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# Structural and Solvent Effects on the Spectroscopic Properties of 1, 8-Naphthalimide Derivatives: A Density Functional Study

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**ABSTRACT:** The molecular structures of 1, 8-naphthalimide derivatives were investigated at density functional theory level within framework of PBE1PBE/6-31G\*. The vertical ionization potential and their delocalization energy of the X-ray solid structure and gas-phase optimized structure were explored. The configuration difference between them was attributed to the  $\pi$ - $\pi$  interaction of the solid effect, which has negligible effect on their absorption spectra. Solid effect also weakens the intramolecular interaction. Their absorption and luminescent spectra in gas and solvent phase were calculated by time-dependent density functional theory (TDDFT) and conductor polarizable continuum models (CPCM)-TDDFT approaches. Obvious red shifts from the solvent effect were found. Substituents on the imides will not improve their spectra properties a lot, whereas substituents on the naphthalene of naphthalimide would modify their properties to emit different spectra. Systematical deviation of vertical excitation energy from absorption and emission spectra, obtained by CPCM-PBEPBE/6-31G\* and CIS-CPCM-PBEPBE/6-31G\* models, were about 0.05 eV and 0.02 eV compared with the experimental values. © 2010 Wiley Periodicals, Inc. *Int J Quantum Chem* 111: 2234–2241, 2011

**Key words:** 1; 8-Naphthalimide derivatives; DFT; solid effect; solvent effect

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## 1. Introduction

**1**,8-naphthalimide derivatives have aroused considerable interest recently because of their optical properties, and thus found wide range of applications in various fields. High electron affinities [1], wide gap [2, 3], and low reduction potentials [4] make them good candidates in OLEDs as n-type materials [5]. They also have applications in numerous systems ranging from sensitizers for Grätzel solar cell [6, 7] to logic gate [8], sensor [9] and charge separation mimics [10], which can act as electron acceptor [11, 12], electron donor [10] or energy donor [13]. They are also made as connected unit in dendrimers, tools for the study of dynamic protein interactions [14].

As we know, structural aspects always determine the optical properties as well as their applications. A series of 1, 8-naphthalimide derivatives come out, with substituent such as oxadiazole [15], diphenylamine [16], dimethylamine, amine [17]. Some semiempirical calculations and DFT calculation have also participated in exploring naphthalimides [18–21] and uncover their electronic properties. Theoretical work shows that calculated structure and experimental solid state structure exhibits difference more or less, which are partly owing to the solid effect [22]. Experimental work demonstrates that the solid state intermolecular  $\pi$ - $\pi$  interaction is closely related to their fluorescent properties [23, 24]. However, there are a few studies about the intramolecular interaction and structural aspect of 1, 8-naphthalimide derivatives [25].

In this work, the aim of this article is to investigate solid effect, solvent effect of a series of 1, 8-naphthalimide derivatives. We have chosen a series of 1, 8-naphthalimide derivatives with the X-ray structures and the absorption and emission properties. Their vertical electronic transition energy were calculated by PBE1PBE/6-31G\* model.

## 2. Computation Methods

All calculations have been carried out with version 2003 of the Gaussian suite of programs [26]. We have selected the parameter-free PBE1 hybrid functional [27, 28] for all DFT and TDDFT computations. 6-31G\* basis sets have been used. The ground-state ( $S_0$ ) and the first singlet excited-state

( $S_1$ ) have been optimized for these derivatives with no symmetry constraint. These minimizations have been performed with PBE1PBE ( $S_0$ ), CIS ( $S_1$ ) approaches. For  $S_1$ , only gas-phase CIS analytic frequency calculations are currently available. Vertical ionization potential (IP) is calculated by subtracting the total energy of the neutral molecular from that of charged molecules at neutral equilibrium geometries. Natural population analysis [29, 30] and natural bond orbitals [31] are carried out to compute atomic charge and energy analysis.

The energetic effect of deleting specific NBO groups or donor-acceptor interaction is determined by including `pop = nbodel` in the route card and `$Del NOSTAR parameter $END` after the coordinate specification as implemented in the NBO 3.1 [32] of Gaussian package. The "NOSTAR" option requests deletion of all non-Lewis orbitals, which lead to the energy of the idealized natural Lewis structure. The electronic delocalization can be assessed by the formula

$$E(\text{NL}) = E(\text{full}) - E(\text{L}),$$

where  $E(\text{full})$  stands for original energy from the ground state geometry and  $E(\text{L})$  is the localized energy with Lewis-type NBOs doubled occupied resulted from "natural Lewis structure".

## 3. Results and Discussion

### 3.1. SOLID STATE EFFECT OF 1, 8-NAPHTHALIMIDE DERIVATIVES

The delocalization energy, vertical ionization potential, dipole moment, bond index, charge calculated by PBE1PBE/6-31G\* with the X-ray crystal structures [16, 25, 33, 34], and theoretical optimized (PBE1PBE/6-31G\*) conformation are shown in Table I. Those compounds are separated into three or two parts: top substituent, naphthalimic ring, and bottom substituent. Their structures are shown in Figure 1 and are numbered in Arabic numerals and Roman numerals for convenience.

For most of them, the delocalization energy and vertical ionization potential (VIP) of the optimized 1, 8-naphthalimides are bigger than those X-rays. In the solid phase, smaller VIP suggests that the electron of the X-rays, owned by the whole crystal instead of single molecule, might be apt to excite more easily. It is natural to deduce

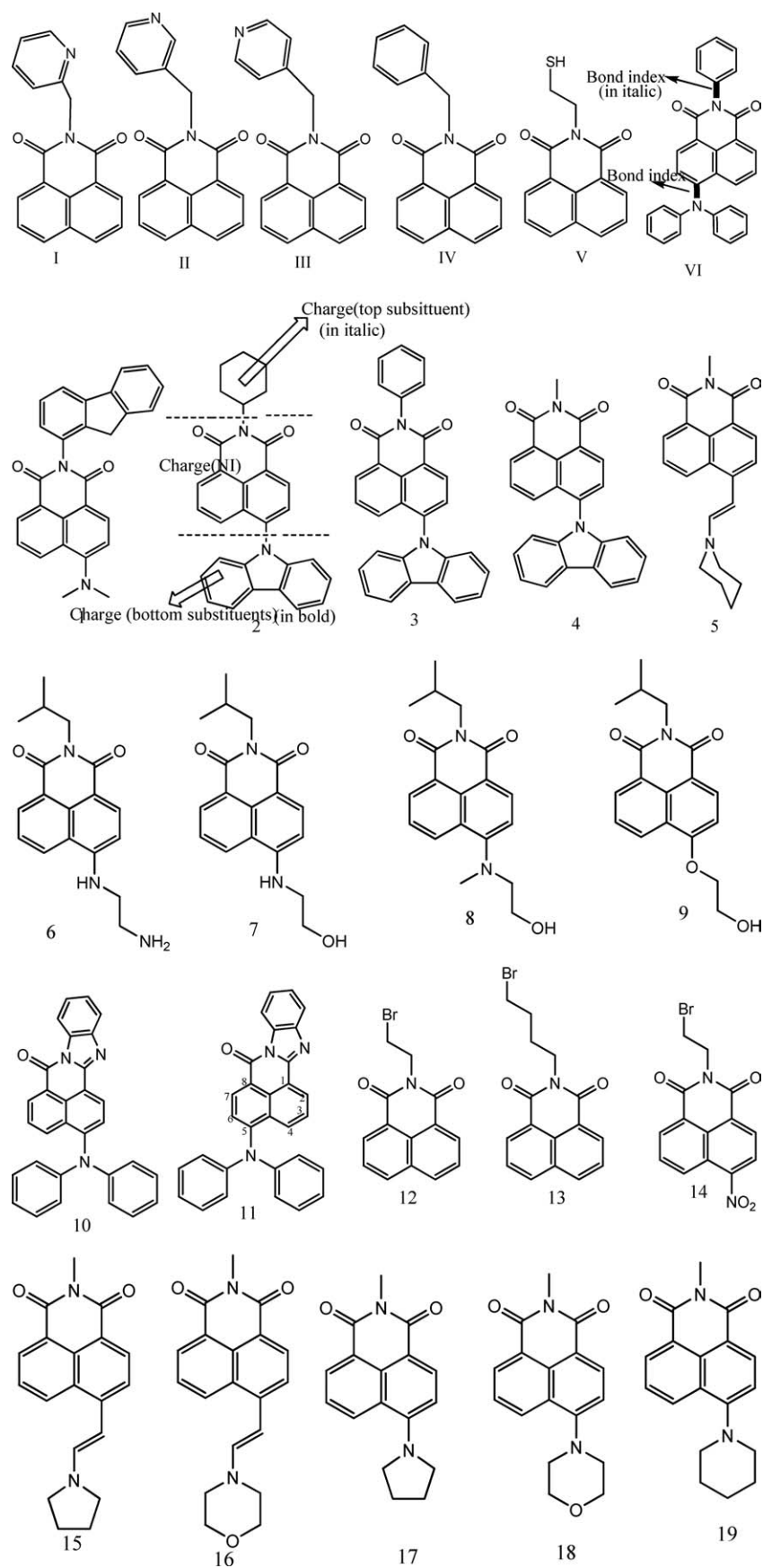
TABLE I

Vertical ionization potential (eV), Delocalization energies (kcal.mol<sup>-1</sup>), Dipole moment (Debye), Bond Indices (au), Charges (a.u.) and Wavelength (nm) for the X-ray crystal structures of 1, 8-naphthalimide derivatives calculated by PBE1PBE/6-31G\* approaches. Electronic excitation energies are in parentheses.

Compounds	Vertical ionization potentials	Delocalization energies	Dipole moment	Bond index <sup>a,b</sup>	Charges <sup>b</sup>	Wavelength (nm)
(a)						
I	8.10	39.24	2.49	<i>0.930</i>	<i>0.242</i>	314(3.95)
II	8.22	36.80	5.50	<i>0.909</i>	<i>0.253</i>	320(3.86)
III	8.25	38.10	6.21	<i>0.913</i>	<i>0.245</i>	315(3.94)
IV	8.09	37.07	4.28	<i>0.905</i>	<i>0.259</i>	315(3.94)
V	8.23	39.47	6.33	<i>0.919</i>	<i>0.148</i>	311(3.99)
VI	6.83	36.91	5.17	<i>0.906</i>	<i>0.261</i>	415(2.90)
		2359.56		1.049	-0.548	
					<b>0.287</b>	
2	7.17	43.72	2.02	<i>0.895</i>	<i>0.260</i>	455(2.72)
		2456.62		0.964	-0.0626	
					<b>0.211</b>	
4	7.23	46.15	2.81	<i>0.926</i>	<i>0.273</i>	465(2.67)
		2142.75		0.964	-0.0745	
					<b>0.1985</b>	
5	6.42	55.85	11.68	<i>0.930</i>	<i>0.262</i>	429(2.89)
		1611.32		1.194	-0.466	
					<b>0.204</b>	
10	6.57	56.25	4.33	1.006	0.137	497(2.50)
11	6.72	50.85	3.46	1.015	0.129	450(2.76)
(b)						
I	14.82	43.86	2.19	0.940	<i>0.236</i>	317(3.91)
					-0.236	
II	14.93	42.53	5.50	0.915	<i>0.246</i>	319(3.88)
					-0.246	
III	15.16	26.81	6.03	0.913	<i>0.241</i>	320(3.88)
					-0.241	
IV	15.14	42.25	4.29	0.912	<i>0.252</i>	319(3.89)
					-0.252	
V	13.16	42.00	5.88	0.919	<i>0.115</i>	328(3.78)
					-0.115	
VI	19.83	44.49	4.84	0.930	0.241	451(2.75)
		2403.23		1.022	-0.494	
					<b>0.253</b>	
2	7.39	46.57	2.43	<i>0.908</i>	0.262	454(2.73)
		2325.07		0.979	-0.0731	
					<b>-0.189</b>	
4	7.24	35.100	2.89	<i>0.937</i>	0.265	456(2.72)
		2112.25		0.979	-0.0767	
					<b>-0.178</b>	
5	6.55	47.33	9.20	<i>0.940</i>	<i>0.262</i>	422(2.94)
		1541.16		1.138	-0.466	
					0.204	
10	6.60	2441.23	4.54	1.014	0.130	495(2.50)
11	6.71	54.43	4.91	1.026	0.115	460(2.69)

<sup>a</sup> Bond indices for the top substituents and naphthalimic ring are in italic.

<sup>b</sup> Charges for top substituents and bottom substituents are in italic and bold, respectively.



**FIGURE 1.** Sketch of 1, 8-naphthalimide derivatives with atom numbering.

TABLE II

Calculated absorption and emission maxima (nm), oscillator strength (f) and molecular configuration of 1, 8-naphthalimide derivatives in the framework of CPCM-TD-PBE1PBE, CPCM-TD-PBE1PBE-CIS and their experimental wavelength in solvent. Electronic excitation energies (eV) are in parentheses. H = HOMO, L = LUMO, L+1 = LUMO+1, etc. Solvent are in parentheses of the experimental value list.

Absorption				Experiment [16,33,35-37]	Emission				Experiment [16,33,35-37]
Excitation Energy	f	Assignment			Excitation Energy	f	Assignment		
1 391(3.17)	0.343	H→L 85.6%		420(CHCl <sub>3</sub> )	434(2.86)	0.377	H→L 82.7%		508(CHCl <sub>3</sub> )
2 490(2.53)	0.252	H→L 91.3%		414(CH <sub>2</sub> Cl <sub>2</sub> )	485(2.55)	0.246	H→L 91.7%		563(CH <sub>2</sub> Cl <sub>2</sub> )
3 482(2.57)	0.309	H→L 91.3%		410(CH <sub>2</sub> Cl <sub>2</sub> )	487(2.55)	0.249	H→L 91.8%		568(CH <sub>2</sub> Cl <sub>2</sub> )
4 464(2.67)	0.0843	H→L 96.8%		419(CH <sub>2</sub> Cl <sub>2</sub> )	487(2.55)	0.228	H→L 91.7%		556(CH <sub>2</sub> Cl <sub>2</sub> )
5 477(2.60)	0.633	H→L 83.8%		494(CH <sub>2</sub> Cl <sub>2</sub> )	498(2.49)	0.689	H→L 80.1%		600(CH <sub>2</sub> Cl <sub>2</sub> )
6 396(3.13)	0.345	H→L 84.6%		428(CH <sub>2</sub> Cl <sub>2</sub> )	430(2.89)	0.333	H→L 82.3%		504(CH <sub>2</sub> Cl <sub>2</sub> )
7 391(3.16)	0.334	H→L+1 84.9%		423(CH <sub>2</sub> Cl <sub>2</sub> )	428(2.89)	0.324	H→L 82.2%		497(CH <sub>2</sub> Cl <sub>2</sub> )
8 406(3.05)	0.367	H→L 84.6%		402(CH <sub>2</sub> Cl <sub>2</sub> )	441(2.81)	0.352	H→L 82.3%		508(CH <sub>2</sub> Cl <sub>2</sub> )
9 353(3.51)	0.345	H→L 84.6%		363(CH <sub>2</sub> Cl <sub>2</sub> )	386(3.21)	0.339	H→L 82.6%		427(CH <sub>2</sub> Cl <sub>2</sub> )
10 531(2.34)	0.374	H→L 91.6%		488(CH <sub>2</sub> Cl <sub>2</sub> )	576(2.15)	0.509	H→L 86.5%		596(CH <sub>2</sub> Cl <sub>2</sub> )
11 494(2.51)	0.433	H→L 90.0%		469(CH <sub>2</sub> Cl <sub>2</sub> )	522(2.37)	0.535	H→L 86.5%		584(CH <sub>2</sub> Cl <sub>2</sub> )
12 330(3.76)	0.294	H→L 83.7%		345(HCN)	332(3.73)	0.294	H→L 83.6%		379(HCN)
13 329(3.77)	0.292	H→L 83.7%		345(HCN)	361(3.44)	0.281	H→L 81.1%		378(HCN)
14 373(3.32)	0.261	H→L 83.9%		350(HCN)	418(2.97)	0.278	H→L 81.7%		450(HCN)
15 477(2.60)	0.631	H→L 83.6%		507(CH <sub>2</sub> Cl <sub>2</sub> )	598(2.07)	0.0004	H→L 92.7%		600(CH <sub>2</sub> Cl <sub>2</sub> )
16 460(2.69)	0.607	H→L 85.3%		505(CH <sub>2</sub> Cl <sub>2</sub> )	484(2.56)	0.674	H→L 81.0%		600(CH <sub>2</sub> Cl <sub>2</sub> )
17 405(3.06)	0.388	H→L 84.5%		443(CH <sub>2</sub> Cl <sub>2</sub> )	441(2.81)	0.360	H→L 82.7%		506(CH <sub>2</sub> Cl <sub>2</sub> )
18 392(3.16)	0.328	H→L 86.5%		394(CH <sub>2</sub> Cl <sub>2</sub> )	433(2.86)	0.350	H→L 83.2%		506(CH <sub>2</sub> Cl <sub>2</sub> )
19 401(3.09)	0.333	H→L 86.3%		410(CH <sub>2</sub> Cl <sub>2</sub> )	440(2.82)	0.355	H→L 83.1%		517(CH <sub>2</sub> Cl <sub>2</sub> )

that the solid effect weakens the intramolecular interaction between substituents and the naphthalimic rings. Shortened bond indices of the X-ray structures also exhibit the weakened intramolecular interaction, which might be explained with the  $\pi$ - $\pi$  packing interaction occurred for the solid geometry. The molecules with two  $\pi$ - $\pi$  system configuration such as benzene and naphthalimic ring, bridged by single bond, have bigger bond index than those with saturated substituents- $\pi$  systems (methyl-naphthalimic ring). Those bigger bond indices and shortened bond lengths verify the charge transfer and intramolecular interaction of X-ray and theoretical optimized structures. Most of the Naphthalimide ring (NI) fragments of the molecules have negative charges except for those of 10 and 11, which might be because of to the benzo group conjugated with the naphthalimic ring. The charge transfer between substituents and naphthalimic rings does occur and modify the excitation energy of 1, 8-naphthalimide derivatives. The excitation energies change a few for two kinds of structure, which is almost negligible. Even it is quite quantitative, it is still of practical

meaning to estimate it theoretically. More accurate results still need to be approved by the solid luminescent spectra. Besides, more accurate models and solid crystal approaches are also necessary if people want to pursue it more deeply.

### 3.2. ABSORPTION AND EMISSION SPECTRA OF 1, 8-NAPHTHALIMIDE DERIVATIVES

The singlet excited states are calculated by CPCM-TDDFT-PBE1PBE/6-31G\* approach at CPCM-PBE1PBE/6-31G\* and CIS/6-31G\* optimized geometries [16, 33, 35–37]. Different solvents are simulated by the CPCM model. The vertical excitation energies and oscillator strength are listed in Table II. Major electronic absorption and emission bands are assigned to those excitations with significant oscillator strength. Herein, we also make a direct linear comparison between the theoretical wavelength and experimental measurement to assess the accuracy of PBE1PBE/6-31G\* approach.

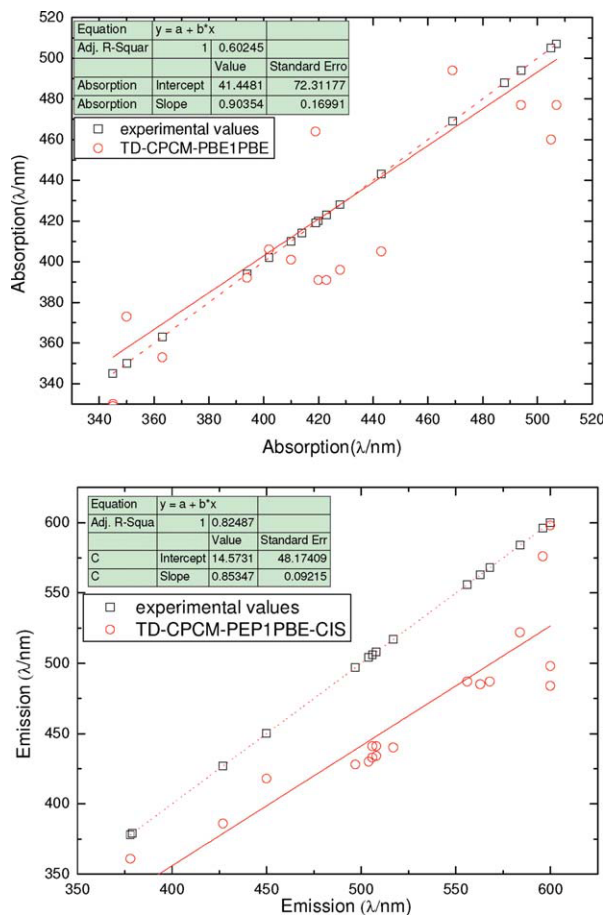
Specifically speaking, the first lowest singlet excitation of the absorption and emission spectra between  $S_0$  and  $S_1$  in solvent phase, as shown in



Table II, corresponds predominantly to the transition of electrons from HOMO-1 to LUMO in Figure 1. HOMOs are mainly localized on the rigid naphthalimic ring for both unsubstituted and substituted naphthalimides, in accordance with the former DFT study [18]. This phenomenon suggests that naphthalimic ring is the main luminescent body. Top substituents seldom contribute to the HOMO and LUMO, whereas bottom substituents mainly act as the antibonding patterns, suggesting the possible cause for different absorption and emission maximum. So it is natural to conclude that top position on imide is a bridge point to keep its origin optical properties and bottom position on naphthene is a modification position for improving spectra properties.

Meanwhile, owing to the extended conjugated structure, the excitation with strong oscillator strength is  $\pi\text{-}\pi^*$  type. The long pair of carbonyl in those 1, 8-naphthalimides also exerts a few contributions, which will not affect the red shifts as a result to the polar solvent. It is reported that 1, 8-naphthalimide with 4 position electron-donating substituents have high quantum yield [38] and the first lowest excited state of 1, 8-naphthalimide with no substituent is  $n\text{-}\pi^*$  type [20]. And there are also near  $\pi\text{-}\pi^*$  type state near it so that increases probability of the inner transition of them. The  $n\text{-}\pi^*$  transition is forbidden. Here the lowest excited state of calculated 1, 8-naphthalimide derivatives is  $\pi\text{-}\pi^*$  type with strong oscillator strength. Maybe we can deduce that the transition type from  $n\text{-}\pi^*$  to  $\pi\text{-}\pi^*$  result in the higher quantum yield from this side.

Obvious red shift as a result of adding  $\text{CH}_2\text{Cl}_2$  (about 35 nm) within framework of CPCM is shown in Table I and Table II. The red shifts and increase of oscillator strength from absorption to emission spectra in  $\text{CHCl}_3$  and HCN suggest the type of the transition is  $\pi\text{-}\pi^*$  type, which is in good agreement trend in the former paper [39, 40]. Those phenomena illustrated that the absorption and emission maxima is of  $\pi\text{-}\pi^*$  type, which is sensitive to the polar solvent and red shifts. For all compounds in this article, CPCM provides a consistent accuracy on absorption and emission wavelength. Comparing with the experimental spectra in Figure 2, the mean absolute error is about 0.05 eV and 0.02 eV for absorption and emission, respectively. These data show that they are rather comparable to the experimental values. TD-PBE1PBE is better than the inspection of TD-B3LYP/6-31G\* approach having a deviation of

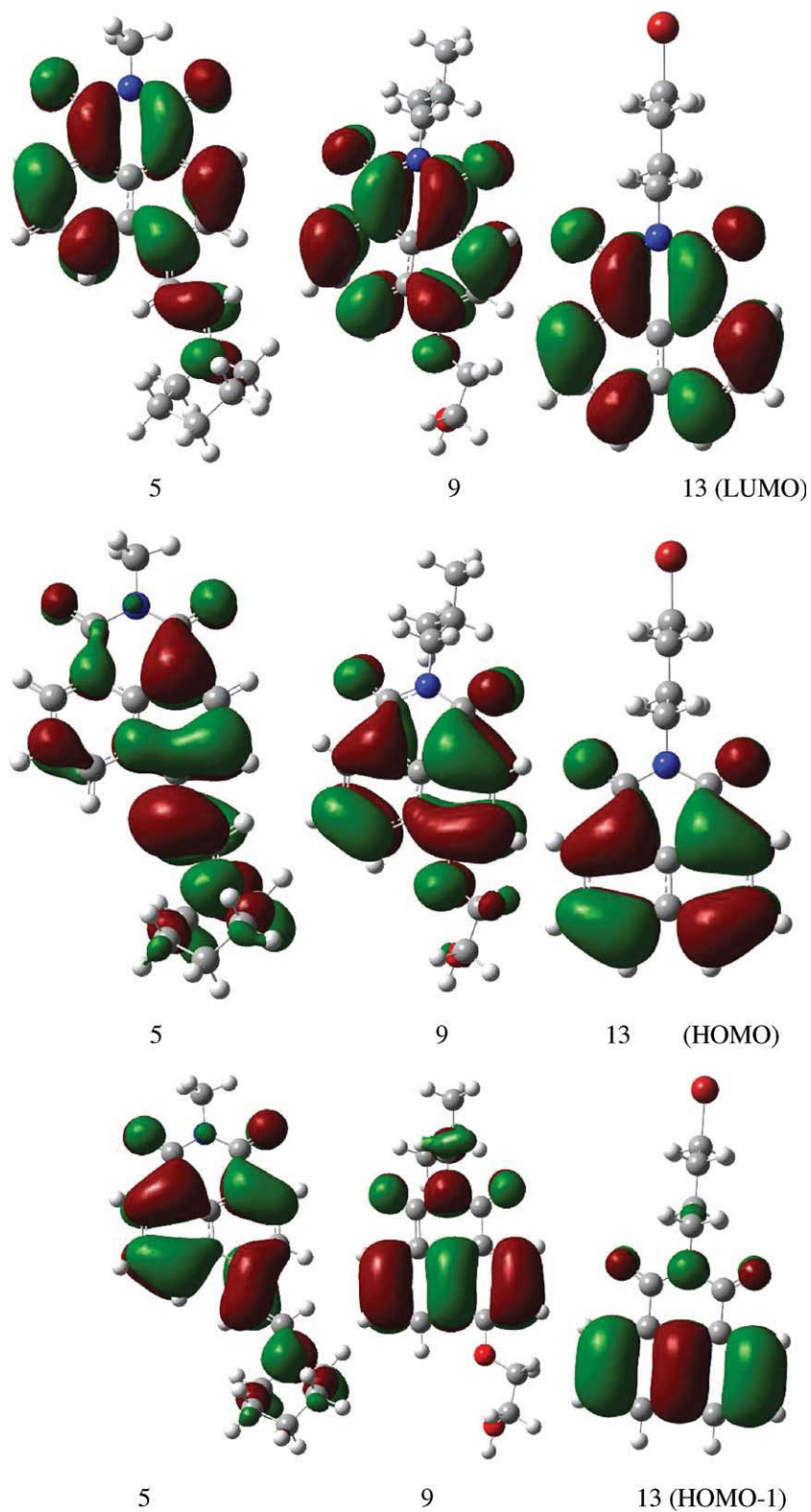


**FIGURE 2.** Comparisons of wavelength between experimental parameters and theoretical calculations. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://www.interscience.wiley.com).]

about 0.25 eV [41]. Figure 3 also shows that the emission spectra are underestimated, which is partly because of the neglect of the electron correlation of CIS approaches and its optimized structure in gas phase.

#### 4. Conclusions

We calculate the absorption and emission spectra of 1, 8-naphthalimide derivatives in gas phase and different solvents by using TD-PBE1PBE/6-31G\* approach and CPCM model. The solid effect from X-ray structure weakened the intramolecular interaction between substituents and the naphthalimic rings in contrast with the optimized molecular structure. X-ray structure has not resulted in the obvious difference of the absorption spectra with optimized structure from PBE1PBE/6-31G\*.



**FIGURE 3.** Schematic drawing of the HOMO-1, HOMO and the LUMOs of 5, 9, and 13. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]



The mean absolute error is about 0.05 eV and 0.02 eV for absorption and emission spectra in solution phase. Most of the vertical transition maximum corresponds to the transition from HOMO to LUMO, which suggests the intramolecular transfer occurs between substituent on the naphthalimic ring and naphthalimic ring. Substituents bridged on imides have little effect on its vertical transition energy, while bottom position on naphthalene of the naphthalimide is a modification position for improving its properties.

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