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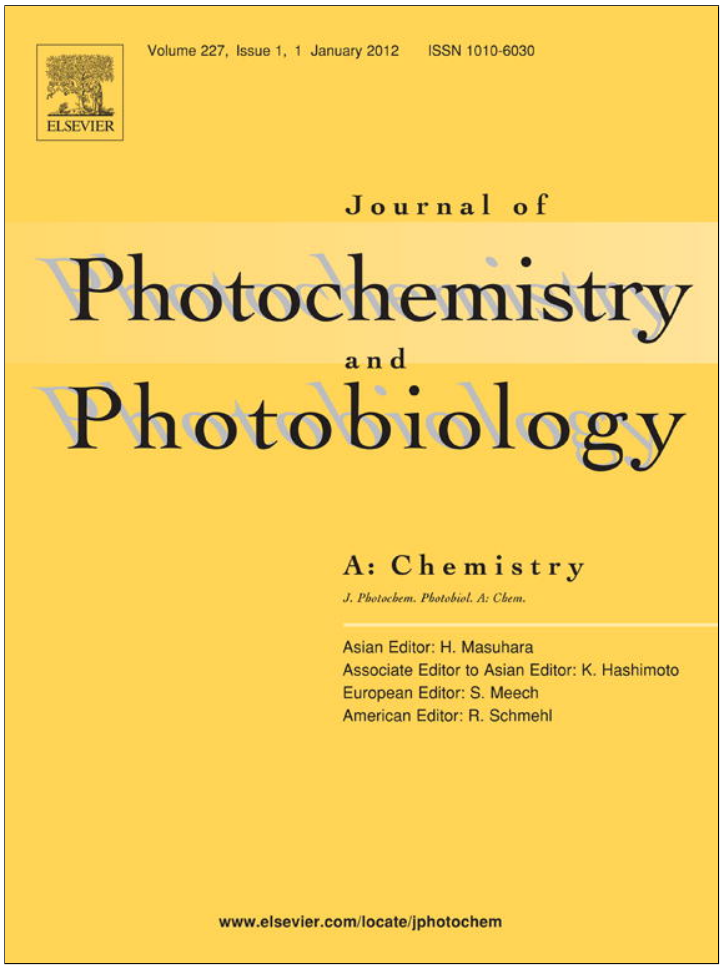

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Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives

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ABSTRACT

We present the CAM (Coulomb Attenuated Method)-B3LYP functional tuned for excitation energies and properties of diarylethene derivatives in the time-dependent density functional theory (TD-DFT) scheme. The CAM-B3LYP parameters are tuned so as to well reproduce the experimental excitation energies and properties of a prototypical diarylethene derivative. The TD-DFT method with the tuned CAM-B3LYP parameters ($\mu = 0.150$, $\alpha = 0.0799$ and $\beta = 0.9201$) is found to semi-quantitatively reproduce several excitation energies obtained from the experimental UV–vis spectra of 15 closed forms of diarylethene derivatives. In contrast, it turns out that the use of default CAM-B3LYP parameters ($\mu = 0.33$, $\alpha = 0.19$, and $\beta = 0.46$) fails to well reproduce these experimental UV–vis spectra. We also clarified that this difference does not originate from the functional dependence of the ground state optimized geometry, but from the CAM-B3LYP parameter dependences of excitation energies and properties in the TD-DFT scheme.

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1. Introduction

Photochromism is defined as reversible isomerization between two isomers, where at least one direction of the reversible reactions is a photoinduced reaction. Since this reaction involves quick property changes such as absorption spectra, refractive indices, dielectric constants, nonlinear optical responses, and redox potentials, the photochromic reactions have attracted much attention due to their potential applications in future optoelectronic devices such as high capacity optical memory and ultra high-speed optical switch [1–4].

Among various photochromic compounds, diarylethene derivatives undergo cyclization and cycloreversion reactions in 6π-electrocyclic systems. One of the most important properties of the diarylethene derivative is the color of the closed form, i.e., its spectrum, which depends on the energy difference between the ground and excited states. Moreover, the photochromic reaction takes place via excited states. Therefore, the reliable evaluation of the excited states is essential for analyzing the photochromic reaction and for constructing the molecular design rule of photochromic compounds. One of the promising methods to calculate the excited states of relatively large size molecules is the time-dependent density functional theory (TD-DFT) method. The TD-DFT method is known to well reproduce the highly-electron-correlated ab initio molecular orbital (MO) results and experimental spectra for organic molecular systems with remarkably low computational costs [5]. Nevertheless, the TD-DFT results are known to strongly depend on the exchange-correlation functional employed in the calculations [6–13]. Jacquemin et al. reported that linear regression of excitation wavelength obtained by TD-DFT calculation could reproduce experimental excitation wavelength of diarylethene derivatives very well [14–16]. Furthermore, our goal is not only reproducing experimental UV–vis spectra, but also establishing methodology to theoretically investigate photochromic reaction via excited state. Therefore, we directly improved exchange-correlation functional.

It is well known that standard DFT functionals have several deficiencies, e.g., (1) underestimation of reaction barriers, (2) non-reproducibility of weak bonds such as van der Waals bond, (3) overestimation of linear and non-linear optical responses, and (4) underestimation of charge transfer and Rydberg excitation energies by TD-DFT calculation. In order to reduce these drawbacks, several treatments have been proposed. For example, Tsuneda et al. developed the long-range-corrected (LC) scheme, where the electron repulsion operator is split into two parts and the long-range exchange part is treated in the exact manner, i.e., using the Hartree-Fock (HF) exchange [17]. The LC scheme is found to achieve great improvement both for the ground and excited state properties [18–25]. Later, Yanai et al. have introduced additional flexible parameters into the LC functional, so-called Coulomb attenuated method (CAM), which depends on three parameters [26]. This functional is also found to give quantitatively good results for the ground state properties.

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Parameters in these functionals are optimized so as to reduce the differences between the calculated and experimental values (ground state structures, ionization energies, atomization energies, a heat of formation, etc.) for several molecular sets [17,26–28]. This implies that the LC/CAM-functional with default parameters does not always reproduce experimental UV spectra quantitatively, so that there still remains a room for tuning these parameters in order to improve the excitation energies and properties of specific molecular sets. In this study, we tune the parameters in CAM-B3LYP, i.e., α, β, and μ, so as to well reproduce the experimental excitation energies and properties of a prototypical diarylethene derivative. Then, using the tuned parameters, we examine its applicability to those quantities of other diarylethene derivatives. The present study not only presents the optimal parameters in the CAM-B3LYP functional tuned for the excitation energies and properties of diarylethene derivatives, but also provides a useful tuning procedure of CAM-B3LYP parameters for excited states of arbitrary molecular systems.

This paper is organized as follows. In Section 2, we provide the theoretical background and explain the tuning methods of parameters in the CAM-B3LYP functional. Details of the numerical results as well as the comparison with experimental results and discussion are given in Section 3. These results are summarized in Section 4.

2. Theoretical background and computational details

In the LC scheme, electron repulsion operator $1/r_{12}$ is split into short-range and long-range parts as follows:

$$\frac{1}{r_{12}} = \frac{1 - erf(\mu r_{12})}{r_{12}} + \frac{erf(\mu_{12})}{r_{12}} \quad (1)$$

where *erf* indicates the error function. The short-range part, the first term of Eq. (1), is treated by the exchange-correlation functional adopted in the DFT, while the long-range part, the second term of Eq. (1), is treated by the exact HF exchange. This functional guarantees correct behavior at an asymptotic ($r_{12} \rightarrow \infty$) region, where the Coulomb and exchange potential should cancel with each other. It is noted here that most of the local density approximation (LDA), the generalized gradient approximation (GGA), even usual hybrid functionals do not fulfill the condition exactly. The default parameters are found to be $\mu = 0.33$ and 0.47 depending on the systems of interest [18,19].

Yanai et al. have generalized Eq. (1) as

$$\frac{1}{r_{12}} = \frac{1 - [\alpha + \beta \cdot erf(\mu r_{12})]}{r_{12}} + \frac{\alpha + \beta \cdot erf(\mu_{12})}{r_{12}} \quad (2)$$

where $0 \le \alpha \le 1$, $0 \le \beta \le 1$, $0 \le \alpha + \beta \le 1$, and α and $\alpha + \beta$ represent the HF exchange fractions in the short- and long-range limits, respectively. Since the above CAM functional includes a larger number of parameters (μ, α, β) than the LC functional including one parameter μ, the CAM functional could be more flexible than the LC one. The functional composed of the Becke 88 exchange functional for the short-range part and VWN5 (19%) + LYP (81%) for the correlation functional is referred to as the CAM-B3LYP functional. The default parameters are chosen to be $\mu = 0.33$, $\alpha = 0.19$, and $\beta = 0.46$, which turn out to well reproduce the ground state properties [26].

In the present calculations, we have employed Gaussian 09 program package [29] to perform the geometry optimization, vibrational analysis, and excited state evaluations. All calculations have been performed by the CAM-B3LYP method with the default (standard) and tuned parameters with triple-ζ polarization basis set, i.e., 6–311G(d, p).

First, the ground-state structures of diarylethene derivatives **1**–**15** (Scheme 1) have been optimized using the standard CAM-B3LYP method followed by the vibrational analysis, which confirms that all vibrational frequencies are real. Second, in order to tune the parameters (α, β, and μ) in the CAM-B3LYP functional, we have evaluated the excited states of a specific derivative **1** (Scheme 1). We here fixed $\alpha + \beta = 1$ in order to ensure the correct asymptotic behavior, i.e., only the HF exact exchange in the long-range limit. The TD-DFT method was then employed to compute 20 low-lying excited states. These sequential calculations, i.e., (i) the geometry optimization, (ii) the vibrational analysis, and (iii) the excited state evaluation, were performed with the several CAM-B3LYP parameters. For each μ, we fitted the α dependences of excitation energies of 5 excited states with large oscillator strengths by means of the 5th order polynomials, and analyzed the difference between the experimental values and the estimated values by the polynomials by a least-squares method in order to tune the parameters.

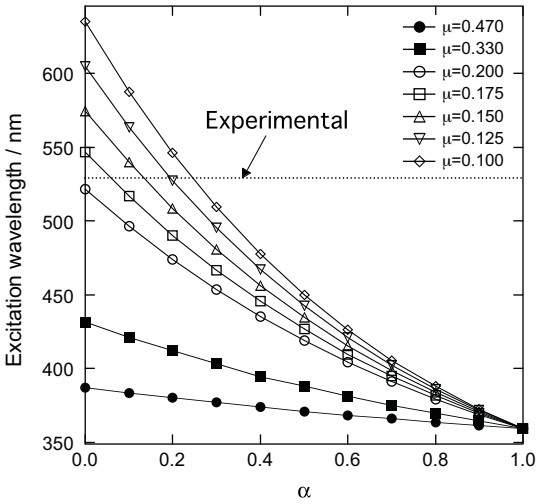

Fig. 1. α dependence of excitation wavelengths for S_1 state of **1** (Scheme 1) at each μ value.

Finally, we examined the excited states of 15 diarylethene derivatives of **1**–**15** (Scheme 1) with these tuned parameters in order to assess the applicability and reliability of the obtained tuned parameters for the calculation of a series of the diarylethene derivatives.

3. Results and discussion

We evaluated the excited states of **1** (Scheme 1) by changing α under the condition of $\alpha + \beta = 1$ at fixed μ values. Fig. 1 shows the α dependence of the excitation wavelengths for the S_1 state at each μ value. The tendency turns out to be the same for all μ values, where the excitation wavelength monotonically decreases with increasing α. In addition, the excitation wavelength is found to monotonically increase with decreasing μ. Judging from these results, there exists an optimal α value to reproduce experimental value (529 nm, Ref. [36]) for μ less than 0.2. This value is much less than the default values ($\mu = 0.33$ and 0.47) and slightly less than those suggested by Jacquemin et al. from the calculation of the excited states of 483 molecules ($\mu = 0.20$) [30] and other studies [31–35]. On the other hand, the default parameter set is found to give 2.6557 eV for S_1 state, which overestimates the experimental value by 0.3157 eV (13.5%).

Fig. 2 shows the α dependences of the 5 excitation energies of **1** at $\mu = 0.175$, 0.150, 0.125 and 0.100. Solid lines are drawn using the 5th order polynomial fitting. We obtained the parameters tuned for each μ by minimizing the sum of squared differences between the experimental values [36] and those estimated by the polynomials. For $\mu = 0.175$, the tuned α value does not exist in $0 \le \alpha \le 1$. It is found that for $\mu = 0.150$, 0.125 and 0.100, the tuned values are (α, β) = (0.0799, 0.9201), (0.1483, 0.8517) and (0.2049, 0.7951), respectively. It is shown that the intensity ratio of the second and third

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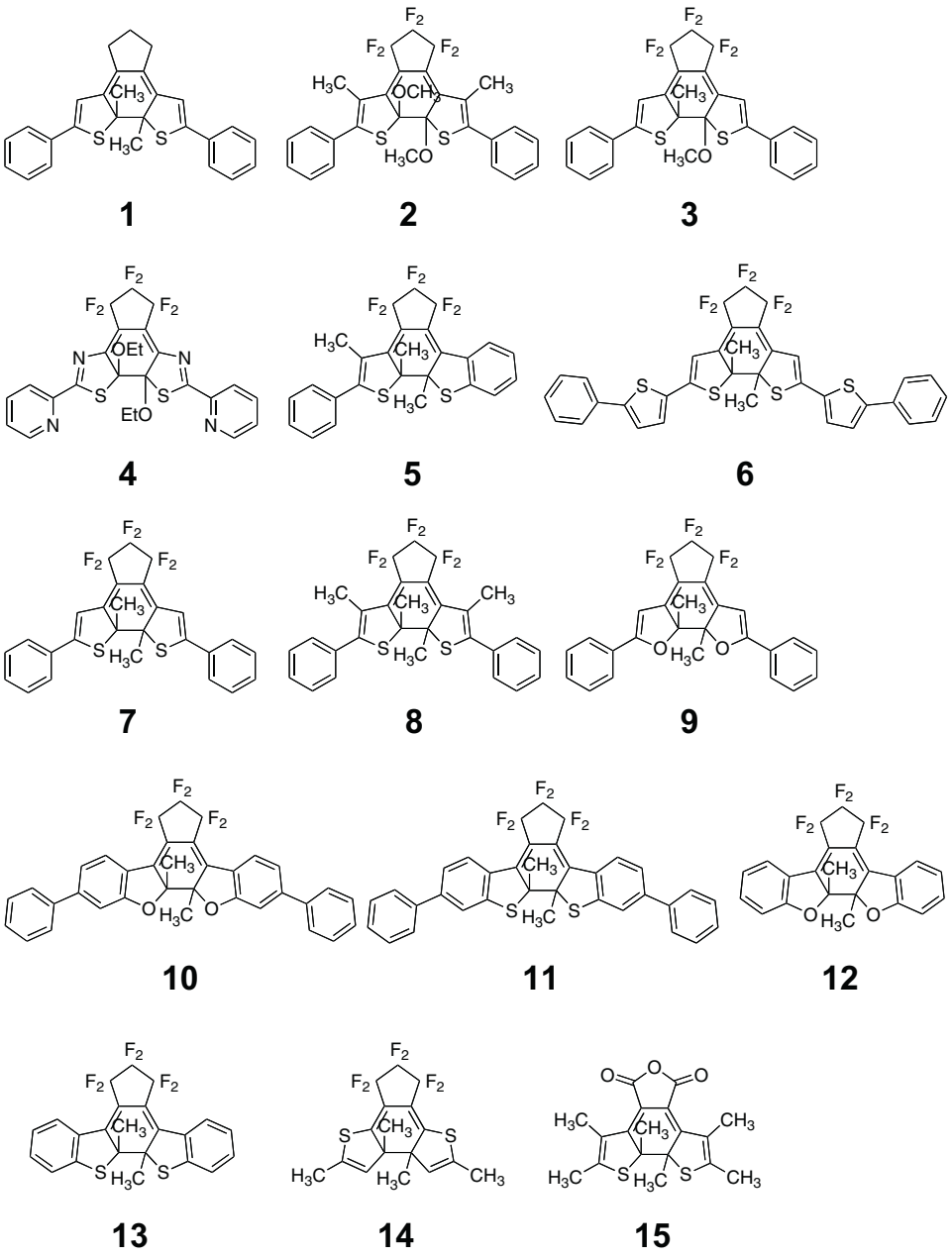

Scheme 1. Structures of diarylethene derivatives.

peaks in the experimental spectrum is about 1:1 [36]. It is found that for $\mu = 0.150$, two peaks are shown to be almost equally weighted, while the oscillator strengths of S_2 and S_3 states become unequally weighted when μ is less than 0.15. As a result, we adopted $\mu = 0.150$, $\alpha = 0.0799$, $\beta = 0.9201$ as the tuned parameters for the following calculations.

Next, we assess the applicability of the tuned parameters using the calculated excitation energies of other diarylethene derivatives. We evaluated the excited states of compounds **1**–**15** using the TD-DFT method with the tuned CAM-B3LYP functional. Fig. 3 shows the comparison between the experimental [36–51] and theoretical excitation wavelengths of totally 50 excited states with large oscillator strengths. The red circle shows the excitation wavelength calculated by the tuned TD-CAM-B3LYP//tuned CAM-B3LYP method, where A//B indicates that method A is adopted for the calculation of excitation energy, while method B for the geometry optimizations. The theoretical excitation wavelengths are found to well reproduce the experimental ones within 1.3% error. On the other hand, the excitation wavelengths calculated by the standard TD-CAM-B3LYP//standard CAM-B3LYP method (black cross) are shown to significantly underestimate the experimental ones by 12.5%. This implies that the tuning of the CAM-B3LYP parameter set is an efficient and powerful method for obtaining reliable excitation spectra at least for a series of molecules with the common molecular backbone, i.e., the diarylethenes in the present case. Moreover, we investigated the effect of the ground state optimized geometries on the excitation wavelength. The black circle shows the excitation wavelength calculated by the tuned TD-CAM-B3LYP//standard CAM-B3LYP method and a red cross shows that calculated by the standard TD-CAM-B3LYP//tuned CAM-B3LYP method. It turns out that the former (black circle) again well reproduces the experimental wavelengths within 1.6% error, while the latter underestimates those by 9.5%. We thus concluded that the functional dependence of the molecular structure is not strong and

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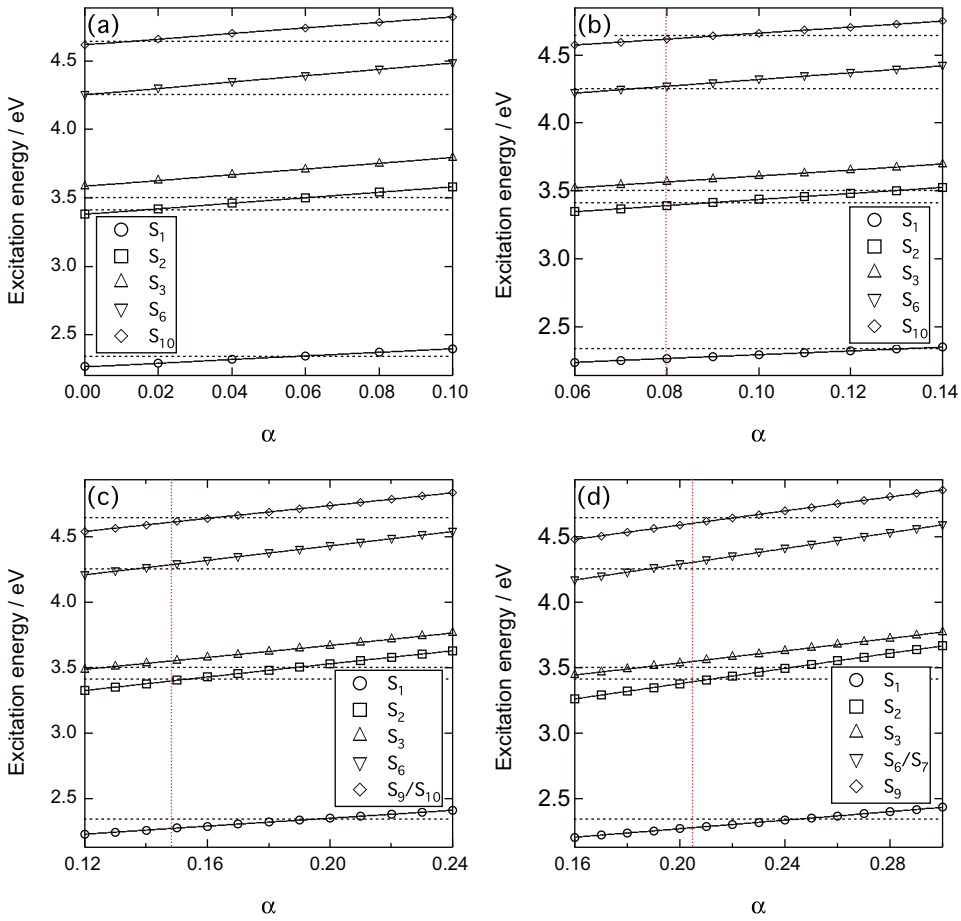

Fig. 2. α dependences of excitation energies for 5 excited states of **1** (Scheme 1): μ = 0.175 (a), 0.150 (b), 0.125 (c), 0.100 (d). Horizontal dashed black and vertical dotted red lines represent the experimental values for these excited states and the optimized α values, respectively.

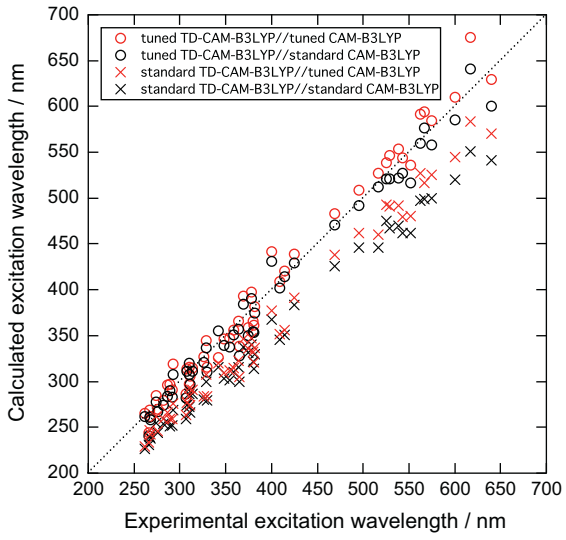

Fig. 3. Comparison between the experimental and theoretical excitation wavelengths of 15 diarylethene derivatives calculated by the TD-CAM-B3LYP method. Red circle, black circle, red cross and black cross represent tuned TD-CAM-B3LYP//tuned CAM-B3LYP, tuned TD-CAM-B3LYP//standard CAM-B3LYP, standard TD-CAM-B3LYP//tuned CAM-B3LYP and standard TD-CAM-B3LYP//standard CAM-B3LYP, respectively. Here, the method in front of (after) "//" indicates that for the calculation of excitation energy (geometry optimization). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

the functional used for calculating the excited states plays an essential role on the reliability of the obtained excitation energies and properties. Moreover, this trend also remains valid in the excited state calculations with the molecular structures optimized by the B3LYP method (see Fig. 1S in Supporting Information). We again confirmed that the theoretical excitation wavelengths calculated by the LC-BLYP (μ = 0.33) method underestimate the experimental excitation wavelengths more significantly than those by the standard CAM-B3LYP method (see Fig. 2S in Supporting Information).

It should be noted here that all of the UV–vis spectra are not always reproduced in the present scheme. Although a certain peak of experimental UV–vis spectrum of **13** splits into 2 peaks [48], the functionals examined in the present study could not reproduce this split. It is expected that the origin of the split might be due to the existence of different conformers or to the effect of large amplitude vibration, since the other derivatives do not exhibit such spectral split. Further investigation is needed to clarify this origin.

Finally, we demonstrate the performance of the tuned CAM-B3LYP method for the ground state properties by comparing with those by the methods with different functionals. Fig. 4 shows the bond lengths of heavy elements and the dihedral angle of a phenyl group in the geometry of **1** optimized by the 4 functionals, i.e., LC-BLYP (μ = 0.33), standard CAM-B3LYP, tuned CAM-B3LYP and B3LYP. Judging from the optimized geometries, the results by the standard CAM-B3LYP are quite similar to those by the LC-BLYP, while those by the tuned CAM-B3LYP are quite close to those by the B3LYP. It is well known that the B3LYP functional well reproduces the ground state geometry of various molecules. Therefore, the tuned CAM-B3LYP has the possibility of reproducing not only

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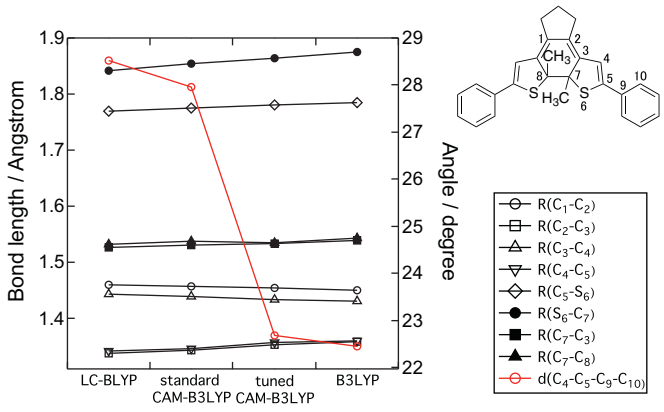

Fig. 4. Bond lengths and dihedral angle of phenyl group in geometry of **1** optimized by 4 functionals: LC-BLYP ($\mu = 0.33$), standard CAM-B3LYP, tuned CAM-B3LYP and B3LYP.

the UV–vis spectra but also the ground state geometries of these species. As seen from the frontier orbital energies of **1** calculated by different functionals (Fig. 5), the orbital energies obtained by the standard and tuned CAM-B3LYP functionals are almost comparable to each other. In contrast, the orbital energies calculated by the tuned CAM-B3LYP are different from those by the B3LYP and LC-BLYP. In particular, it is found that the HOMO–LUMO gap obtained by the B3LYP is smaller, while that by the LC-BLYP is larger than those by the tuned/standard CAM-B3LYP. From these results, it is expected that the present functional gives a well-balanced description for both the molecular structure and frontier orbital energies.

Nevertheless, it is stressed here that there is no guarantee that the present functional always gives good results for arbitrary compounds. In this study, we demonstrate that the tuned parameters in the CAM-B3LYP scheme succeed in reproducing the excitation spectra of at least a series of diarylethenes, where the main contribution of the excited states originates from the common molecular structure. The applicability of the present parameter set to a wide variety of compounds will be reported in future.

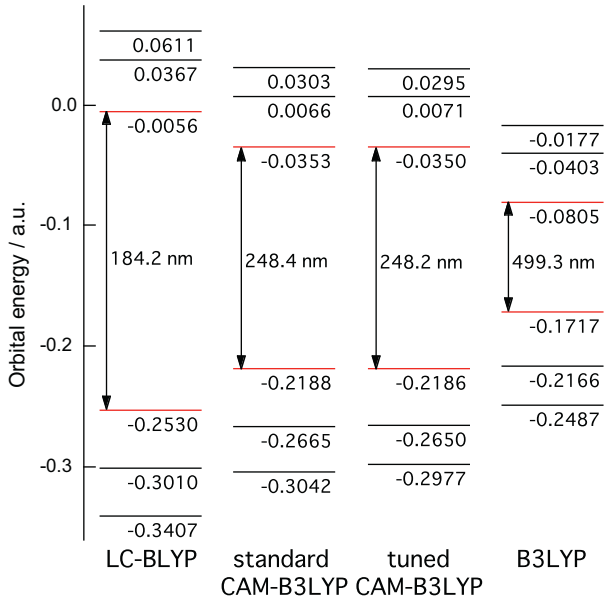

Fig. 5. Frontier orbital energies of **1** calculated by 4 functionals: LC-BLYP ($\mu = 0.33$), standard CAM-B3LYP, tuned CAM-B3LYP and B3LYP.

It is well known that the TD-DFT calculation of excitation spectra also remarkably depends on the choice of the exchange-correlation functional. In general, the exchange-correlation functionals widely employed at present work well for low-lying valence excited states of small organic molecules. Actually, for high-lying, Rydberg, charge transfer, and even some valence excitations, it is crucial that the asymptotic behavior of the exchange-correlation potential is correct, i.e., the Coulombic and exchange contributions are compensated each other. According to Casida et al. [51] and Tozer et al. [52] an asymptotic correction scheme improves TD-DFT performance, i.e., excitation energy. Tawada et al. have shown that the LC functional overcomes several drawbacks appearing in the TD-DFT calculations [18], where the true asymptotic behavior is ensured. In this study, we also chose that $\alpha + \beta = 1$ is the essential constraint condition for the correct asymptotic behavior in our parameter tuning strategy for the excited states. On the other hand, the standard CAM-B3LYP parameters ($\alpha + \beta = 0.65$) do not satisfy this condition. It is likely that the better performance of the present scheme than of the standard CAM-B3LYP partially raises from the correct asymptotic behavior of the functional.

It is also well known that the HF and DFT methods suffer from localization and delocalization error, respectively. So, mixing both HF and DFT exchange terms tends to cancel these errors. In this study, where α is negligible, tuned $\mu = 0.15$ is much smaller than the values tuned in past studies ($\mu = 0.33$ or 0.47), which were optimized by minimizing the error of the calculated equilibrium distances for the dimers of the first to third-row atoms (except rare-gas dimers) [18] and of the atomization energy of G2 set of molecules [19], respectively. Since most molecules in the G2 set are not π-conjugated systems, the conventional μ values are predicted to be more suitable for the σ-bonding molecules whose electronic ground state is well localized. On the other hand, for the excited states of the π-conjugated systems such as C_{60} and pentacene molecules, one of us has determined an optimal μ value for the LC-BLYP exchange-correlation functional by using a many-electron self-interaction free condition [53,54]. This optimal value of μ is about 0.2, which is less than the original ones. Quite interestingly, a tendency of the optimal μ is similar to the present ones. This implies that diarylethene derivatives in this study are more delocalized than the G2 set systems, and the reason why the present μ value works well might be explained from the viewpoint of a cancellation between the localization and delocalization errors despite we have chosen the parameters by minimizing the error between theoretical and experimental UV spectra in the present study. In the future study, we investigate the many-electron self-interaction free condition for the diarylethene derivatives in order to confirm the above conjecture.

4. Conclusions

In this study, we have obtained the tuned CAM-B3LYP parameters ($\mu = 0.150$, $\alpha = 0.0799$ and $\beta = 0.9201$) in the TD-DFT scheme, which can well reproduce the experimental excitation energies of 15 closed forms of diarylethene derivatives. On the other hand, the excitation wavelengths obtained by the standard CAM-B3LYP method are not found to reproduce the experimental values. It turns out that such behavior does not originate from the ground state structural change caused by the tuned functional, but from the direct effect of tuned functional on the excited states. The present tuning procedure of parameters in the TD-CAM-B3LYP scheme also will be useful for the reliable calculation of excited states of a series of molecules with common diarylethene frameworks. Moreover, this result is starting point for further theoretical study on photochromic reaction of diarylethene derivatives.

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Acknowledgements

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jphotochem.2012.03.003.

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