

An *ab initio* scheme for quantitative predictions of the visible spectra of diarylethenes

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Received 1 August 2006; received in revised form 31 August 2006; accepted 15 September 2006

Available online 26 September 2006

Abstract

A fully *ab initio* approach is shown to provide the visible absorption spectra of diarylethene derivatives with a quantitative accuracy. Indeed, a fitted-parameter-free time-dependent density functional theory scheme, combined to the modelling of the surrounding effects, leads to an excellent agreement with the available experimental data. For the λ_{\max} of 17 closed-ring structures, the mean absolute error (MAE) is limited to 9.4 nm (0.036 eV), although no statistical correction has been performed. The present *ab initio* scheme is compared to other theoretical schemes previously proposed for diarylethenes.

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Keywords: Diarylethenes; Photochromism; Density functional theory; Colour; Electronic spectra

1. Introduction

More than a decade ago, Irie and Lehn were the first authors to investigate the photochromic characteristics of diarylethene (DA) derivatives [1–5]. These molecules are indeed excellent candidates for molecular-switch applications, as they can be found in closed-ring and opened-ring forms presenting very different electronic properties, and the conversion between these states is allowed by irradiation at different wavelengths. DA are unconjugated and colourless in the opened-ring form but conjugated and coloured when in the closed-ring state. As several DA compounds are thermally stable, able to undergo many photochromic cycles, and present large quantum yields of conversion as well, they have been the interest of extensive research programs [6–8], that are still vivid today [9–15].

This contribution aims at designing an easy-to-use *ab initio* theoretical approach able to quantitatively predict the visible absorption spectra of DA derivatives. We have focussed our analysis on the λ_{\max} of closed-ring DA compounds, that is often the only reported data in experimental works, while the

opened-ring counterparts almost always absorb light in the UV region. We have selected time-dependent density functional theory (TD-DFT) that has become the most widely used tool for the theoretical simulation of excited state energies [16–27]. This success is due to its efficiency to quickly provide an accurate description of transition energies, with well-understood and predictable limitations [28]. To the best of our knowledge, there are only eight previous theoretical works dealing with the determination of the electronic transition energies of DA compounds. One has been performed with a semi-empirical approach (ZINDO//AM1) but the results have to be significantly corrected, $\lambda^{\text{corr}} = 2.63\lambda^{\text{orig}} - 481$ (in nm), before being comparable to experiments [29]. Other seven used TD-DFT but performed gas-phase calculations with limited basis set, 6–31G or 6–31G(d), that might allow valuable chemical insights but is definitely not adequate for quantitative predictions [30–36]. In Ref. [36], much more accurate gas-phase SAC-CI calculations have been performed. For the neutral DA, the SAC-CI and TD-DFT results are in good agreement with each other [36]. It is also worth to point out the CAS-SCF and CAS-PT2 calculations aiming at determining the reaction path linking the two DA forms [37–39]. The former, lacking of dynamical electronic correlation, provides poor results, while the latter is more accurate but remains a very computationally demanding approach for large molecules.

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2. Computational details

We have selected the Gaussian03 [40] package of programs to perform the geometry optimisations, vibrational analysis and excited state evaluations for the set of DA derivatives of Fig. 1. We have chosen maleic anhydride switches for this investigation, as their symmetry (see below) and moderate size allow systematic calculations on an extended set of molecules. In (TD-)DFT, the choice of the functional is often crucial to yield valuable results. In this contribution, we go for the hybrid PBE0 functional [41] that has been found adequate for various series of industrial organic dyes [27,42–44]. This functional is built on the Perdew–Burke–Ernzerhof pure functional [45], in which the exchange is weighted (75% DFT/25% HF) accordingly to the-

oretical considerations [46], i.e. no experimental input as been used to design PBE0. In the last part of this work, we have also used the well-known B3LYP functional [47], accordingly to the authors of Refs. [30,34–36]. For most organic molecules, the basis set required for accurate predictions of the ground-state properties is smaller than for the calculation of excited states energies. As the use of a smaller basis set for geometry optimizations than for TD-DFT calculations allows a significant gain in *cpu*-time (without loss of accuracy), this procedure has been followed here.

For each molecule, the ground-state structure has been determined by a standard force-minimisation process. Following each optimisation, the vibrational spectrum has been determined, and it has systematically been checked that all vibrational frequen-

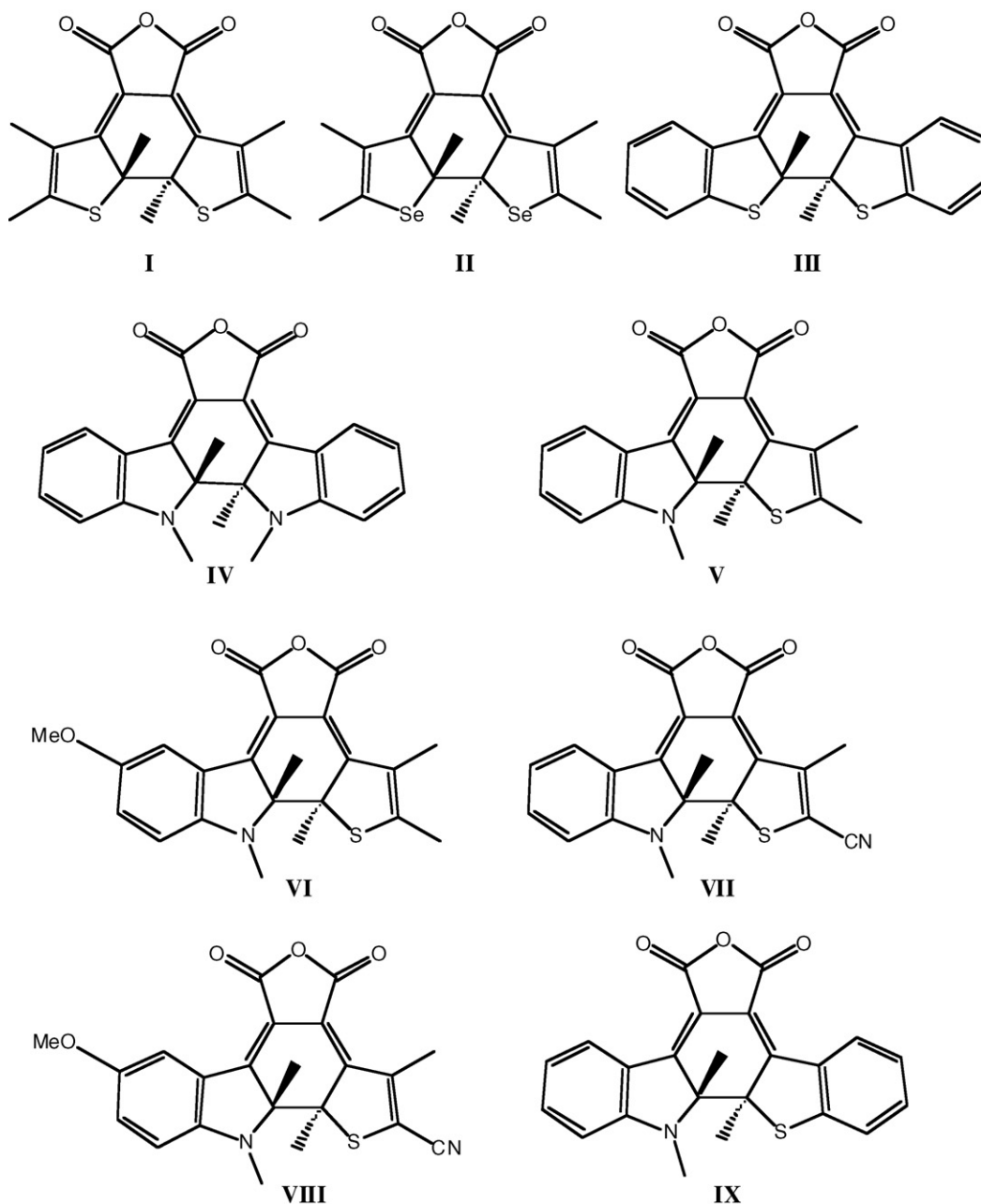


Fig. 1. Sketch of the investigated photochromic molecules.

cies are real. It turns out that the systems **I–IV** belong to the C_2 point group, whereas DA **V–IX** are C_1 .

These ground-state calculations have been performed with a triple- ζ polarised basis set, 6–311G(d,p), that is known for providing converged ground-state structural parameters for a large majority of organic molecules. [48–50]

TD-DFT is then used to compute the three first low-lying excited states of DA. As expected from experimental data, the electronic excitation responsible for the colour presents a typical $\pi \rightarrow \pi^*$ character associated to a large oscillator force. We have selected the 6–311+G(2d, p) basis set for these TD-DFT calculations, as this basis set has been found adequate and accurate for thioindigo dyes, which possess five-member sulphur-containing rings in their chromogenic unit as well [51]. In addition, we demonstrate below that a further extension of the basis set does not alter the λ_{\max} of DA, i.e. 6–311+G(2d,p) provides theoretically converged transition energies, at least for the low-lying states of interest.

As DA UV–vis spectra are often measured in solution, it is essential to include surroundings effects in our simulations. [52,53]. Therefore, at each stage, the bulk solvent effects are evaluated by means of the polarizable continuum model (IEF-PCM) [54]. PCM returns a valid approximation of solvent effects as long as no specific solute-solvent interactions show up. In this study, solvent of various polarities have been chosen: hexane [55], benzene, tetrahydrofuran (THF) and acetonitrile (ACN).

3. Results

Experimental and theoretical λ_{\max} obtained for nine DA in various solvents (17 cases) are listed in Table 1 and compared in Fig. 2. Although the discrepancies between the experimental values that can be found in the literature are limited, they illustrate that experimental values are never error-free. When conflicting measurements do exist, the average value serves as experimental reference.

Table 1
Comparison between experimental and PCM-TD-PBE0/6–311+G(2d, p)/PCM-PBE0/6–311G(d, p) λ_{\max} (in nm). The theoretical oscillator strengths are given between parenthesis

| Molecule | Solvent | Theory | Experiment | Reference |
|-------------|---------|-----------|------------|-----------|
| I | Hexane | 550(0.14) | 552 | [61] |
| | Benzene | 553(0.15) | 560, 564 | [1,61] |
| | THF | 561(0.14) | 560 | [61] |
| | ACN | 563(0.13) | 563 | [61] |
| II | Benzene | 563(0.13) | 565 | [2] |
| | Hexane | 554(0.21) | 538 | [61] |
| III | Benzene | 556(0.22) | 544, 541 | [62,61] |
| | THF | 557(0.20) | 533 | [61] |
| | ACN | 558(0.19) | 535 | [61] |
| IV | Benzene | 611(0.25) | 620 | [2] |
| V | Hexane | 572(0.19) | 578 | [63] |
| | Benzene | 576(0.20) | 595 | [63] |
| VI | Hexane | 609(0.19) | 611 | [64] |
| VII | Hexane | 633(0.21) | 628 | [64] |
| VIII | Hexane | 685(0.21) | 680 | [64] |
| IX | Hexane | 576(0.24) | 583 | [63] |
| | Benzene | 580(0.25) | 597 | [63] |

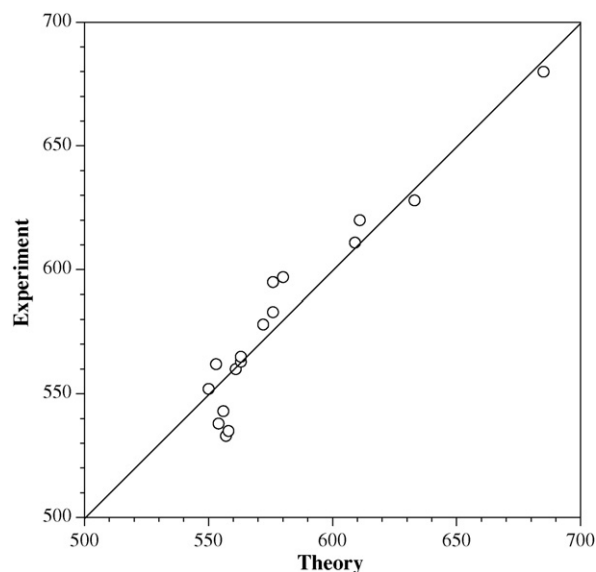


Fig. 2. Comparisons between the experimental and theoretical λ_{\max} (in nm) for the molecules of Table 1 in several solvents. All results have been obtained with PCM-TD-PBE0/6–311+G(2d, p)/PCM-PBE0/6–311G(d, p) approach.

Fig. 2 shows that the agreement between predicted and measured λ_{\max} is exceptional. Indeed, for the complete set, we get a negligible mean signed error (MSE) of 0.8 nm, the theory only very slightly overestimating the wavelengths, and a very small mean absolute error (MAE) of 9.4 nm. The corresponding residual mean square error (RMS) is 12.1 nm. In the energetic scale, the values are: MSE = 0.005 eV, MAE = 0.036 eV and RMS = 0.048 eV. The largest discrepancy is limited to 24 nm, for **III** in THF. It is also worth to highlight that the auxochromic shifts are well reproduced. Indeed, adding a methoxy group to **V** increases λ_{\max} by +33 nm in hexane, an effect correctly foreseen by theory: +37 nm. Likewise going from **V** to **VII** (**VIII**) leads to a variation of +50 nm/+63 nm (+102 nm/+113 nm) in the experiment/with our *ab initio* model. For **I**, the positive solvatochromic effect is also accurately predicted: +13 nm from hexane to acetonitrile instead of the measured +9 nm variation. The influence of the surroundings is smaller for **II** in both theory and experiment, although in that specific case theory does not provide the correct solvatochromic sign. Interestingly for both **I** and **III**, the experimental λ_{\max} in benzene is slightly larger than what could be forecast from the polarity of the solvent. This probably originates in specific solvent–solute interactions that are not accounted for in the PCM model. Nevertheless, one could clearly state that the level of accuracy required for the theoretical design of new DA compounds presenting specific λ_{\max} has been achieved. Of course, for DA substituted by both very strong electron-donor and electron-acceptor groups, i.e. for push–pull derivatives, significant TD-DFT undershooting of the transition energies is still to be expected [28], although for **VIII**, theory is still on the spot.

The oscillator strengths (f) reported in Table 1 are directly related to the absorption intensities (ϵ). One can classify the DA molecules in three categories: in the first (**I** and **II**), f is close to 0.14; in the second (**III** and **V–VIII**), f reaches 0.20 ± 0.01 ; while in the third the absorption is more intense with f attaining

0.25 (IV and IX). Therefore one can conclude that f depends on the number of π electrons in the structure: the larger the number of side aromatic rings, the more intense the absorption, as could be expected.

Chen et al. [35] have investigated the spectra of derivatives I and IV–VIII using a gas-phase B3LYP/6–31G(d) approach. For these six molecules, one can compute a MSE of -18.5 nm and a MAE of 18.5 nm (0.066 eV) with a largest absolute deviation of 32 nm (0.108 eV), i.e. their average error is about twice ours and they systematically underestimated the λ_{\max} . In that contribution, PBE0/6–31G(d) calculations have also been performed and a larger MAE of 33.7 nm (0.120 eV) can be deduced. However, these gas-phase double- ζ results are far from being converged with respect to the basis set extend for the TD-DFT calculation. As an illustration, for I, the λ_{\max} are $530, 543, 542, 547, 550, 551, 550$ and 550 nm with 6–31G(d), 6–31+G(d), 6–311G(d,p), 6–311++G(d,p), 6–311+G(2d,p), 6–311++G(2d,2p), 6–311+G(3d,p) and 6–311++G(2df,2pd) basis sets, respectively. Using the limited 6–31G(d) for the excited-state properties already leads to a 0.09 eV (20 nm) error. In addition, this confirms the adequacy of 6–311+G(2d,p) for DA. The neglect of solvent effects in Refs. [30,35] also results in a small underestimation of the wavelengths. The gas-phase TD-PBE0/6–311+G(2d, p)/PBE0/6–311G(d, p) λ_{\max} of I, II and III are respectively $538, 549$ and 543 nm, that is $15, 14$ and 13 nm smaller than in the unpolar benzene, illustrating the importance of solvent shifts. Therefore, it can be concluded that the statement *the TD-B3LYP/6–31G(d) gaseous calculations are relatively closer to experimental measurements in the current work* in Ref. [35] is, as suggested by the authors themselves, the consequence of a relatively modest level of calculation. As a consequence, gas-phase B3LYP/6–31G(d), that basically works on an error compensation scheme, could be a second choice for a rapid first screening of compounds, but our refined model clearly allows much more quantitative and consistent evaluations.

It is also worth to compare our results with other TD-DFT calculations performed for other classes of molecules. In fact, we are aware of only four studies using a wide panel of organic compounds belonging to several dye families. Two are due to Fabian and co-workers who reported B3LYP/6–31+G(d) MAE of 0.29 and 0.24 eV for $\pi \rightarrow \pi^*$ transitions in sulphur-free and sulphur-bearing molecules, respectively [56,57], one has been performed by Guillaumont and Nakamura who obtained B3LYP/6–31G MAE of 0.19 eV for a very extended set of dyes [58], while the latter by Nguyen and co-workers yields a B3LYP/6–31+G(d) MAE of 0.14 eV for 47 singlet–triplet transitions [59]. If the error obtained in this work are three to six times smaller than in the previous studies, they are in the line of what we recently got for the λ_{\max} accuracy: 0.05 eV for nitroso derivatives [42], 0.07 eV for diazonium salts [43], 0.06 eV for nitro-diphenylaniline [44], 0.02 eV for indigo dyes [26], 0.03 eV for thioindigoids [27], 0.08 eV for anthraquinones [25], and 0.07 eV for thiocarbonyl compounds [60]. This illustrates the paramount importance of using large basis sets and including environmental effects in the calculations, as long as one aims at comparison with experimental values.

4. Conclusions

We have setup a computational procedure allowing a quantitative theoretical determination of the λ_{\max} of DA derivatives. This procedure uses the PBE0 functional, the PCM model and two atomic basis sets, 6–311G(d, p) for the ground-state properties, and 6–311+G(2d, p) for the excited-state properties. For the 17 cases investigated, the experimental λ_{\max} is reproduced with a MAE limited to 9.4 nm, and no cases with a difference exceeding 25 nm has been detected. Consequently, the colour of closed-ring DA can be accurately evaluated by theoretical *ab initio* tools, allowing to evaluate the impact of any substitution pattern before synthesis. We are currently considering perfluoro DA derivatives in order to test the transferability of our methodology.

Acknowledgments

The authors thank the Belgian National Fund for Scientific Research for their research associate positions. EAP and DJ are indebted to Prof. J.M. André for his continuous support. The calculations have been performed on the Interuniversity Scientific Computing Facility (ISCF), installed at the Facultés Universitaires Notre-Dame de la Paix (Namur, Belgium), for which the authors gratefully acknowledge the financial support of the FNRS-FRFC and the “Loterie Nationale” for the convention number 2.4578.02 and of the FUNDP.

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