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STUDIES ON THE EFFECT OF SOLVENTS ON THE ELECTRONIC ABSORPTION SPECTRA OF 4-PHENYLMORPHOLINE AND 1-PHENYLPYRROLE

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ABSTRACT

The Ultraviolet-Visible (UV) spectra of 4-phenylmorpholine and 1-phenylpyrrole in different solvents have been studied. The molar absorptivities and oscillator strengths were determined. Also, quantum chemical calculations were carried out using time-dependent density functional theory with Beck-3-Lee-Yang-Parr exchange-correlation functional with a 6-31G basis set (TDDFT/B3LYP/6-31G*) for the optimized structures of the compounds. On the basis of this, the dipole moment, dihedral angle, oscillator strength, and singlet excited state of these compounds were determined in different solvents of different polarities. It was found that the bands are both n→Π* and Π→Π* transitions for the compounds. The value of the dipole moment and dihedral angles of the compounds increase with increasing polarities of solvents, and it could be predicted theoretically that 4-phenylmorpholine is more planar and reactive than 1-phenylpyrrole. There is a strong agreement between the experimental and theoretical results obtained for 4-phenylmorpholine, while there is a slight disagreement between the experimental and theoretical results in the number of transitions observed for 1-phenylpyrrole due to the collapsing of bands in the excited state in the experimental section.*

Keywords: Solvent effect, 4-phenylmorpholine, 1-phenylpyrrole, oscillator strength

INTRODUCTION

Ultra-violet visible (UV) spectroscopy is concerned with the transition of electrons between orbitals of different energies, usually from the highest occupied molecular orbital (HOMO) of the lowest energy molecular orbital to the lowest unoccupied molecular orbital (LUMO) of the highest molecular energy orbital. The excitation is as a result of absorption of light, and the quantum energy (E), of which is a function of frequency (v). However, not all absorption of radiation by organic molecules results in electronic excitation since the probability of excitation depends on the wave functions of both the ground and excited states of the orbitals concerned. The rule by which a transition is allowed or forbidden is a function of the symmetry and multiplicity (spin) of the ground and excited states of the orbital concerned. The electronic excitation in a molecule is accompanied by a change in vibrational and rotational quantum numbers; therefore, what is supposed to be absorption lines becomes a broad peak containing vibrational and rotational fine structures. However, the interaction of solute and solvent molecules blurred out the fine structures, and as a result, a smooth curve was observed (Booth, 1992;

Kalsi, 2007; Braude & Nachod, 2013; Sharma, 2009; Yadav, 2011).

Moreover, studies have been documented on the effect of solvents on the electronic absorption spectra of different organic compounds. For instance, El-mossalamy *et al.* reported the effect of solvents on the electronic absorption spectra of some sulpha drugs (El-mossalamy *et al*., 2015). Their study showed that the band due to local excitation within the aromatic moiety (п→п* transition) displayed an irregular solvent shift, though the general trend is a red shift with increased solvent polarity. Also, the solvent effects on the electronic absorption spectra of toluene, *o*-bromo and *p*-bromo toluene in different solvents have been reported by Abdul Raheem *et al*. (2010). Their findings revealed that, the electric dipole moments for the excited states (µ*) and the ground states (µ) of these compounds are equal, and the change in dipole moment is zero, implying that there is little or no change in the potential energy surfaces of the ground and the excited states (Abdul Raheem *et al*., 2010). Kosenkov *et al.* (2011) have reported the solvent effect on the electronic transition of *p*-Nitroaniline using the QM/EFP model and their findings accurately predicted the red solvatochromic shift of the charge-transfer $\pi \rightarrow \pi^*$ state of *p*-Nitroaniline in polar water.

Morpholine and pyrrole derivatives have been reported to be important subunits in various natural products and biologically active compounds (Pacorel *et al*., 2010; Bhattarai *et al*., 2012). In addition to their biological application, pyrrole subunits also play an important role in material science as the building blocks of polypyrroles, an important representative class of conducting polymers. This had found wide applications in the area of new materials due to their chemical, thermal, and electrical properties associated with their ease and low cost of production (Street, 1989). The applications of morpholine and pyrrole derivatives as building blocks for many bioactive substances in pharmaceutical industries and in material sciences for the development of conducting polymers make both experimental and theoretical studies of their electronic and molecular properties important. Therefore, understanding of their molecular and electronic properties such as oscillator strength, dihedral angles, dipole moment, vertical transition energy and molar absorptivity has great importance and synergy with the bioactivities of these molecules and other applications. In this work, we report the effect of solvents on the electronic absorption spectra of 4-phenylmorpholine and 1-phenylpyrolle. This study enables us to calculate the important electronic and molecular properties of these compounds.

EXPERIMENTAL SECTION

Materials

All solvents including cyclohexane, 1,2-dichloroethane and methanol were used after distillation. The analytical grade of the reagents; 1-phenylpyrrole and 4-phenylmorpholine were purchased from Sigma Aldrich and used directly.

Methodology

A Lambda 25 UV-Visible spectrophotometer was used to record the electronic spectra of the dilute solution of a compound. A pair of matched quartz cuvettes, one of which contained the sample solution and the other solvent, were located in the sample and reference compartments, respectively and the spectra were recorded at 25^{o}C. The absorbance of a solution was recorded over a wavelength span of 190 nm - 400 nm.

Computational method

The quantum chemical calculations were conducted with the Gaussian 03, revision B.02 software program (Frisch *et al*., 2004). The structures were fully optimized at the DFT level using B3LYP functional with a 6-31G* basis set in each solvent without any symmetry constraints. In the optimized structure, no imaginary vibrational modes were obtained, and this indicates that a true local minimum on the potential energy surface was obtained (Guido *et al*., 2018). Based on the fully optimized structure, TDDFT//B3LYP/6-31G* calculations have been used to determine the singlet excited states of 1-phenylpyrrole and 4-phenylmorpholine in methanol, 1,2-dichloroethane and cyclohexane respectively.

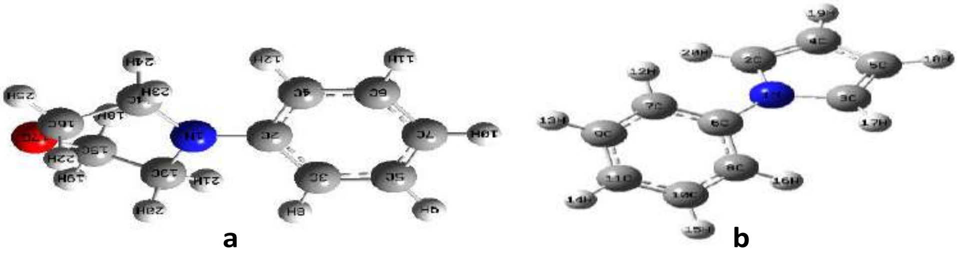

Figure 1: (a) Optimized structure for 4-Phenylmorpholine (b) Optimized structure for 1-Phenylpyrrole

RESULTS AND DISCUSSION

Solvent effects on the UV-Visible spectra of 4-phenylmorpholine

In general, two to three bands are observed in the spectra of 4-phenylmorpholine as shown in Figure 2. These bands can be designated as $S_0 \rightarrow S_1$, $S_0 \rightarrow S_2$ and $S_0 \rightarrow S_3$ in the order of increasing energy (decreasing wavelength). Table 1 summarizes the determined spectrum properties. In 4-phenylmorpholine, three bands were observed in 1,2- dichloroethane and cyclohexane. In methanol, two major bands; the $S_0 \rightarrow S_2$ and $S_0 \rightarrow S_3$, were observed, while the $S_0 \rightarrow S_1$ band did not appear. The absence of the $S_0 \rightarrow S_1$ band may be due to methanol not being transparent in the ultra-violet region where the band should have been observed. No vibrational fine structure was observed for the UV-Visible spectra of the compound in all the solvents. This may be due to the non-rigidity of the compound. The low intensity of the $S_0 \rightarrow S_1$ transition (band I) makes it designated as ^1L_b and it is quantum mechanically forbidden, overlap forbidden and symmetrically forbidden as well. This is supported by the generally observed low values of the oscillator strength for this band (Table 1). The forbidden nature of this transition is exhibited more in 1,2-dichloroethane than in the other solvents as seen from its very low oscillator strength values of 0.007 in (Table 1). The low value of oscillator strength observed for the compound in 1,2-dichloroethane, may be due to 1,2-dichloroethane shielding the molecule away from the influence of applied light (Obi-Egbedi et al., 1998). The $S_0 \rightarrow S_2$ transition (band II) is designated as ^1L_a, the $S_0 \rightarrow S_3$ is designated as ^1B_b respectively and the $S_0 \rightarrow S_1$ stands for the ground state (Abdul Raheem *et al*., 2010). It can be observed in Figure 2 that, $S_0 \rightarrow S_3$ transition (band III), $S_0 \rightarrow S_2$ (band II) and $S_0 \rightarrow S_1$ (band I) are red-shifted. This allows the classification of all the bands as $\Pi \rightarrow \Pi^*$. The transition intensity recorded in the form of oscillator strength in different solvents revealed that for 4-phenylmorpholine, the oscillator strength follows the order: $f_{S0 \rightarrow S3} > f_{S0 \rightarrow S2} > f_{S0 \rightarrow S1}$.

Table 1: Wavenumber of absorption maxima (cm^{-1}), molar absorption coefficient and oscillator strengths of 4-phenylmorpholine in different solvents

	I			II			III		
Solvent	**V**$_{max}$ **(cm^{-1})**	**E**$_{max}$ **(M^{-1}cm^{-1})**	f	**V**$_{max}$ **(cm^{-1})**	**E**$_{max}$ **(M^{-1}cm^{-1})**	f	**V**$_{max}$ **(cm^{-1})**	**E**$_{max}$ **(M^{-1}cm^{-1})**	f
Cyclohexane	34965.05	1480.31	0.013	40004.80	12105.97	0.121	49390.03	17121.85	0.263
1,2-dichloroethane	34843.21	1741.24	0.007	39682.54	12783.79	0.264	45454.55	5558.78	-
Methanol	-	-	-	40643.78	4040.51	0.036	48633.40	5887.02	0.058

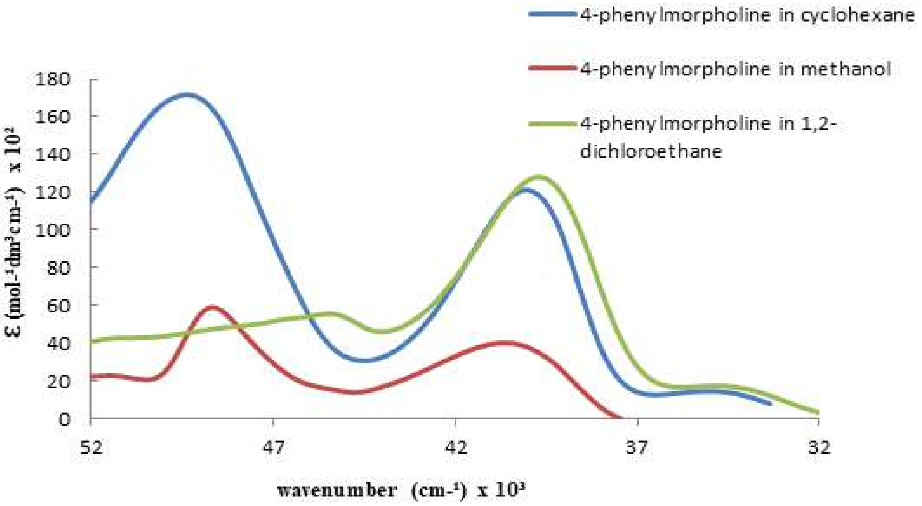

Figure 2: Electronic absorption spectra of 4-phenylmorpholine in cyclohexane, methanol and 1,2-dichloroethane

Solvent effects on the UV-Visible spectra of 4-phenylmorpholine generated computationally

For 4-phenylmorpholine, TD-DFT calculations predicted one intense band and two less intense bands in all the solvents. It can be deduced from **Table 2** that bands I and III in all the solvents had low values for oscillator strength (f). This means that the two bands are of low intensity and have a forbidden transition. However, band II in all the solvents has moderate values for oscillator strengths. This indicates that band II is more intense than band I and III and it is an allowed transition, i.e. an electronic transition at 4.56eV (271.81nm), 5.32eV(233.26nm) and 6.34eV (195.51) for $S_o \rightarrow S_1$, $S_o \rightarrow S_2$ and $S_o \rightarrow S_3$ respectively, has oscillator strength of 0.0459, 0.4194 and 0.0220 in cyclohexane. In all the bands, it was observed that as the solvent transit from non-polar solvent to polar solvent (cyclohexane to methanol), there is an increase in wavelength; i.e. from 271.81 nm to 274.18 nm for band I, 233.26 nm to 233.9 nm for band II and 195.51 nm to 195.86 nm for band III respectively. This indicates that all the bands are of $\Pi \rightarrow \Pi^*$ transition. In Table 3, it can be deduced that the polarity of the solvent is directly proportional to the dihedral angle. Methanol having the highest polarity out of all the solvents employed has the highest dihedral angle (166.55^o) while cyclohexane having the lowest polarity has the lowest dihedral angle (165.457^o). The value of dipole moments depends on the polarity of the solvent used i.e. dipole moments increase with the increase in polarity of a solvent (Islam *et al*., 2011; Kosar *et al*., 2012). From **Table 3**, it is observed that the dipole moment of 4-phenylmorpholine has the highest value in methanol and the lowest value in cyclohexane solvent. This indicates that the compound has a high charge distribution in methanol and a low charge distribution in cyclohexane which makes it more reactive in polar solvents than in non-polar solvents (Targema *et al*., 2013).

Table 2: Calculated parameters for 4-phenylmorpholine in cyclohexane, 1,2-dichloroethane and methanol using TDDFT/B3LYP/6-31G*.

Excitation	CI Coefficient	Wavelength(nm) calculated	Oscillator strength (f)	Energy (eV)
Cyclohexane				
$S_o\rightarrow S_1$		271.81	0.0457	4.5616
43→46	0.21413			
44→45	0.65798			
$S_o\rightarrow S_2$		233.26	0.4194	5.3153
43→46	-0.16039			
44→45	0.63835			
$S_o\rightarrow S_3$		195.51	0.0220	6.3415
41→45	-0.31951			
42→45	0.37429			
43→46	0.43515			
44→47	0.23399			
1,2-dichloroethane				
$S_o\rightarrow S_1$		274.00	0.0458	4.5249
43→46	0.20777			
44→45	0.65798			
$S_o\rightarrow S_2$		234.46	0.4305	5.2880
43→46	-0.15671			
44→45	0.63835			
$S_o\rightarrow S_3$		195.51	0.0221	6.3310
41→45	-0.31929			
42→45	0.43704			
43→46	0.43189			
Methanol				
$S_o\rightarrow S_1$		274.18	0.0424	4.5220
43→46	0.20926			
44→45	0.65849			
$S_o\rightarrow S_2$		233.98	0.4100	5.2989
43→46	-0.16315			
44→45	0.63647			
$S_o\rightarrow S_3$		195.86	0.0189	6.3303
41→45	-0.31569			
42→45	0.45235			
43→46	0.42245			

Table 3: Total energy, dipole moment and dihedral angle ($C_{14}N_1C_2C_3$) of the optimized structure of 4-phenylmorpholine in different solvents as calculated at DFT/B3LYP level using the basis set of 6-31G* in the excited state.

Solvent	Total energy (a.u)	Dipole moment (D)	Dihedral angle
Cyclohexane	-518.8407	0.3559	165.547°
1,2 Dichloroethane	-518.8453	0.4049	166.202°
Methanol	-518.8465	0.4175	166.551°

Solvent effects on the UV-Visible spectra of 1-phenylpyrrole

For 1-phenylpyrrole, two major bands which can be designated as the $S_0 \rightarrow S_1$ transition (band I) and $S_0 \rightarrow S_2$ transition (band II) appeared in the spectra in order of increasing energy in all the solvents (**Figure 3**). In polar solvents such as methanol and 1,2-dichloroethane, the band II is of lower intensity than the band I which can be rationalized on the basis of charge transfer at higher energies. However, in a non-polar solvent like cyclohexane, the band II is more intense than band I. This is supported by the molar absorptivity and oscillator strength values higher in band II than in band I (**Table 4).** In the UV spectra of 1-phenylpyrrole, the shift to a longer wavelength (199 nm) for band II observed in a highly non-polar solvent (cyclohexane) relative to (207 nm) highly polar solvent (methanol) indicate that the band is Π→Π* transitions (Yadav *et al.*, 2011). This implies that the excited state of this transition is more polar or has more charge character, which makes it more stabilized in the excited state than in the ground state, hence resulting in lower energy. Contrary to band II, the shift to a shorter wavelength (255 nm) for band I observed for the spectra of the compound in the same highly non-polar solvent (cyclohexane) relative to the highly polar solvent (methanol) at 251 nm, indicates that the band is n→Π* transition. This indicates that the ground state of this transition is more polar or has more charge character than the excited state, which makes it more stabilized than the excited state. Hence a more stabilized ground state results in higher energy. The transition intensity recorded in the form of oscillator strength in non-polar solvent (cyclohexane) revealed that for 1-phenylpyrrole, the oscillator strength is in general order of $f_{S0 \rightarrow S2} > f_{S0 \rightarrow S1}$ while for polar solvents (methanol and 1,2 dichloroethane) the oscillator strength is in general order of $f_{S0 \rightarrow S1} > f_{S0 \rightarrow S2}$ respectively.

Table 4: Wavenumber of absorption maxima (cm^{-1}), molar absorption coefficient and oscillator strengths of 1-Phenylpyrrole in different solvents

	Band I ($S_0 \rightarrow S_1$)			Band II ($S_o \rightarrow S_2$)		
Solvents	$V_{max}(cm^{-1})$	$E_{max}(M^{1}cm^{-1})$	f	$V_{max}(cm^{-1})$	$E_{max}(M^{-1}cm^{-1})$	f
Cyclohexane	39215.69	15140.41	0.269	50251.26	24973.82	0.546
1,2dichloroethane	39062.50	14271.89	0.212	45662.10	7175.01	-
Methanol	39840.64	13029.78	0.168	47846.89	11719.85	0.120

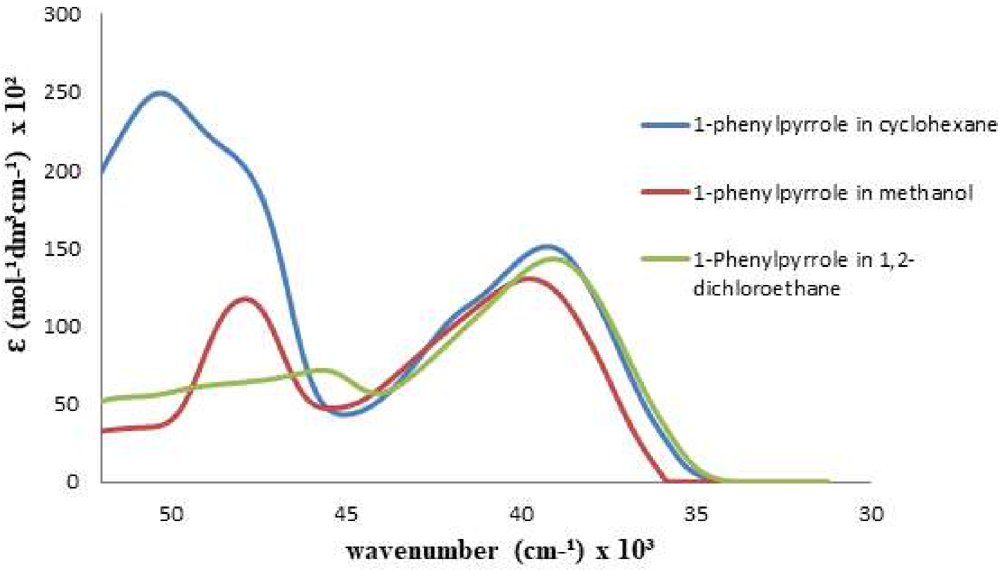

Figure 3: Electronic absorption spectra of 1-phenylpyrrole in cyclohexane, methanol and 1,2-dichloroethane

Solvent effects on the UV-Visible spectra of 1-phenylpyrrole generated computationally

For 1-phenylpyrrole, TD-DFT calculations predicted one intense band and five less intense bands in all the solvents. **Table 5** shows that apart from band IV, all other bands have low values of oscillator strength i.e. electronic transition at 4.70 eV (263.69 nm), 4.79 eV (250.51 nm), 4.95 eV (250.51 nm), 5.07 eV(244.73 nm), 5.97 eV(207.56 nm) and 6.40 eV(193.84 nm) for $S_o \rightarrow S_1$, $S_o \rightarrow S_2$, $S_o \rightarrow S_3$, $S_o \rightarrow S_4$, $S_o \rightarrow S_5$ and $S_o \rightarrow S_6$ respectively; with oscillator strength of 0.0093, 0.0005, 0.0114, 0.4709, 0.0517 and 0.0729 respectively in 1,2-dichloroethane. This indicates that band I, II, III, V and VI have low intensity and forbidden transitions. However, band IV in all the solvents has moderate values for oscillator strength. This implies that band IV transitions are allowed. From **Table 5**, all the bands were shifted to shorter wavelengths from non-polar solvent (cyclohexane) to polar solvent (methanol); i.e. 263.69 nm to 258.89 nm for band I, 258.85 nm to 253.14 nm for band II, 250.51 nm to 248.13 nm for band III, 244.73 nm to 242.07 nm for band IV, 207.56 nm to 206.04 nm for band V and 193.84 nm to 193.31 nm for band VI respectively. This indicates that all the bands are $n \rightarrow \Pi^*$ transitions. **Table 6** also shows that 1-phenylpyrrole has the highest dihedral angle (144.68^{o}) in methanol and the least dihedral (143.39^{o}) in cyclohexane. This signifies that 1-phenylpyrrole is more planar in methanol than in other solvents (Islam *et al*., 2011; Kosar *et al*., 2012). It also shows that 1-phenylpyrrole has the highest dipole moment (2.00 Debye) in methanol and the least dipole moment (1.70 Debye) in cyclohexane. From Table 3 and 6, it can be observed that 4-phenylmorpholine has a higher dihedral angle relative to 1-phenylpyrrole, implying that 4-phenylmorpholine is more planar than 1-phenylpyrrole. The reason for this might be due to the presence of hydrogen bonding interactions between 4-phenylmorpholine and the solvents which might be absent in the interaction between 1-phenypyrrole and the solvents. Moreover, the more planar a molecule is, the smaller the optical (EHOMO - ELUMO gap) of the molecule is. This in turn leads to an increase in intra-molecular charge transfer in the molecule; which is responsible for the reactivity of that particular molecule (Targema *et al*., 2013). In light of this, it can be said that 4-phenylmorpholine is more reactive than 1-phenylpyrrole.

Table 5: Calculated parameters for 1-phenylpyrrole in cyclohexane, 1,2-dichloroethane and methanol using TDDFT/B3LYP/6-31G*

Excitation	CI Coefficient	Wavelength (nm) calculated	Oscillator strength (f)	Energy (eV)
$S_o\rightarrow S_1$		263.69	0.0086	4.7020
38→39	0.68591			
38→41	-0.10269			
$S_o\rightarrow S_2$		258.85	0.0002	4.7897
38→40	0.70494			
$S_o\rightarrow S_3$				
36→39	-0.29953	250.51	0.0122	4.9492
37→40	0.63869			
$S_o\rightarrow S_4$		244.73	0.4627	5.0662
37→39	0.65789			
$S_o\rightarrow S_5$		207.56	0.0442	5.9733
35→40	-0.44390			
36→39	0.49038			
37→40	0.22156			
$S_o\rightarrow S_6$		193.84	0.0633	6.3963
37→38	-0.47481			
36→40	0.47123			
1,2-dichloroethane				
$S_o\rightarrow S_1$		259.89	0.0095	4.7707
38→39	0.68497			
38→41	-0.10600			
$S_o\rightarrow S_2$		254.20	0.0006	4.8774
38→40	0.70373			
$S_o\rightarrow S_3$				
36→39	-0.31727	248.42	0.0109	4.9909
37→40	0.63073			
$S_o\rightarrow S_4$		243.03	0.4702	5.1016
37→39	0.65590			
$S_o\rightarrow S_5$		206.58	0.0544	6.0017
35→40	-0.42958			
36→39	0.48925			
37→40	0.24050			
$S_o\rightarrow S_6$		193.65	0.0743	6.4024
35→39	0.47562			
36→40	0.47058			
Methanol				
$S_o\rightarrow S_1$		258.89	0.0091	4.7891
38→39	0.68403			
38→41	-0.10916			
$S_o\rightarrow S_2$		253.14	0.0011	4.8978
38→40	0.70107			
$S_o\rightarrow S_3$				
36→39	-0.32316	248.13	0.0096	4.9966
37→40	0.62789			
$S_o\rightarrow S_4$		242.07	0.4533	5.1217
37→39	0.65185			
$S_o\rightarrow S_5$		206.04	0.0527	6.0175
35→40	0.42750			

36→39	0.48793			
37→40	-0.24451			
$S_0 \rightarrow S_6$		193.31	0.0717	6.4137
35→39	0.47583			
36→40	0.47049			

Table 6: Total energy, dipole moment and dihedral angle ($C_{14}N_1C_2C_3$) of optimized structure of 4-phenylmorpholine in different solvents calculated by DFT/B3LYP level using the basis set of 6-31G* in the excited state

SOLVENT	TOTAL ENERGY (a.u)	DIPOLE MOMENT (D)	DIHEDRAL ANGLE
Cyclohexane	-441.2223	1.7047	143.39°
1,2 dichloroethane	-441.2270	1.9641	143.58°
Methanol	-444.2283	2.0049	144.68°

Comparison between experimental and computational studies of the effect of solvents on 4-phenylmorpholine and 1-phenylpyrrole.

The experimental and theoretical results for the effect of solvents on the electronic absorption spectra of 4-phenylmorpholine in different solvents correlate fairly well. Three major bands were observed in both methods. The transitions were classified as Π→Π* in all the bands observed in both methods. However, in the case of 1-phenylpyrrole, six bands were observed when the theoretical method was employed while two bands were observed when employing the experimental method. The reason for this difference could be due to the perturbation effect on some of the bands by solvents which may lead to collapsing of those bands or the mixing of bands at the excited states. In the theoretical analysis, all the bands were as a result of n→Π* transition while in the experimental studies, band II emerged as a result of Π→Π* transition and band I emerged as a result of n→Π*. The experimental low-energy bands of 4-phenylmorpholine and 1-phenylpyrrole at 34965.05 cm^{-1} and 39215.69 cm^{-1}, respectively in cyclohexane are equivalent to optical band gaps of 4.33 eV and 4.86 eV which suggest that the compounds are potential insulators.

CONCLUSION

Experimentally, three major bands were observed for the electronic absorption spectra of 4-phenylmorpholine in different solvents, while two major bands were observed for 1-phenylpyrrole. For 4-phenylmorpholine, all the bands were red-shifted, which indicates that they are Π→Π* transition. However, in 1-phenylpyrrole, band II was red-shifted, indicating Π→Π* transition while band I was blue-shifted, signifying n→Π* transition. Theoretically, three major bands were observed for 4-phenylmorpholine and all the bands were red-shifted, implying Π→Π* transition. This shows that there is a strong agreement between the experimental and theoretical results obtained for the electronic absorption spectra of 4-phenylmorpholine in different solvents. However, six bands were observed for 1-phenylpyrrole in all the solvents used for the calculation in this study and all the bands were blue-shifted, signifying n→Π* transition. In this case, there is a disagreement between the experimental result and the theoretical result in the number of transitions observed. Dihedral angles and dipole moments increase with the polarity of the solvents. 4-phenylmorpholine is also observed to be more planar and more reactive than 1-phenylpyrrole.

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