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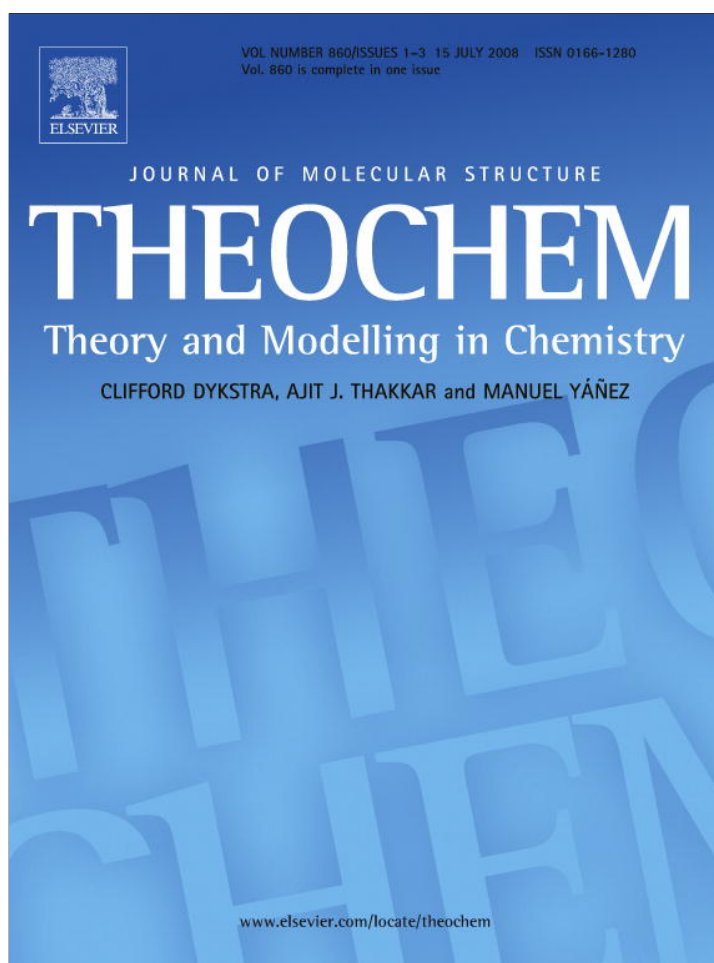
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## Study of intramolecular charge transfer of Michler's ketone using time dependent density functional theory

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## ABSTRACT

Intramolecular charge transfer of Michler's ketone (MK) in vacuum and in six different aprotic solvents has been studied by using time dependent density functional theory (TDDFT). Dynamic process and spectrum feature of a molecule is strongly influenced by the solvent–solute interactions. Therefore, in this work the explicit consideration of solvent–solute interaction has been taken in to account by using the polarizable continuum model (PCM). We have constructed the potential energy curve by taking a combination of two different types of torsional motion; first, an anti-twisting ( $\sim 23^\circ$ ) of *N,N*-dimethylanilino group to bring back the pre-twisted molecule to a nearly planar geometry and second, a twisting ( $\sim 180^\circ$ ) of *N,N*-dimethylamino moiety with respect to the phenyl ring (to which it is attached). A large bathochromic shift in our calculated emission and absorption energies for polar solvents is a clear remnant of charge transfer nature in the excited state. Finally, our results are in agreement with experimental findings and other available theoretical data.

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## 1. Introduction

During the last few decades, an accruable measure of interest on twisted intermediate charge transfer (TICT) process has been achieved in both theoretical and experimental fields of research [1–18]. Although these studies propose many interesting models and hitherto features of TICT process, but till, none of these models fully enable provision of a unified interpretation of the ICT process from donor to an acceptor within a same molecule. Some aromatic organic molecules with a donor and an acceptor group exhibit a characteristic feature of dual-fluorescence in its emission spectrum. Lippert first observed such kind of dual-fluorescence from 4-*N,N*-dimethylamino benzonitrile (DMABN) [1]. After some years, Grabowski explained this phenomenon by introducing TICT model [2]. The implicit assumption of this model is a twisting motion of the donor group to a plane perpendicular to the acceptor group that takes the initially generated locally excited (LE) state to another minimum on the excited state potential energy surface (PES) [2,12,13,17]. Zachariasse and his co-workers extended this model to a planar geometry by assuming a solvent-induced vibronic coupling which is supposed to takes place between locally excited (LE) and charge transferred (CT) state and finally they proposed a planar intramolecular charge transfer (PICT) model [3,4]. Besides these two models, a wagged intramolecular charge transfer

(WICT) and rehybridized intramolecular charge transfer (RICT) have also been proposed by some other groups [5,6].

Dual-fluorescence strongly depends on the energy gap between the first two excited states ( $n\pi^*$  and  $\pi\pi^*$ ), which is significantly influenced by the substituted donor strength and the solvent polarity. For instance, in 4-*N,N*-dimethylamino benzonitrile (DMABN) comparatively strong donor disubstituted amino group modifies the excited states ( $S_1$  and  $S_2$ ) by tuning their energy level and shows a dual emission, whereas a relatively weak donor primary amino group in 4-aminobenzonitrile (ABN) cannot tune the excited state energy level and is thus unable to show dual-fluorescence even in highly polar solvent [4]. Apart from substitution, solvent polarity also has a significant influence on the excited state energy levels. In non-polar aprotic solvent the energy gap between  $n\pi^*$  (LE) and  $\pi\pi^*$  (CT) state is significantly small. In this situation  $S_1$  state is expected to have both the  $\pi\pi^*$  and  $n\pi^*$  character. However, in polar aprotic solvent, more stable  $\pi\pi^*$  dominates over  $n\pi^*$  in  $S_1$  state, thus inverting their relative energies even at the primary geometry. Furthermore, a remarkable redshift in the fluorescence maxima of Michler's ketone in polar solvent implying a strong intramolecular charge transfer is supposed to takes place in the  $S_1$  state. The conclusion is further supported by an experimentally detected large dipole-moment change ( $\Delta\mu = 10.4$  D) in the CT state, that is obtained from the relaxation of  $S_1$  state immediately after photo excitation of the ground state [8].

The phenomenal success of DFT [15–18,22,23] motivated us to employ this method for examination of the small energy gap be-

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tween the lower excited states ( $S_1$  and  $S_2$ ) of Michler's ketone. In particular, the accuracy achieved for the ground state and the excited state calculation using TDDFT is good enough to aid in assigning experimental spectra for these systems [15–18,22,23]. The observation of TICT process by using DFT calculation has been proven to be quite challenging [15–21]. A theoretical knowledge of intramolecular charge transfer process is based primarily on ensemble computational studies. Therefore, the evolution of ensemble average may be used to explain the TICT feature.

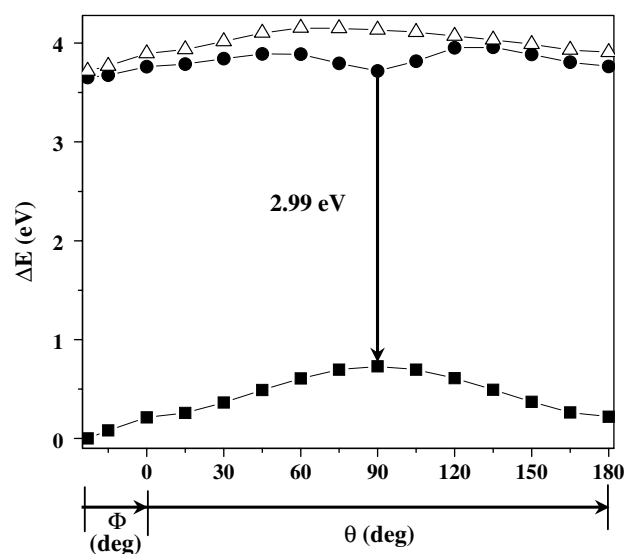
## 2. Computational methods

Ground state optimizations of Michler's ketone (Scheme 1) have been performed by using B3LYP hybrid function with 6-31G (d) basis set at a DFT level [15–17]. A rigorous formalism (TDDFT) is used for transition energy calculation within a DFT framework using same function with 6-31G (d, p) and 6-311G (2d, p) basis set, respectively, for the solvated and the vacuum phase [15–21]. Solvation energy calculations have been performed using time dependent density functional theory–polarizable continuum model (TDDFT–PCM) [22,23]. All calculations were performed using Gaussian 03w package [24]. In analogy to some recent works, we have considered the optimized structure obtained in vacuum to hold good for the solution phase as well as for the excited state calculations assuming not much change in the corresponding geometries [16–18]. Absorption energy obtained from TDDFT calculation is the vertical excitation energy without zero point correction [16–18]. We have used a less complicated basis set in the solvated phase compared to vacuum, in order to save our computational time and also since the system itself becomes complicated when solvation effect is incorporated within the DFT framework. However, several authors have shown that such a little change in basis set does not affect the computed values significantly [16,17]. Potential energy surface (PES) of Michler's ketone is obtained by pursuing an intramolecular rotation along twist coordinate at the donor side within a DFT framework. The details of twisting motions are described in Section 3.2.

## 3. Results and discussion

### 3.1. Ground state properties and vertical excited states of MK

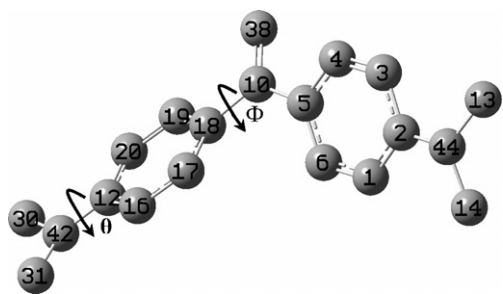
Ground state optimized structure of Michler's ketone (MK) is totally asymmetric; therefore symmetry element could not be applied to identify the different energy levels. In ground state optimized structure of MK, the dihedral angle ( $\phi$ ) between *N,N*-dimethylamino group and benzene moiety is  $\sim 8.5^\circ$  (Fig. 1), and the angle ( $\theta$ ) between phenyl plane of the *N,N*-dimethylanilino moiety and the carbonyl group is  $\sim 23^\circ$  (Fig. 1). From the calculated values of the geometrical parameters, it is clear that the benzophenone moiety within Michler's ketone molecule is not planar; the



**Fig. 1.** Potential energy surface (PES) of Michler's ketone in vacuum for the ground and first two excited states along the twist coordinate of the donor moiety;  $\phi$  and  $\theta$ , describe the rotation of *N,N*-dimethylanilino and *N,N*-dimethylamino group, respectively.

dihedral angle between two phenyl rings is  $\sim 47^\circ$ , which is close to that ( $\sim 51^\circ$ ) reported previously by Mondal et al. [12]. The ground state dipole-moment of Michler's ketone in vacuum was found to be  $\sim 4.98$  D which is slightly greater than that (4.1 D) reported previously by Mondal et al. [12]. The small discrepancy arises mainly because they used GAMESS program with different approximations for ground state optimization. Interestingly, a high dipole-moment ( $\sim 4.98$  D) indicates the unsymmetrical charge distribution in the ground state. We have detected a larger ground state dipole-moment in polar aprotic solvent compared to that observed in vacuum. This is because a polar solvent always stabilizes the polar state by dipole–dipole interaction.

The calculation of vertical excitation energy using TDDFT is not zero point energy corrected [16–18]. In this section, we will try to address the absorption energy (vertical energy) of Michler's ketone in vacuum and in different aprotic solvents. We did not consider protic solvent in order to avoid the complicity that arises in the excited state on account of hydrogen bond formation [12,13,16–18]. An analysis of TDDFT wave function in vacuum shows that the  $S_1$  and  $S_2$  states are mainly composed of  $n\pi^*$  (HOMO–1 to LUMO; HOMO – highest occupied molecular orbital, LUMO – lowest unoccupied molecular orbital) and  $\pi\pi^*$  (HOMO to LUMO) nature of transition. In vacuum, the energy gap between these two states is significantly small ( $\sim 0.07$  eV, Table 1). Therefore, the forbidden  $n\pi^*$  transition in  $S_1$  state becomes partially allowed due to mixing up with energetically close  $S_2$  ( $\pi\pi^*$ ) state (Fig. 1). In non-polar aprotic solvent (similar to vacuum), due to the energetic proximity of the  $S_1$  (LE) and  $S_2$  (CT) state, the absorption bands arising from the two transitions are almost overlap [12–14]. In vacuum, polar  $S_2$  (CT) state has larger oscillator strength with predominantly  $\pi\pi^*$  (HOMO to LUMO) transition character (Table 1). However, in the presence of polar solvent, the highly polar charge transfer (CT) state is significantly stabilized by dipole–dipole interactions and switch over to the first excited state ( $S_1$ ). With increase in solvent polarity, the energy gap between LE and CT state increases quite drastically ( $\sim 4$  times) from 0.07 eV in vacuum to  $\sim 0.27$  eV in most polar DMSO (Table 1). In polar solvent, Mondal et al. [12] observed an additional low intensity band at the blue end ( $\sim 320$  nm) in the absorption spectrum of Michler's ketone that becomes more prominent and well separated from the high intensity



**Scheme 1.** Optimized geometry of Michler's ketone (MK) in the ground electronic state.

**Table 1**  
Computed excited state parameters and absorption energy of Michler's ketone in vacuum and other aprotic solvents using DFT and TDDFT method with B3LYP hybrid function

Medium/Solvent	State	Oscillator strengths ( <i>f</i> )	Computed absorption energies ( $\Delta E$ , eV)	Experimental absorption energies ( $\Delta E$ , eV) <sup>c</sup>
Vacuum <sup>a</sup>	S <sub>1</sub> (LE)	0.0082	3.65	–
	S <sub>2</sub> (CT)	0.6525	3.72	
Cyclohexane <sup>b</sup>	S <sub>1</sub> (CT)	0.7653	3.62	–
	S <sub>2</sub> (LE)	0.0186	3.70	
CHCl <sub>3</sub> <sup>b</sup>	S <sub>1</sub> (CT)	0.7837	3.54	3.51
	S <sub>1</sub> (LE)	0.0316	3.74	
CH <sub>2</sub> Cl <sub>2</sub> <sup>b</sup>	S <sub>1</sub> (CT)	0.7859	3.52	3.51
	S <sub>1</sub> (LE)	0.0381	3.75	
Acetone <sup>b</sup>	S <sub>1</sub> (CT)	0.7785	3.50	3.60
	S <sub>1</sub> (LE)	0.0416	3.76	
Acetonitrile <sup>b</sup>	S <sub>1</sub> (CT)	0.7774	3.49	3.56
	S <sub>2</sub> (LE)	0.0435	3.76	
DMSO <sup>b</sup>	S <sub>1</sub> (CT)	0.8010	3.48	3.46
	S <sub>2</sub> (LE)	0.0490	3.75	

<sup>a</sup> Basis set 6-311G (2d, p).

<sup>b</sup> Basis set 6-31G (d, p).

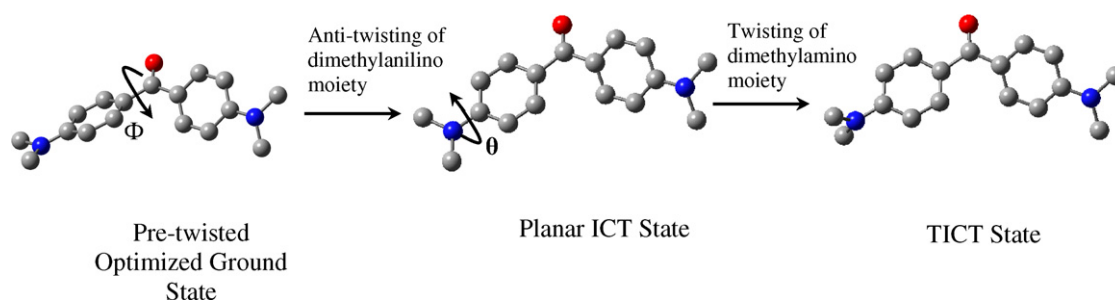
<sup>c</sup> Values taken from Ref. [7].

one with increase in solvent polarity [12]. Note, the low intensity band originates from a forbidden (HOMO-1 to LUMO) transition. The position of the band hardly shows any solvent polarity dependence due to its weakly polar nature in the excited state [12]. With increase in solvent polarity, the energy difference between LE and CT state increases and the transition energy involved with these two states becomes significantly different that resulting in two well separated bands in the absorption spectrum. Evidently, from our calculated values, we have detected a very little change in LE (HOMO-1 to LUMO) state energy with change in solvent polarity (Table 1). Note, our calculated average transition energy ( $\sim 3.74$  eV) for the LE state is not very different from the reported experimental value ( $\sim 3.87$  eV, 320 nm) [8,12]. Besides vacuum, we have also performed our DFT/TDDFT calculations on a series of six aprotic solvents with different polarity. Due to low solubility of Michler's ketone in cyclohexane, we did not find a steady state experimental data to compare [12], for other aprotic solvents our calculated results nicely correlate with the experimental values, which is a strong support towards the reliability of our computed values and also appropriate choice of basis sets (Table 1) [8].

### 3.2. Twisting dynamics and emission property in vacuum and in aprotic solvents

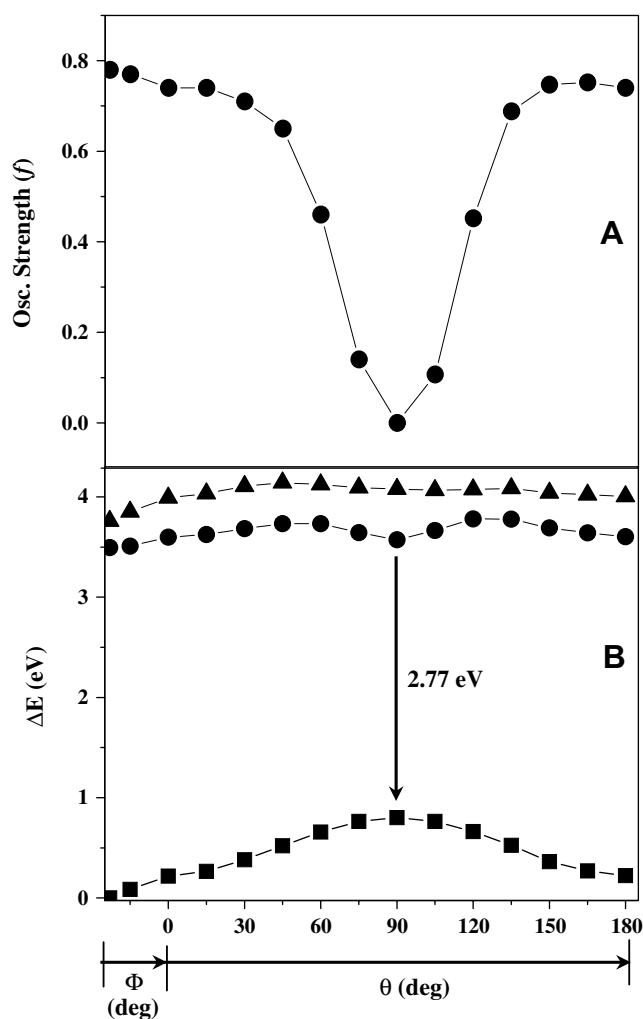
Several experimental observations of Michler's ketone in aprotic solvent as such, low fluorescence quantum yield, blue shifted absorption maximum in time resolved transient spectra and significantly short lifetime in the excited states is a clear indication of a relaxation involving a change of molecular conformation in the S<sub>1</sub> state [12]. Mondal et al. [12] tried to correlate this relaxation pro-

cess by taking a combination of an anti-twisting and twisting motion of the donor moiety. In brief, immediately after photo excitation, the Michler's ketone molecule first shows an anomalously fast (few picoseconds) anti-twisting relaxation of *N,N*-dimethylanilino group to bring back the pre-twisted molecule to a nearly planar geometry with high mesomeric interaction and intramolecular charge transfer (ICT) character [12,13,26–30]. In polar solvent the *N,N*-dimethylamino moiety of Michler's ketone exhibits a further twisting of  $\sim 90^\circ$  with respect to the phenyl ring to which it is attached. Such kind of twisting motion is the prerequisite condition for the relaxation of ICT to TICT state. Therefore, in this section we will discuss the potential energy curve via anti-twisting and twisting motion of the donor moiety (Scheme 2). The twisting dynamics is described by two torsional parameters  $\Phi$  and  $\theta$ , respectively, to describe the anti-twisting and twisting motion of the *N,N*-dimethylanilino and *N,N*-dimethylamino groups. In Scheme 1,  $\theta$  and  $\Phi$  represent, respectively, the dihedral angle  $<30$ – $42$ – $12$ – $20$  and  $<19$ – $18$ – $10$ – $38$ . Ground state optimized structure of Michler's ketone is non-planar; dihedral angle ( $\theta$ ) between *N,N*-dimethylamino group and the phenyl ring (to which it is attached) is  $\sim 8.5^\circ$  (Fig. 1), which we define as an arbitrary zero position for  $\theta$  during PES calculation. The same logic is also applied for dihedral angle ( $\Phi$ ) between *N,N*-dimethylanilino and carbonyl group, with an optimized value of  $\sim -23^\circ$  which is used as an initial value for  $\Phi$  in PES calculation (Figs. 1 and 2B). During the PES calculation all geometrical parameters are kept frozen to that optimized for the ground state at all the points and for every electronic states, except their twisting angles ( $\Phi$  and  $\theta$ ), they are varied  $\sim 15^\circ$  in each steps. A nearly planar structure (with ICT character) can be achieved by an anti-twisting ( $\sim 23^\circ$ ) of *N,N*-dimethylanilino



**Scheme 2.** Twisting dynamics of Michler's ketone (MK) in the S<sub>1</sub> state.





**Fig. 2.** (A) Plot of oscillator strength of  $S_1$  state for Michler's ketone (MK) along the twisting coordinate of the donor moiety in acetonitrile solvent. (B) Potential energy surface (PES) of MK for the ground and first two excited states along the twist coordinate of donor moiety in acetonitrile.  $\Phi$  and  $\theta$  describe the rotation of  $N,N$ -dimethylanilino and  $N,N$ -dimethylamino group.

moiety in the pre-twisted ground state geometry. Further, a torsional motion ( $\sim 90^\circ$ ) of the  $N,N$ -dimethylamino group is essential to yield a minimum on the energy surface from a nearly planar ICT state. Potential energy surface (PES) of Michler's ketone in vacuum is depicted in Fig. 1, whereas Fig. 2A and B, respectively, shows the oscillator strength and PES of Michler's ketone in a polar aprotic solvent (acetonitrile). Besides vacuum and acetonitrile, we have also calculated the PES in some other solvents with different

polarity, such as cyclohexane,  $\text{CHCl}_3$ ,  $\text{CH}_2\text{Cl}_2$ , acetone and DMSO. In both vacuum and solvent medium the ground state energy gradually increases along the twist coordinate and reaches a maximum at  $\theta \sim 90^\circ$ . On the contrary, the energy of CT state decreases in the same direction and ultimately reaches to a local energy minimum at  $\theta \sim 90^\circ$ ; resulting a smallest gap ( $\Delta E_{1s}$ ) between the ground and the first excited state. In addition to this a second local minimum at a nearly planar structure ( $\theta \sim 0^\circ$ ,  $\Phi \sim 0^\circ$ ) is also observed (Figs. 1 and 2B). A red-shifted emission and lowering of oscillator strength along the donor twist coordinate is a clear reminiscent of lowering of vertical transition energy ( $\Delta E_{1s}$ ) and increasing of  $n-\pi^*$  character of the emitting species (Figs. 1 and 2). The assumption is further supported by the study of molecular orbital picture (not shown). In the ground state optimized geometry, predominantly  $\pi-\pi^*$  nature of transition (HOMO to LUMO) is observed and the donor lone pair is delocalized through resonance with the attached phenyl group. However, the twisted conformer ( $\theta \sim 90^\circ$ ,  $\Phi \sim 0^\circ$ ) shows  $n-\pi^*$  transition character (HOMO-1 to LUMO) with localized donor lone pair which becomes available for charge transfer to the  $\pi^*$  orbital of the acceptor ( $\text{C}=\text{O}$ ) moiety (Scheme 2). This is a clear feature of charge transfer that takes place when donor group become orthogonal to the acceptor group, i.e., decoupling is maximum. In the observed second local minimum ( $\Phi \sim 0$ ,  $\theta \sim 0$ ), an intramolecular charge transfer is supposed to takes place at a nearly planar geometry (Figs. 1 and 2B). The calculated vertical transition energy at this point is  $\sim 3.55$  and  $3.38$  eV in vacuum and in acetonitrile, respectively. Note our calculated value ( $\sim 3.38$  eV) for acetonitrile is much higher than that ( $\sim 2.57$  eV) observed for 1-propanol in an experimental study [12]. The discrepancy mainly arises because of the hydrogen bond forming ability of 1-propanol that makes the excited state inherently stable. In general polar protic solvents exhibit an efficient non-radiative relaxation from the TICT state to the ground state and not a radiative emission; the only radiative emission obtained is from the ICT state [12,13]. In Table 2 we have compared the computed emission energies and the corresponding reported experimental values. In all the solvents mentioned our calculated values are little bit higher than the experimental values, which is maximum ( $\sim 0.36$  eV) in the case of acetonitrile and minimum ( $\sim 0.15$  eV) for  $\text{CHCl}_3$ . Recently some other groups have also reported a higher computed emission energy obtained from PES calculation [16–18]. The small discrepancy between the calculated values and the experimental results may be attributed to the non-optimized excited state geometry of Michler's ketone. This is due to lack of an analytical gradient in the TDDFT method and hence it is beyond our scope to optimize the excited state geometry. Furthermore, we used the ground state optimized structure in vacuum and applied it to the solvent phase assuming not much change in geometry [16–18]. Therefore it is not surprising to observe a small discrepancy that may originate from the small geometrical change in the solvent phase compared to the vacuum.

**Table 2**

Computed excited state parameters and emission energies of Michler's ketone in vacuum and other aprotic solvents using DFT and TDDFT method with B3LYP hybrid function

Medium/Solvent	$\epsilon^c$	State	Oscillator strengths ( $f$ )	Computed emission energies ( $\Delta E$ , eV)	Experimental emission energies ( $\Delta E$ , eV) <sup>d</sup>
Vacuum <sup>a</sup>		$S_1$ (CT)	0.00	2.99	–
Cyclohexane <sup>b</sup>	2.0	$S_1$ (CT)	0.00	2.93	–
$\text{CHCl}_3$ <sup>b</sup>	4.8	$S_1$ (CT)	0.00	2.84	2.69
$\text{CH}_2\text{Cl}_2$ <sup>b</sup>	9.1	$S_1$ (CT)	0.00	2.81	2.58
Acetone <sup>b</sup>	20.7	$S_1$ (CT)	0.00	2.78	2.52
Acetonitrile <sup>b</sup>	37.5	$S_1$ (CT)	0.00	2.77	2.41
DMSO <sup>b</sup>	46.7	$S_1$ (CT)	0.00	2.76	2.42

<sup>a</sup> Basis set 6-311G (2d, p).

<sup>b</sup> Basis set 6-31G (d, p).

<sup>c</sup> Static dielectric constant; values taken from Ref. [25].

<sup>d</sup> Values taken from Ref. [7].

#### 4. Conclusion

In this work, using TDDFT method we have calculated the absorption and emission energies of Michler's ketone in vacuum and in six aprotic solvents with different static polarity. From our study it is evident that immediately after photo excitation Michler's ketone initially undergoes an anomalously fast intramolecular anti-twisting motion to bring back the pre-twisted geometry to a nearly planar one, followed by a twisting of the *N,N*-dimethyl-amino group at an angle  $\sim 90^\circ$  to yield a minimum on the energy surface curve. This type of twisting may leads to an excited state relaxation from LE to ICT and finally to a TICT state. In vacuum, highly polar CT state becomes less stable compared to less polar LE state and resides to an energetically high  $S_2$  state. Polar solvent stabilizes the CT state to a greater magnitude compared to the LE state that inverts the CT state to an energetically more stable  $S_1$  state, which is responsible for the observed red shift in the calculated emission and absorption energy in polar solvent compared to vacuum.

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