega_1 t}\phi_1+c_2(t)e^{-i\omega_2 t}\phi_2 \tag{2}$$

This is a method that has made unidirectional angular momentum of low-symmetry aromatic ring molecules (Mineo et al., 2016). However, in this method, authors did not calculate the vibrational effect, hence we will construct the time-dependent angular momentum equation of low-symmetry aromatic ring molecules involved vibrational effect.

2.2. Theory of nuclear vibration

2.2.1. Born-Oppenheimer approximation

For multi-particle systems, its Schrödinger equation cannot be solved analytically. To overcome this difficulty, we adopt the Born-Oppenheimer approximation. In real molecules, because of the great difference in masses of electrons and nuclei, the electron can respond almost instantaneously to the displacement of the nuclei. Therefore, instead of trying to calculate the Schrödinger equation for all the particles simultaneously, we regard the nuclei as fixed in position and calculate the Schrödinger equation for the electrons in the static electric potential arising from the nuclei in that particular arrangement.

The full Hamitonian is

$$\hat{H} = -\frac{1}{2m_e}\hbar^2 \sum_{i=1,2,...} \frac{\partial^2}{\partial r_i^2} - \frac{1}{2}\hbar^2 \sum_{j=1,2,...} \frac{\partial^2}{\partial Q_j^2} + V(r,Q) \qquad (3)$$

where $r_i = (\vec{r}_1, \vec{r}_2, ...)$ is coordinates of electrons in molecules, $Q_j = (Q_1, Q_2, ...)$ is normal modes coordinates (unit: a.u), $V(r,Q)$ is potential energy of molecule.

The wavefunction of systems is written as a combination of the electronic wavefunction and nuclear wavefunction.

$$\phi(r,Q,t) = \sum_i c_i(t)\psi_i(r,Q)\exp(-i\omega_i t) \qquad (4)$$

From Eq (4), we can separated wavefunction of the system to be electronic wavefunction and the nuclear wavefunction.

$$\psi(r,Q) = \sum_\alpha \psi_\alpha(r,Q)\Theta_\alpha(Q) \qquad (5)$$

here $\psi_\alpha(r,Q)$ is the electronic wavefunction and $\Theta_\alpha(Q)$ is the vibrational wavefunction. The notation $\psi_\alpha(r,Q)$ means that the wavefunction for the electron is a function of its position r and depends parametrically on the coordinates of the normal modes, each fixed possition of normal modes Q.

2.2.1. Vibrational overlap integrals (Franck-Condon overlap integral)

Because nuclear masses are larger than the mass of an electron; as a result, the nuclear locations remain unchanged during the actual transition, but then readjust once the electrons have adopted their final distribution.

In other words, when an electronic transition takes place, new arrangement of vibronic states in each electronic state occurs. In real molecules, the ground vibronic state is not the highest contribution. Therefore, we should solve this problem within the contributions of vibronic states in each electronic state.

Franck-Condon overlap integral is approached from many different ways (Kupka & Cribb, 1986), (Lin, Li, Yamaki, Hayashi, & Lin, 2010), depend on initial conditions and parameter in the calculation.

The Franck-Condon overlap integral between $\alpha' v'$ and αv vibronic states is given by

$$I_{\alpha v,\alpha' v'} = \langle \Theta_{\alpha' v'} | \Theta_{\alpha v} \rangle \qquad (6)$$

where $\Theta_{\alpha v}$ is vibronic wavefunction in α electronic state, $\Theta_{\alpha' v'}$ is vibronic wavefunction in α'electronic state, with v and v' present vibronic state in α and α' electronic states, respectively. In this calculation, we utilize harmonic oscillator wavefunction to replace for molecular wavefunction because it had an analytical solution which defined in almost textbook of quantum mechanics.

3. Time-dependent angular momentum equation in low-symmetry aromatic ring molecules considering vibrational effect

In section 2.1, we introduced unidirectional angular momentum of π-electron in low-symmetry aromatic ring molecules (Mineo et al., 2016). However, the vibrational effect is not involved in Eq (1). Therefore, in this section, we present a time-dependent angular momentum of π-electron in low-symmetry aromatic ring molecules considering the vibrational effect.

In involvement of vibrational effect, the molecular wavefuntion is the superposition of electronic motion and vibronic states

$$\phi(r,Q,t)=\sum_{\alpha,v}c_{\alpha v}(t)\psi_{\alpha v}(r,Q)\exp(-i\omega_{\alpha v}t) \tag{7}$$

In Eq (7), molecular wavefunction involved in nuclear and electronic coordinates, hence we utilized Born-Oppenheimer approximation in order to separated wavefunction becomes multiplication of electronic wavefunction and nuclear wavefunction.

$$\psi_{\alpha v}(r,Q)=\psi_{\alpha}(r,Q)\Theta_{\alpha v}(Q) \tag{8}$$

The interaction between the system and two laser fields within the dipole approximation, is expressed as

$$V(t)=\boldsymbol{\mu}\cdot\mathbf{e}_aF_a\cos(\omega_a t-\xi_a)+\boldsymbol{\mu}\cdot\mathbf{e}_bF_b\cos(\omega_b t-\xi_b) \tag{9}$$

where $\boldsymbol{\mu}$ is electronic dipole moment operator, $\boldsymbol{\mu}=-e\mathbf{r}$ in which $\mathbf{r}$ denotes the electron coordinates, $\mathbf{e}$ is the photon polarization vector, F is the laser amplitude, ω_a,ω_b are the frequency of two linear laser polarized, respectively, In eq (9), the two linearly polarized electric fields F_a,F_b induce nonresonant trasitions between the ground and the two excited states, resprectively. The condition of the selective transitions is to set the photon-polarization vectors $(\mathbf{e}_a,\mathbf{e}_b)$ to satisfy $\boldsymbol{\mu}_{02}\perp\mathbf{e}_a$ and $\boldsymbol{\mu}_{01}\perp\mathbf{e}_b$.

The time-dependent Schrödinger equation including electronic states and vibronic states is given as

$$\frac{\partial c_{\alpha v}}{\partial t}=-\frac{i}{\hbar}\sum_{\alpha' v'}V_{\alpha v,\alpha' v'}(t)\exp(-i\omega_{\alpha' v',\alpha v}t)c_{\alpha' v'}(t) \tag{10}$$

where $\omega_{\alpha' v',\alpha v}$ is the frequency difference between αv and $\alpha' v'$ states, $V_{\alpha v,\alpha' v'}(t)$ is the element matrix which denotes association between α and α' states through interaction field is given by

$$V_{\alpha v,\alpha' v'}(t)=\langle\psi_{\alpha v}|-\boldsymbol{\mu}\cdot F(t)|\psi_{\alpha' v'}\rangle \tag{11}$$

The combination between eq (8) and eq (11), we have

$$V_{\alpha v,\alpha' v'}(t)=\langle\Theta_{\alpha v}|-\boldsymbol{\mu}_{\alpha\alpha'}\cdot F(t)|\Theta_{\alpha' v'}\rangle \tag{12}$$

here $\boldsymbol{\mu}_{\alpha\alpha'}$ is dipole moment operator, $F(t)$ is laser amplitude. As a result, eq (12) have became

$$V_{\alpha v,\alpha' v'}(t) \approx -\boldsymbol{\mu}_{\alpha\alpha'}(Q_0)\cdot F(t)\langle \Theta_{\alpha v}|\Theta_{\alpha' v'}\rangle \tag{13}$$

here $\boldsymbol{\mu}_{\alpha\alpha'}(Q_0)$ denotes dipole moment operator is calculated in equilibrium point $(Q = Q_0)$ in the electronic ground state.

Eq (13), $\langle \Theta_{\alpha v}|\Theta_{\alpha' v'}\rangle$ is the Franck-Condon overlap integral in eq (6), which has the general from as written in Eq (5). For this reason, eq (11) is expressed as

$$V_{\alpha v,\alpha' v'}(t) \approx -\boldsymbol{\mu}_{\alpha\alpha'}(Q_0)\cdot F(t) I_{\alpha v,\alpha' v'} \tag{14}$$

From eq (1), we defined the value of time-dependent angular momentum including the vibrational effect

$$L(t) = \langle \phi|\hat{l}_z|\phi\rangle = -2\hbar\sum_{\alpha v}\mathrm{Im}\left(c^*_{1u}(t)c_{2v}(t)\exp\left(-i\omega_{2v,1u}t\right)\right)\mathrm{Im}\left(\langle \psi_{1u}|l|\psi_{2v}\rangle\right) \tag{15}$$

Utilizing Condon approximation $\psi_{\alpha v}(r,Q) \approx \psi_{\alpha}(r,Q_0)\Theta_{\alpha v}(Q)$ and $l_{12} = \langle \psi_1|l|\psi_2\rangle$ which is pure imaginary, thus $\langle \psi_{1u}|l|\psi_{2v}\rangle$ in eq (14) as

$$\langle \psi_{1u}|l|\phi_{2v}\rangle = \langle \psi_1(t)|l|\psi_2(t)\rangle\langle \Theta_{1u}|\Theta_{2v}\rangle = l_{12}I_{1u,2v} \tag{16}$$

The combination between eq (15) and eq (16), we have the unidirectional time-dependent angular momentum of π-electron in low-symmetry aromatic ring molecules including vibrational effect.

$$L(t) \approx -2\hbar\sum_{uv} I_{1u,2v}\,\mathrm{Im}\left(c^*_{1u}(t)c_{2v}(t)\exp\left(-i\omega_{2v,1u}t\right)\right)\mathrm{Im}\,l_{12} \tag{17}$$

In the next section, we present the detailed calculation for a particular low-symmetry aromatic ring molecule, it is Toluene.

4. Results and discussion

In the previous section, we derived an analytical expression for the expectation value of the angular momentum operator including the vibrational effect, $L(t)$ for, an aromatic ring molecule with low-symmetry in a three-electronic state model. We now apply the formula to a real molecular system, Toluene. The three-electronic state model is valid for toluene in lower excited, π-electronic states since the π-electronic structure in toluene is close to that in benzene: a pair of optically allowed excited states in toluene originates from the doubly degenerate E_{1u} excited state of benzene (D_{6h}). In order to calculate the value of time-dependent angular momentum in toluene, we have built the Fortran code based on Runge-Kutta numerical method.

Firstly, to ensure the high reliability of our Fortran code, we show and compare our result for time-dependent angular momentum of toluene for the case of without vibrational effect with the result of another author (Mineo et al., 2016). Particular, the Franck-Condon overlap integral is zero $\left(I_{\alpha v,\alpha' v'} = 0\right)$ in without vibrational effect case. Fig. 1 illustrates the results that was calculated according to our Fortran code. Fig. 1, expectatoin values of the angular momentum operator for toluene, $L(t)$, in units of $\hbar$, with $\xi\left(\equiv \xi_a - \xi_b\right)$ is the laser relative phase.Two linear polarized laser control the Stark shift of two excited states in laser amplitude is $F_a = 1.5GV/m$, $F_b = 1.4GV/m$, respectively. As in Fig. 1, our results for expectation value of time-dependent angular momentum, that was calculated according to out Fortran code, are basically similar to another author's one (Mineo et al., 2016). This means that our Fortran code is high reliability.

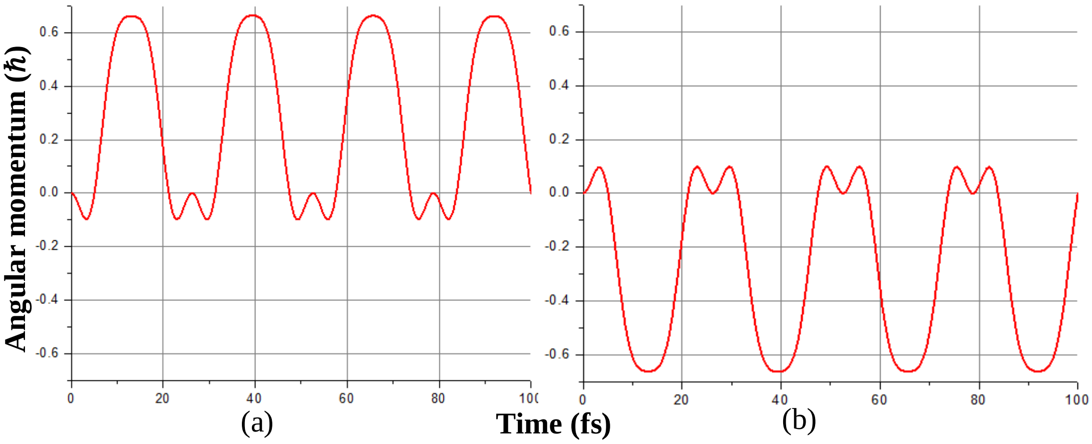

Fig. 1. *Expectation values of the angular momentum operator for toluene, $L(t)$ (unit: $\hbar$), (a) $\xi = -\pi/2$; (b) $\xi = \pi/2$*

Fig. 1a, the magnitude of the unidirectional angular momentum with $\xi = -\frac{\pi}{2}$ is positive, $L(t) > 0$, it means the direction of angular momentum is counterclockwise. In other words, rotation of π-electron in toluene is counterclockwise at that time. Likewise, Fig. 1b for those with $\xi = \frac{\pi}{2}$; in this case, the magnitude of the unidirectional angular momentum is negative, $L(t) < 0$, and direction of which is clockwise. Thus, the formation of degenerate dressed states with a relative phase of $\xi = \pm\frac{\pi}{2}$ is the origin of the unidirectional π-electron rotation.

In addition, we present the expectation value of unidirectional angular momentum operator, $L(t)$, including the vibrational effect. As seen in eq (17), it depends on $c_{1u}(t)$ and $c_{2v}(t)$ parameters, which have been calculated based on eq (10) with initial conditions are $c_{00}(0)=1$ and $c_{10}(0)=c_{20}(0)=0$; and laser amplitute is $F_a=1.5GV/m$, $F_b=1.4GV/m$, respectively.

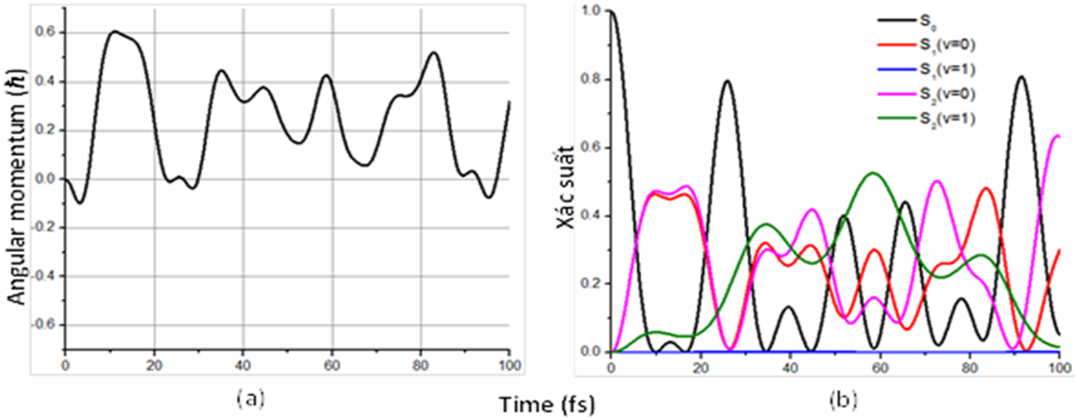

Fig. 2. *a) Expectation values of the angular momentum operator for toluene, $L(t)$ (unit: $\hbar$), including vibrational effect; b) temporal population of the unidirectional angular momentum in toluene.*

Fig. 2 gives information about the expectation values of the angular momentum for toluene, $L(t)$, including vibrational effect; we can see these values is not stable. It can be seen in Fig. 1 and Fig. 2 that the oscillation periods of angular momentum pulses are slight differences. Specifically, the oscillation periods of angular momentum are the same between 0 fs and 10 fs, due to the popultation of $S_1(v=1)$ and $S_2(v=1)$ is quite small. This demonstrates that the value of unidirectional angular momentum operator, $L(t)$, in toluene has been affected hardly under vibrational effect as soon as the interaction between laser and molecule. When the time is greater than 10 fs, the oscillation periods of unidirectional angular momentum, $L(t)$, in Fig.2a is not stable that compared with which of Fig. 1. Because of the time is greater than 10 fs, two excited states of toluene have excited is closer and closer each other; at that time, the magnitude of the unidirectional angular momentum operator, $L(t)$, are affected under vibrational states within electronic states in toluene. The population of $S_1(v=1)$ and $S_2(v=1)$ is increasing, but the population of $S_1(v=1)$ experienced moderate increase, it is approximately zero; hence $S_2(v=1)$ is the state that mainly affected the oscillation periods of angular momentum. That is the main reason which impacted on changing of the oscillation periods of angular momentum pulses, $L(t)$, in toluene compared with the neglect vibrational effect in Fig. 1. Moreover, it is interesting to see the $L(t)$-dependence of the population of $S_2(v=1)$. It can be seen from comparison between Fig. 2a and Fig. 2b that the oscillation periods of unidirectional angular momentum pulses, $L(t)$, have decreased, so the population of $S_2(v=1)$ have also decreased.

5. Conclusion

In this paper, we proposed the equation of unidirectional time-dependent angular momentum operator including vibrational effect, Eq (17), that is combination between vibrational computational methods. The wavefunction was separated into electronic wavefunction and vibrational wavefunction under Born-Oppenheimer approximation. The vibrational states have been presented by Franck-Condon overlap integral. In addition, results show the changing of the oscillation periods of unidirectional angular momentum and comparision between within vibrational effects and without vibrational effect. Moreover, from these results, we consider carefully the vibronic coupling that affects the oscillation periods of unidirectional angular momentum in toluene.

- ***Conflict of Interest:*** *Authors have no conflict of interest to declare.*
- ***Acknowledgement:*** *This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.03-2018.60.*

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HIỆU ỨNG DAO ĐỘNG CỦA MÔMEN ĐỘNG LƯỢNG ĐƠN HƯỚNG PHỤ THUỘC THỜI GIAN TRONG PHÂN TỬ VÒNG THƠM ĐỐI XỨNG THẤP ĐƯỢC TẠO RA KHI SỬ DỤNG HAI LASER PHÂN CỰC THẲNG

***La Dũng Kiệt*[1*], *Hirobumi Mineo*[2]**

Trường Đại học Sư phạm Thành phố Hồ Chí Minh

Viện Khoa học Vật liệu tiên tiến – Trường Đại học Tôn Đức Thắng

[*] *Tác giả liên hệ: La Dũng Kiệt – Email: ladungkiet@gmail.com*

Ngày nhận bài: 20-01-2019; ngày nhận bài sửa: 30-01-2019; ngày duyệt đăng: 24-5-2019

TÓM TẮT

Trong nghiên cứu này, chúng tôi trình bày kết quả của một nghiên cứu tính toán lí thuyết về phương trình mômen động lượng phụ thuộc thời gian cho phân tử vòng thơm đối xứng thấp bao gồm hiệu ứng dao động khi sử dụng hai laser phân cực thẳng. Để khảo sát điều đó, chúng tôi xem xét hiệu ứng dao động trong phân tử Toluene và mô tả ảnh hưởng của hiệu ứng dao động đến sự thay đổi dao động theo thời gian của mômen động lượng đơn hướng.

Từ khóa: hiệu ứng dao động, phân tử vòng thơm đối xứng thấp, π-electron.