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Research Article

PCM-DFT Investigation on the Linear and Nonlinear Optical Properties of Two Triazole Derivatives in Different Solvents

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Abstract. This effort was performed to investigate the linear and nonlinear optical (NLO) properties of two 1,2,3-triazole derivatives in several solvent media and in gas-phase at PCM/DFT/CAM-B3LYP/6-311+G(d) level of theory. The static and dynamic NLO parameters as the total dipole moment, the average linear polarizability, the *Hyper-Rayleigh Scattering* (HRS) first hyperpolarizability, and the average second hyperpolarizabilityare calculated as function of static dielectric constant of the solvents. The computational linear and nonlinear optical studies revealed that both the triazoles derivatives are promising materials for NLO applications.

Keywords. Polarizable continuum model, Dipole moment, Linear polarizability, Hyper-Rayleigh Scattering (HRS), Second hyperpolarizability

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1. Introduction

The study of organic materials exhibiting nonlinear optical properties has been of great interest in the recent years, partly due to the ease handlingof these compounds as compared with inorganic materials.Organic materials with large third-order nonlinear optical (NLO) properties are promising for several applications in photonic technologies [1,6,7,14,17,30,31]. Triazole and its derivatives, as the 1,2,3-triazole, have a simple structure exhibiting interesting nonlinear optical properties [1, 5, 28] and in addition present a number of functionalities in the fight against pathologies, such as antimycotic [12], antiviral [15], anticonvulsant [8], antidepressant [26], anti-inflammatory [16], antifungal [9] and analgesic [22].

In this work a study of the solvent media effects on the geometrical and nonlinear optical (NLO) properties of two 1,2,3triazole derivatives, namely: 1-(3,4-dimethylphenyl)-4-(3-methoxyphenyl)-5-trifluoromethyl-1H-1,2,3-triazole (DMTT) with molecular formula $C_{18}H_{16}F_3N_3O$ and 3-[4-(3),4-dimethoxyphenyl)-5-(trifluoromethyl)-1H-1,2,3-triazol-1-yl] phenol (DTTP) with molecular formula $C_{17}H_{14}F_3N_3O_3$ [10] is reported. The solvent media are modelled using the Polarizable Continuum Model (PCM) and the NLO parameters were calculated at DFT/CAM-B3LYP/6-311+G(d) level in gas-phase and in nineteen solvent media. The total dipole moment, the average linear polarizability and the first and second hyperpolarizabilities were studied as function of the static dielectric constant of the solvent media. Also, complementary studies of the bond-anglesand torsion-angles, of the frontier molecular orbitals (HOMO and LUMO) and the global reactivity descriptorswerecalculated as function of the static dielectric constant for DMTT and DTTP (see Figure 1).

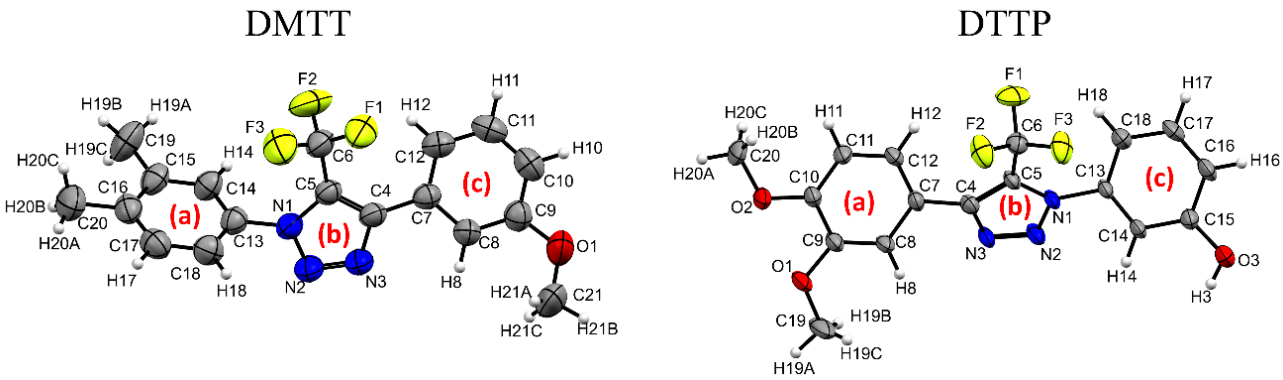

Figure 1. Ortep diagram of 1,2,3-triazole derivatives, DMTT and DTTP

2. Material and Methods

Solvent Media

In our theoretical calculation the solvent media are modelled through the *Polarizable Continuum Model* (PCM) [4, 20, 24] and the NLO parameters were calculated using the Density Functional Theory (DFT) with the functional CAM-B3LYP, that combines the hybrid qualities of B3LYP and the long-range correction, being more convenient for the calculation of the static and dynamic NLO parameters, as discussed in reference [27] for several basis set. Here the large 6-311+G(d) Pople split-valence basis set is used combined with the CAM-B3LYP. In favor of usingthe PCM model, recent theoretical studies of NLO properties of molecules immersed in solvent media have shown a good agreement with the experimental data for the Hyper-Rayleigh Scattering first hyperpolarizability [5, 13, 21, 25].

Organic solvents are divided into polar (protic and aprotic) and nonpolar; in this work solvents having values of the static dielectric constant (ϵ) below 5 will be considered as nonpolar solvents. The solvent media used in the present calculation were: Argon ($\epsilon = 1.43$); Heptane ($\epsilon = 1.91$); Toluene ($\epsilon = 2.37$); Chloroform ($\epsilon = 4.71$); ChloroBezene ($\epsilon = 5.70$); Tetrahydrofuran ($\epsilon = 7.43$); DichloroMethane ($\epsilon = 8.93$); DiChloroEthane ($\epsilon = 10.13$); 2-Methyl_2_Propanol ($\epsilon = 12.47$); 1-Butanol ($\epsilon = 17.33$); Acetone ($\epsilon = 20.49$); Ethanol ($\epsilon = 24.85$); Methanol ($\epsilon = 32.61$); Acetonitrile ($\epsilon = 35.69$); DMSO ($\epsilon = 46.83$); FormicAcid ($\epsilon = 51.10$); Water ($\epsilon = 78.36$); Formamide ($\epsilon = 108.94$); *n*-MethylFormamide-mixture ($\epsilon = 181.56$). Also, results for the Gas-phase ($\epsilon = 1.00$) were computed.

Geometric Optimization

The molecular geometry optimization of the title compounds was performed in a diverse set of solvents and in gas phase. The similarities between the X-ray diffraction result obtained by Farrán *et al*. [10] and the optimized molecular structures were analysed calculating the root mean square deviation (RMSD) using the Mercury software [18].

HOMO and LUMO

From the values of the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) the gap energies as function of the static dielectric constants of several solvent media were calculated. Also, the reactivity descriptors were calculated in three chosen solvent media.

NLO Parameters

The total dipole moment (μ), the average linear polarizability ($\langle\alpha\rangle$) the first hyperpolarizability parallel to the moment dipole (taken as z-direction) ($\beta_{\|z}$) and the average second hyperpolarizability are given by the following expressions,

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{\frac{1}{2}}, \tag{2.1}$$

$$\langle\alpha\rangle = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}, \tag{2.2}$$

$$\beta_{\|z} = \frac{1}{5}\sum_{i=1}^{3}(\beta_{zii} + \beta_{izi} + \beta_{iiz}), \tag{2.3}$$

$$\langle\gamma\rangle = \frac{1}{5}[\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2(\gamma_{xxyy} + \gamma_{xxzz} + \gamma_{yyzz})]. \tag{2.4}$$

The Hyper-Rayleigh Scattering (HRS) first hyperpolarizability ($\langle\beta_{HRS}\rangle$) is given by,

$$\langle\beta_{HRS}\rangle = \sqrt{\langle\beta_{ZZZ}^2\rangle + \langle\beta_{XZZ}^2\rangle}, \tag{2.5}$$

where X, Y, and Z are the coordinates of the laboratory reference system. The light beam propagation is assumed in X-direction and polarized in Z-direction [3, 23]. $\langle\beta_{ZZZ}^2\rangle$ and $\langle\beta_{XZZ}^2\rangle$ are the macroscopic averages calculated from β_{ijk} and calculated from the expressions,

$$\langle\beta_{ZZZ}^2\rangle = \frac{1}{210}(30\delta_1 + 12(\delta_2 + \delta_3 + \delta_5) + 6(\delta_4 + \delta_6) + 2(\delta_7 + \delta_8 + \delta_{11}) + 4\delta_9 + \delta_{10}), \tag{2.6}$$

$$\langle\beta_{XZZ}^2\rangle = \frac{1}{210}(6(\delta_1 - \delta_3 - \delta_5 + \delta_7) + 8\delta_2 + 18\delta_4 + 4\delta_6 - \delta_8 - 2\delta_9 + 3\delta_{10} - \delta_{11}), \tag{2.7}$$

where the coefficients δ_n are defined in Table 1.

Table 1. The δ_n ccoefficients used for the calculation of HRS first hyperpolarizability

$$\delta_1 = \sum_i \beta_{iii}^2 ;$$
$$\delta_2 = \sum_{ij} \beta_{iii}\beta_{ijj} ;$$
$$\delta_3 = \sum_{ij} \beta_{iii}(\beta_{jij} + \beta_{jji}) ;$$
$$\delta_4 = \sum_{ij} \beta_{ijj}^2 ;$$
$$\delta_5 = \sum_{ij} \beta_{ijj}(\beta_{jij} + \beta_{jji}) ;$$
$$\delta_6 = \sum_{ij} (\beta_{jij} + \beta_{jji})^2 ;$$
$$\delta_7 = \sum_{ijk} \beta_{ijj}\beta_{ikk} ;$$
$$\delta_8 = \sum_{ijk} (\beta_{jij} + \beta_{jji})(\beta_{kik} + \beta_{kki}) ;$$
$$\delta_9 = \sum_{ijk} \beta_{ijj}(\beta_{kik} + \beta_{kki}) ;$$
$$\delta_{10} = \sum_{ijk} (\beta_{ijk} + \beta_{ikj})^2 ;$$
$$\delta_{11} = \sum_{ijk} (\beta_{ijk} + \beta_{ikj})(\beta_{jjk} + \beta_{jki}).$$

All computational calculations were performed using the Gaussian 09 program package [11] and converted to electrostatic units (esu).

3. Results and Discussion

Molecular Analysis in Solvent Media

The similarities between the optimized molecular structurein a solvent medium and the molecular structure obtained by X-ray diffraction were analysedcalculating the Root Mean Square Deviation (RMSD). The anchoring pointswere chosen at the benzene ring (a) and at the benzenering (c) for DMTT and DTTPrespectively. Figure 2 shows the overlap between the X-ray molecular structure (in red) and the optimized molecular geometry in DMSO (in yellow) for both triazole derivatives. The anchoring points can be seen clearly in Figure 2.

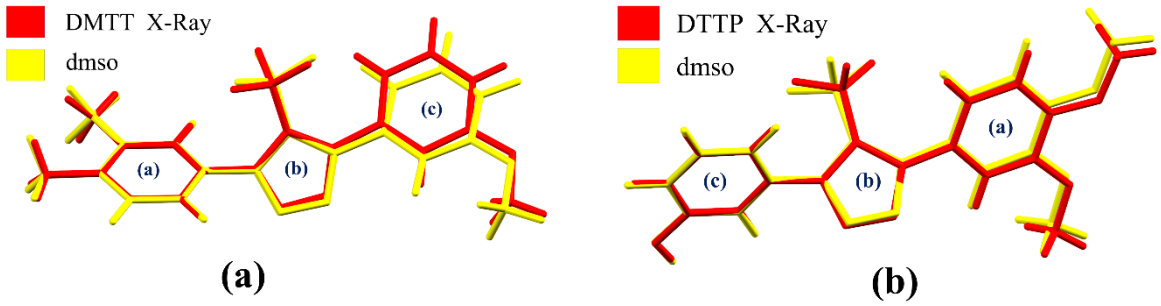

Figure 2. Overlap between the X-ray diffraction results and the PCM/DFT optimized structures for DMTT and DMTT both in DMSO

Figure 3 shows the RMSD-values for DMTT and DTTP, as function of the static dielectric constant (ϵ) of the solvent media. As can be seen the RMSD-values for DTTP increases monotonically with the increasing of the ϵ-values. For DMTT, in the range of $1 \leq \varepsilon \leq 5.70$ a decreasing of the RMSD-value with the increasing of ε-value is observed in the Figure 3 and a smooth increasing of the RMSD-value is observed for $5.7 < \varepsilon \leq 30$. For solvent medium with $\varepsilon > 30$ the curves tend to stability, for both compounds.

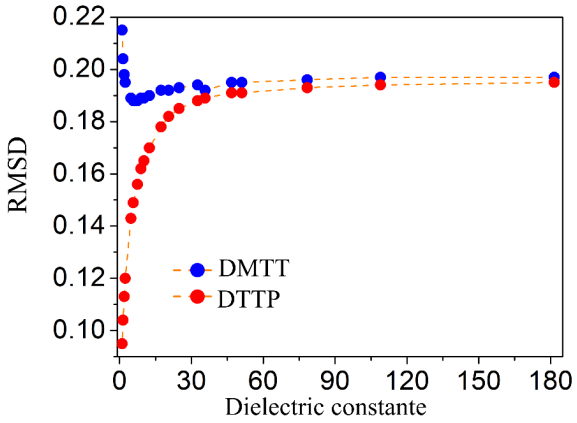

Figure 3. RMSD-values for DMTT and DTTP as function of ϵ-values

Table S41 (Support Information) shows the results for the bond-angles and torsion-angles for DMTP and DTTP molecules in gas-phase and solvent media. The X-ray diffraction results are also shown for comparison. As can be seen in Table S41 the solvent medium effects on the bond-angles for both molecules are weak, the changes are smaller than 2%. The changes in the torsion-angles in general are also not significant, as can be seen in Table S41, however the torsion-angle N2-N1-C13-C18 (N2-N1-C13-C14) for DMTT (DTTP), increases with the increasing of the ϵ-value ($1 \leq \varepsilon \leq 181.56$) going from 54° (51°) to 64° (61°) showing a considerable variation of 10° due to the solvent media effects.

The CHELPG partial charges of the compounds also can be seen in the Support Information Tables S42–S43. For DMTT the methoxy group O1-C21 has a charge of −0.202e and the benzene ring (a) has 0.067e in DMSO. Also, in DMSO, for the DTTP the charges of the methoxy group O1-C19 and the hydroxyl (O3-H3) are of −0.162e and −0.230e respectively.

HOMO-LUMO

Figure 4 shows the plots of the frontier molecular orbitals, HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) for DMTT and DTTP in DMSO, the blue and red colours, represent the positive and negative regions, respectively. HOMO and LUMO energies are important parameters to help our understanding about the molecular chemical reaction. While HOMO behaves as an electron donor, LUMO behaves as an electron acceptor. The HOMO and LUMO for DMTT and DTTPin gas-phase and in various solvent media can be seen in the Figures S1-S19 (Support Information).

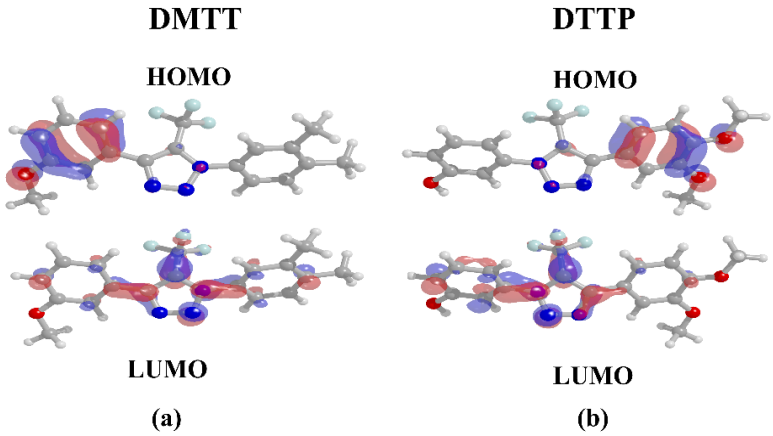

Figure 4. The HOMO and LUMO orbitals of the compounds in DMSO

Table 2 shows the values of the HOMO-energy (ε_{HOMO}) and LUMO-energy (ε_{LUMO}) for both DMTT and DTTP in Chloroform, DMSO and Water. From these parameters the global reactivity descriptors as, the ionization energy ($I_E = -\varepsilon_{HOMO}$), the electron affinity ($A_E = -\varepsilon_{LUMO}$), the global hardness ($\eta = (I_E - A_E)/2$), the chemical potential ($\mu = -(I_E + A_E)/2$), the global electrophilicity ($\omega = \mu^2/2\eta$), the global softness ($S = 1/\eta$) and additional electronic charge ($\Delta N = -\mu/\eta$) were calculated. These global quantities can be used as complementary tools in the description of thermodynamic aspects of chemical reactivity in connection with minimum polarizability and maximum hardness principles.

Table 2. Chemical parameters of the DMTT and DTTP in some solvent media

	Chloroform		DMSO Water		Water	
	DMTT	DTTP	DMTT	DTTP	DMTT	DTTP
ε_{HOMO} (eV)	−7.81	−7.37	−7.88	−7.45	−7.89	−7.46
ε_{LUMO} (eV)	−0.47	−0.55	−0.48	−0.53	−0.48	−0.53
Ionization energy (I_E) (eV)	7.81	7.37	7.88	7.45	7.89	7.46
Electron affinity (A_E) (eV)	0.47	0.55	0.48	0.53	0.48	0.53
Global hardness (μ)	3.67	3.41	3.70	3.46	3.70	3.46
Chemical potential (μ_p)	−4.14	−3.96	−4.18	−3.99	−4.18	−3.99
Global electrophilicity (ω)	2.34	2.30	2.36	2.30	2.37	2.30
Global softness (S)	0.27	0.29	0.27	0.29	0.27	0.29
Additional electronic charge (ΔN)	1.13	1.16	1.13	1.15	1.13	1.15

As can be seen in Table 2 the global quantities present small variations with the increasing of the static dielectric constant values. Particularly the global softness and the additional electronic charge are practically insensible to the change of the solvent medium for both compounds. The values of the ionization energy, global hardness, and chemical potential for DMTT are greater than for the DTTP although this difference is small. However, the value of the electron affinity energy (A_E) of DTTP is greater than of DMTT.

Other important parameter to be considered is the gap energy, defined as the difference between the HOMO-LUMO energies. The gap energies results for the two 1,2,3-triazole derivatives as function of the static dielectric constant of the solvent media are shown in Figure 5. As can be seen the values of the gap energy increases with the increasing of the ϵ-values, this increase is more significant for ϵ in the range of $1 < \varepsilon < 20$; for $\varepsilon > 20$ the increase

is smaller, and the gap energies tends asymptotically to the values of 7.41 eV (DMTT) and 6.93 eV (DTTP). The fact that the DTTP gap energies in solvent media are smaller than for DMTT molecule (Figure 5) indicates that the DTTP molecule is more polarizable and more reactive than DMTT [29]. An analysis of the reactivity parameters of the compounds, suggests that the DTTP has potential to present better nonlinear optical properties than DMTT.

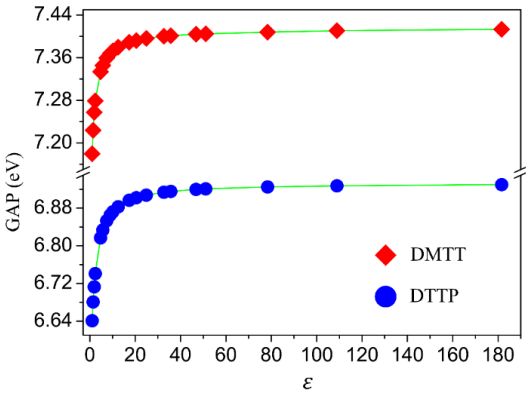

Figure 5. Gap energy as function of the ϵ-values of solvent medium for the two 1,2,3-triazole derivatives

Nonlinear Optical Properties

The DFT/CAM-B3LYP/6-311+G(d) static results for the dipole moment (μ), the average linear polarizability ($\langle\beta(0;0)\rangle$), the first hyperpolarizability parallel to the dipole moment ($\beta_{\|z}(0;0,0)$) and the average second hyperpolarizability ($\langle\gamma(0;0,0,0)\rangle$) for both DMTT and DTTP are shown in Figure 6. As can be seen the values of μ, $\langle\beta(0;0)\rangle$, and $\langle\gamma(0;0,0,0)\rangle$, increase with the increasing of the ϵ-values, this increasing is more significant in the region where $\epsilon < 20$.

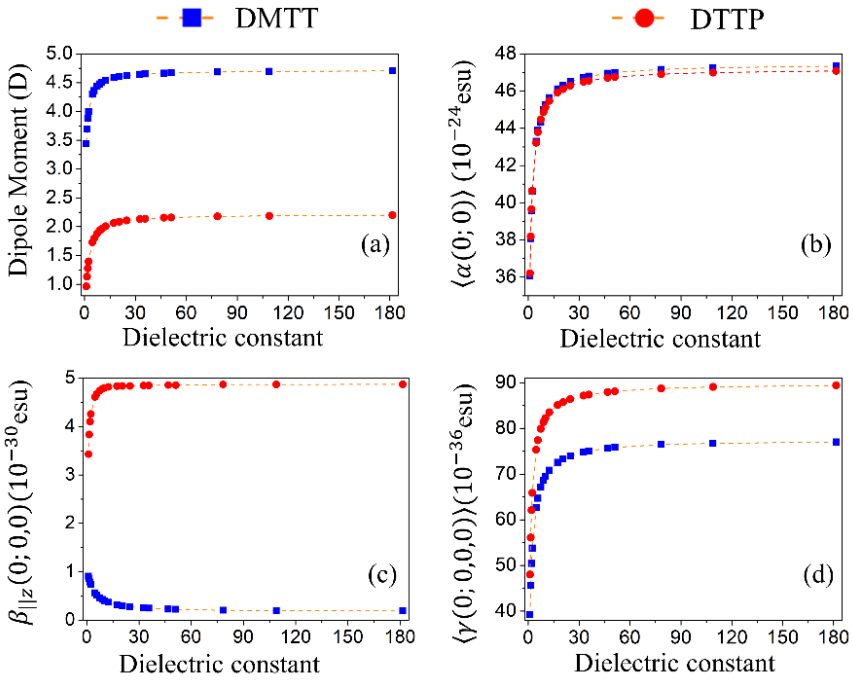

Figure 6. Static electric parameters:μ, $\langle\beta(0;0)\rangle$, $\beta_{\|z}(0;0,0)$ and $\langle\gamma(0;0,0,0)\rangle$ for DMTT and DTTP, as function of the ϵ-values

The μ-values for DMTT are greater than for DTTP and go from 3.44 D to 4.70 D (DMTT) and goes from 0.963 D to 2.20 D (DTTP). However, the $\langle\beta(0;0)\rangle$-values for DMTT and DTTP in a determined solvent medium are practically the same. For example, in DMSO the α-values are 46.95×10^{-24} esu (DMTT) and 46.70×10^{-24} esu (DTTP) and in Water 47.2×10^{-24} esu (DMTT) and 47.0×10^{-24} esu (DTTP). Differently the $|\beta_{\|z}(0;00)|$-values show a significant variation as function of ϵ-value. With the increasing of the ϵ-value for DMTT the $|\beta_{\|z}(0;00)|$-values decrease, while for DTTP increase (see Figure 6). These results for the static parameters show that the NLO properties of DTTP are better than of DMTT.

Figure 7 shows the HRS first hyperpolarizability as function of the static dielectric constant in the static and dynamic (at $\lambda = 1064$ nm) cases for both the compounds. As we can note the β_{HRS}-value in both cases (static and dynamic) for DTTP are greater than those for DMTT in all solvent media. The behaviour of the β_{HRS}-value as function of ϵ-value is similar for both compounds. Particularly the β_{HRS}-values (static case) in Chloroform are 1.63×10^{-30} esu (DMTT) and 6.77×10^{-30} esu (DTTP) and in DMSO are 2.02×10^{-30} esu (DMTT) and 7.26×10^{-30} esu (DTTP). The β_{HRS}-values at $\lambda = 1064$ nm are greater than the static values, in Chloroform, for DMTT (+5%) and DTTP (+1.8%), however in DMSO the values are smaller −18.5% (DMTT) and −17% (DTTP).

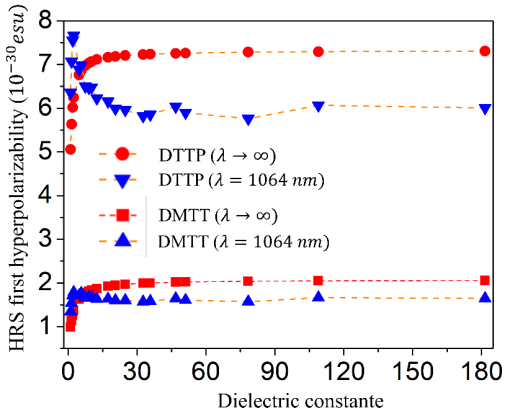

Figure 7. Static and dynamic β_{HRS}-values for DTTP and for DMTT as function of the dielectric constant

Figure 8 shows the DFT/CAM-B3LYP/6-311+G(d) results for the dynamic average second hyperpolarizabilities $\langle\gamma(-\omega;\omega,0,0)\rangle$ and $\langle\gamma(-2\omega;\omega,\omega,0\rangle$ corresponding to Kerr effect and second harmonic generation (dc-SHG) respectively for both compounds at 1064nm.As can be seen the results for the DTTP are greater than those for the DMTT, and the dispersion curves present similar behaviour. The $\langle\gamma(-\omega;\omega,0,0)\rangle$-values in Chloroform (nonpolar), DMSO (polar, aprotic) and Water (polar, protic) for DTTP are 22.0%, 18.7% and 18.5% respectively greater than the values for DMTT. Likewise, the $\langle\gamma(-2\omega;\omega,\omega,0\rangle$-values in the same solvent media for DTTP are greater than those for DMTT of 31.3%, 25.8% and 25.4% respectively.

The standard compound to compare the values of the HRS first hyperpolarizability is the P-nitroaniline (pNA), that presents good NLO properties and have β_{HRS}-value well-known experimentally. The HRS first hyperpolarizability of pNA in DMSOat $\lambda = 1064$ nm is 25.3×10^{-30} esu, this value is greater than the values of DMTT(1.64×10^{-30} esu) and of DTTP (6.04×10^{-30} esu). However, the value of the second hyperpolarizability ($\langle\gamma(-2\omega;\omega,\omega,0\rangle$) for pNA is $\langle\gamma_{pNA}\rangle = 8.0\times10^{-36}$ esu [2], this value is smaller those obtained for both, DMTT and DTTP, $\langle\gamma_{DMTT}\rangle = 69.2\times10^{-36}$ esu and $\langle\gamma_{DTTP}\rangle = 87.0\times10^{-36}$ esu, that aremore than ten times greater than pNA-value, suggesting that these molecules could be promising for NLO applications.

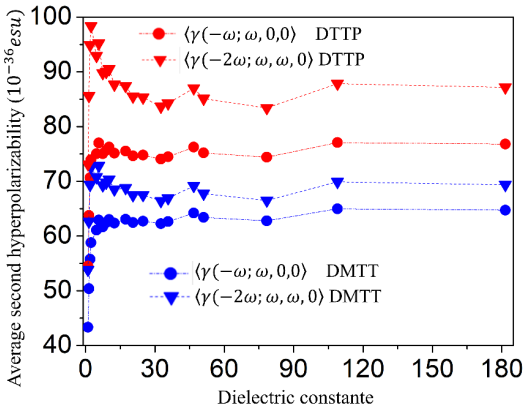

Figure 8. Average second hyperpolarizabilities $\langle\gamma(-\omega;\omega,0,0)\rangle$ and $\langle\gamma(-2\omega;\omega,\omega,0\rangle$, as function of the dielectric constant

The difference in the NLO responses of the two compounds studied is directly related to the transition energies toward the most absorbing excited state. In addition, the presence of two methoxy groups in the molecule (DTTP) which are groups with a high capacity to donate electrons, i.e.,ğ-donor character, since it has the oxygen with negative partial charge linked to the aromatic ring and therefore increases the electron density in phenolic hydroxyl, while the molecule (DMTT) presents two methyl groups which are weak electron donor groups. Thus, the DMTT compound becomes more symmetrical (see Figure 3) and therefore reduces its second order NLO response. Conversely, the use of two methoxy groups improves the push-pull character of DTTP and, in turn, its first hyperpolarizability. Also, the energy difference between the HOMO and LUMO orbitals for DTTP is smaller than for DMTT.

4. Conclusions

The static and dynamic first and second hyperpolarizability of two 1,2,3-triazole derivatives: 1-(34-dimethylphenyl)-4-(3-methoxyphenyl)-5-trifluoromethyl-1H-123-triazole (DMTT) and 3-[4-(3)4-dimethoxyphenyl)-5-(trifluoromethyl)-1H-123-triazol-1-yl] phenol (DTTP) as function of the dielectric constant of the solvent media were investigated at PCM/DFT/CAM-B3LYP/6-311+G(d) level of theory. The static values of the parallel first hyperpolarizability and the average second hyperpolarizability, $\beta_{\|z}(0;0,0)$ and $\langle\gamma(0;0,0,0)\rangle$, for DTTP are greater than for DMTT in all solvent media and increase with the dielectric constant increasing. The HRS first hyperpolarizability valuesin both cases (static and dynamic) for DTTP are greater than those for DMTT in all solvent media and present similarbehaviouras function of ϵ-value for both compounds. The values of the second hyperpolarizability, ($\langle\gamma(-2\omega;\omega,\omega,0\rangle$), obtained for both, DMTT and DTTP, in DMSO at electric field frequency of 0.0426 a.u. (1064 nm), are more than eight times greater than for P-nitroaniline (pNA), that is a compound commonly used as reference. The results of the present study on the nonlinear optical (NLO) properties of the molecular compounds, DMTT and DTTP, suggest that these compounds present favourable conditions for applications as nonlinear optical materials.

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Appendix: Supporting Information

Table S1. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in Gas Phase

	Coordinates		
	x	y	z
C4	1.2405	–0.3393	–0.3254
C5	0.0243	0.2079	0.0722
C6	–0.2978	1.4814	0.7870
C7	2.6173	0.1863	–0.3232
C8	3.6709	–0.7142	–0.0776
H8	3.4302	–1.7508	0.1189
C9	4.9931	–0.2628	–0.1009
C10	5.2710	1.0870	–0.3696
H10	6.3052	1.4151	–0.3807
C11	4.2250	1.9679	–0.6226
H11	4.4435	3.0084	–0.8436
C12	2.8976	1.5284	–0.6059
H12	2.0961	2.2235	–0.8293
C13	–2.3372	–0.7572	–0.0944
C14	–3.0909	0.2551	–0.6906
H14	–2.5893	1.0487	–1.2353
C15	–4.4860	0.2535	–0.5966
C16	–5.1290	–0.7986	0.0953
C17	–4.3490	–1.8117	0.6673
H17	–4.8405	–2.6239	1.1959
C18	–2.9569	–1.8032	0.5840
H18	–2.3608	–2.5902	1.0318
C19	–5.2845	1.3621	–1.2404
H19A	–4.6307	2.0803	–1.7416
H19B	–5.8779	1.9106	–0.4990
H19C	–5.9883	0.9715	–1.9851
C20	–6.6335	–0.8390	0.2153
H20A	–6.9591	–1.7098	0.7901
H20B	–7.1151	–0.8880	–0.7689
H20C	–7.0223	0.0572	0.7137
C21	5.8703	–2.4420	0.3859
H21A	5.2824	–2.5926	1.2998
H21B	6.8636	–2.8720	0.5192
H21C	5.3686	–2.9340	–0.4563
F1	0.7626	1.9356	1.4841
F2	–0.6647	2.4817	–0.0670
F3	–1.3166	1.3298	1.6654
N1	–0.9081	–0.7567	–0.2171
N2	–0.2949	–1.8425	–0.7366
N3	0.9811	–1.5985	–0.7961
O1	6.0805	–1.0578	0.1271

Table S2. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Argon*

	Coordinates		
	x	*y*	*z*
C4	1.2399	–0.3398	–0.3453
C5	0.0255	0.2012	0.0660
C6	–0.2939	1.4629	0.8026
C7	2.6168	0.1862	–0.3358
C8	3.6704	–0.7113	–0.0800
H8	3.4318	–1.7475	0.1213
C9	4.9920	–0.2571	–0.0964
C10	5.2684	1.0925	–0.3684
H10	6.3017	1.4238	–0.3745
C11	4.2222	1.9707	–0.6307
H11	4.4400	3.0109	–0.8536
C12	2.8955	1.5282	–0.6207
H12	2.0935	2.2207	–0.8509
C13	–2.3383	–0.7542	–0.1046
C14	–3.0938	0.2515	–0.7095
H14	–2.5948	1.0355	–1.2702
C15	–4.4883	0.2537	–0.6051
C16	–5.1277	–0.7873	0.1074
C17	–4.3453	–1.7935	0.6886
H17	–4.8341	–2.5966	1.2331
C18	–2.9537	–1.7891	0.5943
H18	–2.3561	–2.5701	1.0509
C19	–5.2901	1.3539	–1.2591
H19A	–4.6391	2.0626	–1.7770
H19B	–5.8758	1.9145	–0.5208
H19C	–6.0011	0.9528	–1.9911
C20	–6.6312	–0.8231	0.2392
H20A	–6.9540	–1.6839	0.8301
H20B	–7.1193	–0.8865	–0.7410
H20C	–7.0141	0.0821	0.7256
C21	5.8701	–2.4342	0.4050
H21A	5.2768	–2.5815	1.3157
H21B	6.8634	–2.8613	0.5465
H21C	5.3754	–2.9297	–0.4388
F1	0.7730	1.9113	1.4945
F2	–0.6745	2.4736	–0.0318
F3	–1.3018	1.2942	1.6906
N1	–0.9091	–0.7557	–0.2379
N2	–0.3005	–1.8314	–0.7802
N3	0.9769	–1.5888	–0.8397
O1	6.0793	–1.0491	0.1419

Table S3. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Heptane*

	Coordinates		
	x	y	z
C4	1.2394	–0.3388	–0.3613
C5	0.0267	0.1972	0.0608
C6	–0.2909	1.4495	0.8140
C7	2.6167	0.1868	–0.3456
C8	3.6695	–0.7093	–0.0817
H8	3.4316	–1.7449	0.1232
C9	4.9910	–0.2539	–0.0925
C10	5.2674	1.0954	–0.3671
H10	6.3002	1.4283	–0.3690
C11	4.2218	1.9722	–0.6369
H11	4.4400	3.0120	–0.8613
C12	2.8954	1.5285	–0.6324
H12	2.0936	2.2194	–0.8681
C13	–2.3389	–0.7511	–0.1128
C14	–3.0969	0.2496	–0.7230
H14	–2.6006	1.0272	–1.2949
C15	–4.4909	0.2537	–0.6102
C16	–5.1264	–0.7798	0.1169
C17	–4.3412	–1.7808	0.7037
H17	–4.8272	–2.5777	1.2596
C18	–2.9501	–1.7786	0.6006
H18	–2.3506	–2.5549	1.0627
C19	–5.2961	1.3475	–1.2705
H19A	–4.6477	2.0508	–1.7990
H19B	–5.8777	1.9151	–0.5343
H19C	–6.0111	0.9390	–1.9942
C20	–6.6290	–0.8132	0.2581
H20A	–6.9488	–1.6681	0.8591
H20B	–7.1225	–0.8852	–0.7186
H20C	–7.0078	0.0971	0.7379
C21	5.8681	–2.4298	0.4211
H21A	5.2703	–2.5739	1.3290
H21B	6.8610	–2.8552	0.5692
H21C	5.3786	–2.9279	–0.4240
F1	0.7813	1.8949	1.5001
F2	–0.6844	2.4672	–0.0050
F3	–1.2888	1.2665	1.7105
N1	–0.9098	–0.7534	–0.2547
N2	–0.3049	–1.8209	–0.8149
N3	0.9736	–1.5794	–0.8743
O1	6.0775	–1.0442	0.1542

Table S4. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Toluene*

	Coordinates		
	x	*y*	*z*
C4	1.2391	–0.3379	–0.3715
C5	0.0274	0.1948	0.0575
C6	–0.2888	1.4412	0.8211
C7	2.6167	0.1872	–0.3519
C8	3.6688	–0.7081	–0.0828
H8	3.4312	–1.7433	0.1246
C9	4.9903	–0.2521	–0.0901
C10	5.2669	1.0969	–0.3663
H10	6.2994	1.4307	–0.3656
C11	4.2218	1.9729	–0.6409
H11	4.4403	3.0124	–0.8663
C12	2.8956	1.5287	–0.6398
H12	2.0940	2.2187	–0.8790
C13	–2.3393	–0.7490	–0.1180
C14	–3.0991	0.2487	–0.7311
H14	–2.6047	1.0226	–1.3097
C15	–4.4928	0.2537	–0.6130
C16	–5.1256	–0.7754	0.1228
C17	–4.3384	–1.7731	0.7128
H17	–4.8224	–2.5664	1.2755
C18	–2.9476	–1.7720	0.6041
H18	–2.3467	–2.5454	1.0694
C19	–5.3002	1.3436	–1.2769
H19A	–4.6536	2.0440	–1.8112
H19B	–5.8798	1.9148	–0.5419
H19C	–6.0174	0.9306	–1.9959
C20	–6.6276	–0.8076	0.2700
H20A	–6.9453	–1.6593	0.8766
H20B	–7.1246	–0.8842	–0.7045
H20C	–7.0040	0.1055	0.7464
C21	5.8665	–2.4273	0.4315
H21A	5.2656	–2.5692	1.3376
H21B	6.8590	–2.8518	0.5840
H21C	5.3803	–2.9271	–0.4143
F1	0.7868	1.8847	1.5036
F2	–0.6900	2.4632	0.0119
F3	–1.2805	1.2494	1.7228
N1	–0.9103	–0.7515	–0.2654
N2	–0.3078	–1.8137	–0.8371
N3	0.9713	–1.5729	–0.8964
O1	6.0761	–1.0416	0.1620

Table S5. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Choroform*

	Coordinates		
	x	*y*	*z*
C4	1.2381	–0.3348	–0.3956
C5	0.0293	0.1897	0.0506
C6	–0.2831	1.4211	0.8399
C7	2.6166	0.1886	–0.3668
C8	3.6667	–0.7056	–0.0865
H8	3.4291	–1.7398	0.1264
C9	4.9883	–0.2487	–0.0855
C10	5.2660	1.0996	–0.3650
H10	6.2980	1.4352	–0.3582
C11	4.2225	1.9747	–0.6499
H11	4.4423	3.0135	–0.8772
C12	2.8964	1.5296	–0.6567
H12	2.0956	2.2181	–0.9031
C13	–2.3404	–0.7425	–0.1299
C14	–3.1051	0.2449	–0.7534
H14	–2.6159	1.0079	–1.3508
C15	–4.4979	0.2518	–0.6227
C16	–5.1236	–0.7643	0.1377
C17	–4.3308	–1.7513	0.7389
H17	–4.8094	–2.5337	1.3209
C18	–2.9409	–1.7525	0.6168
H18	–2.3359	–2.5165	1.0925
C19	–5.3117	1.3291	–1.2991
H19A	–4.6696	2.0219	–1.8485
H19B	–5.8884	1.9100	–0.5696
H19C	–6.0322	0.9023	–2.0065
C20	–6.6240	–0.7938	0.2995
H20A	–6.9359	–1.6365	0.9214
H20B	–7.1293	–0.8837	–0.6694
H20C	–6.9949	0.1267	0.7657
C21	5.8615	–2.4225	0.4550
H21A	5.2534	–2.5585	1.3567
H21B	6.8530	–2.8450	0.6181
H21C	5.3832	–2.9269	–0.3922
F1	0.8002	1.8585	1.5149
F2	–0.7014	2.4538	0.0550
F3	–1.2605	1.2076	1.7525
N1	–0.9117	–0.7456	–0.2904
N2	–0.3155	–1.7939	–0.8908
N3	0.9652	–1.5551	–0.9502
O1	6.0724	–1.0365	0.1785

Table S6. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Chlorobenzene*

	Coordinates		
	x	*y*	*z*
C4	1.2378	–0.3339	–0.4010
C5	0.0297	0.1887	0.0491
C6	–0.2817	1.4167	0.8442
C7	2.6166	0.1890	–0.3702
C8	3.6661	–0.7051	–0.0874
H8	3.4284	–1.7390	0.1268
C9	4.9878	–0.2481	–0.0846
C10	5.2659	1.1000	–0.3650
H10	6.2978	1.4358	–0.3569
C11	4.2228	1.9749	–0.6523
H11	4.4431	3.0135	–0.8800
C12	2.8967	1.5298	–0.6607
H12	2.0962	2.2181	–0.9087
C13	–2.3407	–0.7409	–0.1325
C14	–3.1065	0.2444	–0.7580
H14	–2.6184	1.0052	–1.3590
C15	–4.4991	0.2515	–0.6246
C16	–5.1231	–0.7620	0.1408
C17	–4.3290	–1.7468	0.7440
H17	–4.8063	–2.5271	1.3300
C18	–2.9393	–1.7483	0.6191
H18	–2.3334	–2.5103	1.0968
C19	–5.3144	1.3263	–1.3032
H19A	–4.6734	2.0177	–1.8555
H19B	–5.8906	1.9089	–0.5747
H19C	–6.0356	0.8967	–2.0083
C20	–6.6232	–0.7912	0.3057
H20A	–6.9337	–1.6320	0.9306
H20B	–7.1303	–0.8838	–0.6621
H20C	–6.9931	0.1307	0.7698
C21	5.8600	–2.4215	0.4606
H21A	5.2503	–2.5559	1.3613
H21B	6.8512	–2.8436	0.6264
H21C	5.3835	–2.9272	–0.3867
F1	0.8034	1.8527	1.5174
F2	–0.7039	2.4517	0.0649
F3	–1.2557	1.1982	1.7593
N1	–0.9121	–0.7440	–0.2959
N2	–0.3173	–1.7892	–0.9027
N3	0.9637	–1.5508	–0.9622
O1	6.0714	–1.0356	0.1821

Table S7. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Tetrahydrofuran*

	Coordinates		
	x	*y*	*z*
C4	1.2375	–0.3326	–0.4078
C5	0.0302	0.1877	0.0470
C6	–0.2799	1.4112	0.8493
C7	2.6166	0.1896	–0.3745
C8	3.6653	–0.7045	–0.0885
H8	3.4272	–1.7379	0.1275
C9	4.9871	–0.2475	–0.0834
C10	5.2658	1.1003	–0.3650
H10	6.2977	1.4363	–0.3553
C11	4.2235	1.9751	–0.6554
H11	4.4443	3.0134	–0.8839
C12	2.8973	1.5301	–0.6658
H12	2.0971	2.2181	–0.9159
C13	–2.3409	–0.7389	–0.1359
C14	–3.1082	0.2443	–0.7628
H14	–2.6216	1.0031	–1.3677
C15	–4.5006	0.2515	–0.6261
C16	–5.1225	–0.7595	0.1443
C17	–4.3268	–1.7420	0.7493
H17	–4.8025	–2.5201	1.3394
C18	–2.9373	–1.7438	0.6210
H18	–2.3301	–2.5038	1.1004
C19	–5.3177	1.3237	–1.3066
H19A	–4.6780	2.0139	–1.8619
H19B	–5.8933	1.9078	–0.5788
H19C	–6.0397	0.8914	–2.0091
C20	–6.6221	–0.7884	0.3129
H20A	–6.9310	–1.6275	0.9410
H20B	–7.1314	–0.8837	–0.6534
H20C	–6.9909	0.1349	0.7751
C21	5.8579	–2.4204	0.4680
H21A	5.2460	–2.5525	1.3675
H21B	6.8487	–2.8420	0.6372
H21C	5.3836	–2.9278	–0.3794
F1	0.8074	1.8458	1.5201
F2	–0.7074	2.4491	0.0771
F3	–1.2496	1.1865	1.7677
N1	–0.9125	–0.7419	–0.3028
N2	–0.3194	–1.7832	–0.9174
N3	0.9619	–1.5453	–0.9771
O1	6.0701	–1.0347	0.1868

Table S8. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Dichloromethane*

	Coordinates		
	x	*y*	*z*
C4	1.2373	–0.3317	–0.4120
C5	0.0305	0.1871	0.0457
C6	–0.2789	1.4080	0.8524
C7	2.6166	0.1900	–0.3772
C8	3.6647	–0.7041	–0.0890
H8	3.4263	–1.7372	0.1280
C9	4.9867	–0.2472	–0.0826
C10	5.2659	1.1003	–0.3650
H10	6.2977	1.4364	–0.3543
C11	4.2240	1.9752	–0.6574
H11	4.4453	3.0132	–0.8863
C12	2.8977	1.5303	–0.6691
H12	2.0979	2.2181	–0.9205
C13	–2.3410	–0.7377	–0.1380
C14	–3.1093	0.2444	–0.7655
H14	–2.6236	1.0023	–1.3723
C15	–4.5015	0.2517	–0.6268
C16	–5.1221	–0.7581	0.1464
C17	–4.3253	–1.7395	0.7520
H17	–4.8001	–2.5166	1.3443
C18	–2.9360	–1.7414	0.6215
H18	–2.3280	–2.5003	1.1017
C19	–5.3198	1.3226	–1.3078
H19A	–4.6810	2.0122	–1.8648
H19B	–5.8949	1.9073	–0.5802
H19C	–6.0423	0.8889	–2.0090
C20	–6.6214	–0.7870	0.3172
H20A	–6.9292	–1.6252	0.9470
H20B	–7.1320	–0.8837	–0.6483
H20C	–6.9895	0.1370	0.7785
C21	5.8565	–2.4197	0.4728
H21A	5.2431	–2.5504	1.3715
H21B	6.8469	–2.8411	0.6441
H21C	5.3835	–2.9282	–0.3747
F1	0.8098	1.8418	1.5215
F2	–0.7097	2.4474	0.0845
F3	–1.2458	1.1793	1.7728
N1	–0.9127	–0.7406	–0.3071
N2	–0.3207	–1.7794	–0.9265
N3	0.9609	–1.5419	–0.9862
O1	6.0691	–1.0343	0.1899

Table S9. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Dichloroethane*

	Coordinates		
	x	*y*	*z*
C4	1.2372	–0.3311	–0.4146
C5	0.0307	0.1868	0.0448
C6	–0.2783	1.4060	0.8542
C7	2.6166	0.1902	–0.3789
C8	3.6644	–0.7038	–0.0894
H8	3.4258	–1.7367	0.1283
C9	4.9864	–0.2470	–0.0821
C10	5.2659	1.1003	–0.3650
H10	6.2978	1.4365	–0.3537
C11	4.2244	1.9752	–0.6586
H11	4.4460	3.0131	–0.8878
C12	2.8980	1.5305	–0.6711
H12	2.0984	2.2182	–0.9234
C13	–2.3411	–0.7370	–0.1394
C14	–3.1099	0.2446	–0.7670
H14	–2.6248	1.0019	–1.3749
C15	–4.5021	0.2519	–0.6270
C16	–5.1218	–0.7574	0.1476
C17	–4.3244	–1.7381	0.7535
H17	–4.7985	–2.5146	1.3470
C18	–2.9352	–1.7401	0.6217
H18	–2.3268	–2.4983	1.1022
C19	–5.3211	1.3220	–1.3083
H19A	–4.6828	2.0114	–1.8662
H19B	–5.8959	1.9071	–0.5807
H19C	–6.0440	0.8876	–2.0086
C20	–6.6210	–0.7862	0.3198
H20A	–6.9282	–1.6239	0.9505
H20B	–7.1324	–0.8836	–0.6452
H20C	–6.9887	0.1382	0.7807
C21	5.8555	–2.4194	0.4759
H21A	5.2412	–2.5491	1.3740
H21B	6.8458	–2.8406	0.6485
H21C	5.3834	–2.9286	–0.3717
F1	0.8113	1.8394	1.5222
F2	–0.7112	2.4464	0.0890
F3	–1.2434	1.1749	1.7759
N1	–0.9129	–0.7398	–0.3098
N2	–0.3215	–1.7771	–0.9321
N3	0.9602	–1.5397	–0.9917
O1	6.0685	–1.0341	0.1918

Table S10. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *2-Methyl-2-Propanol*

	Coordinates		
	x	*y*	*z*
C4	1.2370	–0.3302	–0.4185
C5	0.0310	0.1864	0.0435
C6	–0.2774	1.4031	0.8569
C7	2.6166	0.1907	–0.3813
C8	3.6638	–0.7034	–0.0899
H8	3.4248	–1.7361	0.1288
C9	4.9860	–0.2468	–0.0813
C10	5.2660	1.1003	–0.3649
H10	6.2979	1.4364	–0.3526
C11	4.2250	1.9752	–0.6604
H11	4.4471	3.0129	–0.8901
C12	2.8986	1.5307	–0.6741
H12	2.0993	2.2184	–0.9277
C13	–2.3412	–0.7359	–0.1414
C14	–3.1109	0.2450	–0.7691
H14	–2.6266	1.0017	–1.3784
C15	–4.5029	0.2522	–0.6272
C16	–5.1214	–0.7563	0.1494
C17	–4.3231	–1.7362	0.7554
H17	–4.7963	–2.5120	1.3506
C18	–2.9340	–1.7382	0.6217
H18	–2.3248	–2.4957	1.1026
C19	–5.3230	1.3214	–1.3086
H19A	–4.6855	2.0106	–1.8677
H19B	–5.8973	1.9068	–0.5810
H19C	–6.0464	0.8860	–2.0077
C20	–6.6203	–0.7852	0.3236
H20A	–6.9265	–1.6223	0.9556
H20B	–7.1329	–0.8835	–0.6406
H20C	–6.9875	0.1397	0.7840
C21	5.8540	–2.4189	0.4804
H21A	5.2383	–2.5472	1.3777
H21B	6.8439	–2.8400	0.6551
H21C	5.3831	–2.9291	–0.3672
F1	0.8134	1.8359	1.5233
F2	–0.7135	2.4449	0.0956
F3	–1.2399	1.1684	1.7804
N1	–0.9131	–0.7385	–0.3137
N2	–0.3226	–1.7736	–0.9403
N3	0.9593	–1.5365	–1.0000
O1	6.0676	–1.0338	0.1947

Table S11. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *1-Butanol*

	Coordinates		
	x	*y*	*z*
C4	1.2368	–0.3290	–0.4235
C5	0.0314	0.1859	0.0417
C6	–0.2762	1.3994	0.8602
C7	2.6167	0.1913	–0.3846
C8	3.6631	–0.7029	–0.0905
H8	3.4236	–1.7352	0.1295
C9	4.9854	–0.2466	–0.0801
C10	5.2662	1.1001	–0.3648
H10	6.2981	1.4362	–0.3512
C11	4.2259	1.9751	–0.6627
H11	4.4488	3.0125	–0.8931
C12	2.8994	1.5310	–0.6780
H12	2.1006	2.2186	–0.9333
C13	–2.3413	–0.7346	–0.1441
C14	–3.1121	0.2457	–0.7715
H14	–2.6289	1.0018	–1.3823
C15	–4.5039	0.2527	–0.6272
C16	–5.1209	–0.7551	0.1517
C17	–4.3213	–1.7342	0.7575
H17	–4.7933	–2.5093	1.3545
C18	–2.9325	–1.7361	0.6213
H18	–2.3223	–2.4927	1.1024
C19	–5.3254	1.3210	–1.3083
H19A	–4.6890	2.0100	–1.8688
H19B	–5.8992	1.9065	–0.5803
H19C	–6.0496	0.8846	–2.0061
C20	–6.6195	–0.7841	0.3284
H20A	–6.9244	–1.6206	0.9618
H20B	–7.1336	–0.8834	–0.6349
H20C	–6.9859	0.1412	0.7885
C21	5.8518	–2.4184	0.4865
H21A	5.2344	–2.5448	1.3827
H21B	6.8414	–2.8392	0.6640
H21C	5.3827	–2.9299	–0.3612
F1	0.8162	1.8316	1.5245
F2	–0.7165	2.4430	0.1040
F3	–1.2353	1.1600	1.7861
N1	–0.9133	–0.7368	–0.3189
N2	–0.3241	–1.7690	–0.9509
N3	0.9580	–1.5322	–1.0107
O1	6.0663	–1.0336	0.1986

Table S12. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Acetone*

	Coordinates		
	x	*y*	*z*
C4	1.2367	–0.3285	–0.4256
C5	0.0315	0.1857	0.0410
C6	–0.2757	1.3980	0.8615
C7	2.6167	0.1915	–0.3859
C8	3.6627	–0.7027	–0.0907
H8	3.4230	–1.7348	0.1299
C9	4.9851	–0.2466	–0.0797
C10	5.2663	1.1000	–0.3648
H10	6.2982	1.4360	–0.3507
C11	4.2263	1.9751	–0.6638
H11	4.4494	3.0123	–0.8944
C12	2.8997	1.5311	–0.6797
H12	2.1011	2.2187	–0.9357
C13	–2.3413	–0.7340	–0.1452
C14	–3.1126	0.2461	–0.7723
H14	–2.6298	1.0021	–1.3836
C15	–4.5043	0.2530	–0.6271
C16	–5.1207	–0.7547	0.1525
C17	–4.3206	–1.7336	0.7581
H17	–4.7921	–2.5085	1.3556
C18	–2.9318	–1.7354	0.6210
H18	–2.3212	–2.4917	1.1019
C19	–5.3264	1.3211	–1.3078
H19A	–4.6904	2.0101	–1.8688
H19B	–5.8998	1.9065	–0.5795
H19C	–6.0510	0.8844	–2.0050
C20	–6.6191	–0.7838	0.3303
H20A	–6.9235	–1.6201	0.9641
H20B	–7.1338	–0.8835	–0.6327
H20C	–6.9854	0.1417	0.7901
C21	5.8509	–2.4182	0.4890
H21A	5.2326	–2.5438	1.3848
H21B	6.8402	–2.8390	0.6677
H21C	5.3825	–2.9303	–0.3587
F1	0.8174	1.8298	1.5249
F2	–0.7177	2.4422	0.1074
F3	–1.2334	1.1567	1.7885
N1	–0.9134	–0.7361	–0.3210
N2	–0.3246	–1.7671	–0.9553
N3	0.9575	–1.5304	–1.0151
O1	6.0658	–1.0335	0.2002

Table S13. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Ethanol*

	Coordinates		
	x	y	z
C4	1.2366	–0.3279	–0.4278
C5	0.0317	0.1855	0.0402
C6	–0.2752	1.3964	0.8629
C7	2.6167	0.1918	–0.3873
C8	3.6624	–0.7025	–0.0910
H8	3.4224	–1.7345	0.1301
C9	4.9849	–0.2465	–0.0792
C10	5.2665	1.0999	–0.3647
H10	6.2984	1.4358	–0.3501
C11	4.2268	1.9750	–0.6648
H11	4.4503	3.0121	–0.8956
C12	2.9001	1.5313	–0.6814
H12	2.1018	2.2189	–0.9382
C13	–2.3413	–0.7334	–0.1464
C14	–3.1131	0.2465	–0.7732
H14	–2.6309	1.0023	–1.3851
C15	–4.5048	0.2533	–0.6270
C16	–5.1204	–0.7542	0.1534
C17	–4.3198	–1.7328	0.7588
H17	–4.7908	–2.5075	1.3571
C18	–2.9311	–1.7345	0.6207
H18	–2.3201	–2.4905	1.1016
C19	–5.3275	1.3209	–1.3075
H19A	–4.6920	2.0100	–1.8690
H19B	–5.9007	1.9064	–0.5790
H19C	–6.0524	0.8839	–2.0041
C20	–6.6188	–0.7834	0.3323
H20A	–6.9226	–1.6196	0.9667
H20B	–7.1341	–0.8834	–0.6302
H20C	–6.9847	0.1422	0.7921
C21	5.8499	–2.4180	0.4916
H21A	5.2308	–2.5428	1.3869
H21B	6.8390	–2.8388	0.6715
H21C	5.3822	–2.9307	–0.3562
F1	0.8186	1.8280	1.5254
F2	–0.7189	2.4414	0.1110
F3	–1.2315	1.1531	1.7909
N1	–0.9135	–0.7353	–0.3233
N2	–0.3253	–1.7651	–0.9598
N3	0.9570	–1.5285	–1.0197
O1	6.0652	–1.0335	0.2019

Table S14. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Methanol*

	Coordinates		
	x	*y*	*z*
C4	1.2365	–0.3272	–0.4302
C5	0.0318	0.1854	0.0393
C6	–0.2746	1.3947	0.8645
C7	2.6168	0.1921	–0.3888
C8	3.6620	–0.7023	–0.0913
H8	3.4217	–1.7340	0.1305
C9	4.9846	–0.2465	–0.0786
C10	5.2666	1.0998	–0.3646
H10	6.2986	1.4356	–0.3494
C11	4.2273	1.9749	–0.6659
H11	4.4512	3.0119	–0.8971
C12	2.9005	1.5314	–0.6833
H12	2.1025	2.2190	–0.9410
C13	–2.3414	–0.7327	–0.1477
C14	–3.1137	0.2469	–0.7742
H14	–2.6320	1.0027	–1.3866
C15	–4.5053	0.2536	–0.6268
C16	–5.1202	–0.7538	0.1544
C17	–4.3189	–1.7321	0.7595
H17	–4.7893	–2.5066	1.3585
C18	–2.9304	–1.7337	0.6202
H18	–2.3188	–2.4894	1.1010
C19	–5.3287	1.3210	–1.3069
H19A	–4.6937	2.0101	–1.8689
H19B	–5.9015	1.9064	–0.5781
H19C	–6.0540	0.8837	–2.0029
C20	–6.6183	–0.7831	0.3346
H20A	–6.9215	–1.6190	0.9694
H20B	–7.1344	–0.8834	–0.6276
H20C	–6.9840	0.1427	0.7943
C21	5.8488	–2.4178	0.4946
H21A	5.2287	–2.5417	1.3894
H21B	6.8376	–2.8385	0.6759
H21C	5.3819	–2.9312	–0.3532
F1	0.8199	1.8260	1.5259
F2	–0.7204	2.4404	0.1151
F3	–1.2292	1.1491	1.7936
N1	–0.9137	–0.7344	–0.3258
N2	–0.3259	–1.7628	–0.9650
N3	0.9564	–1.5264	–1.0248
O1	6.0645	–1.0335	0.2039

Table S15. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Acetonitrile*

	Coordinates		
	x	*y*	*z*
C4	1.2364	–0.3270	–0.4309
C5	0.0319	0.1853	0.0391
C6	–0.2745	1.3942	0.8649
C7	2.6168	0.1922	–0.3893
C8	3.6619	–0.7022	–0.0914
H8	3.4215	–1.7339	0.1306
C9	4.9845	–0.2465	–0.0784
C10	5.2666	1.0997	–0.3646
H10	6.2986	1.4355	–0.3492
C11	4.2275	1.9749	–0.6663
H11	4.4514	3.0118	–0.8975
C12	2.9007	1.5315	–0.6839
H12	2.1027	2.2190	–0.9418
C13	–2.3414	–0.7325	–0.1481
C14	–3.1139	0.2471	–0.7744
H14	–2.6323	1.0028	–1.3870
C15	–4.5054	0.2537	–0.6267
C16	–5.1201	–0.7536	0.1547
C17	–4.3187	–1.7319	0.7597
H17	–4.7889	–2.5063	1.3588
C18	–2.9301	–1.7335	0.6200
H18	–2.3185	–2.4891	1.1008
C19	–5.3290	1.3211	–1.3067
H19A	–4.6942	2.0102	–1.8688
H19B	–5.9017	1.9064	–0.5778
H19C	–6.0544	0.8837	–2.0026
C20	–6.6182	–0.7830	0.3352
H20A	–6.9213	–1.6189	0.9701
H20B	–7.1345	–0.8833	–0.6268
H20C	–6.9837	0.1428	0.7949
C21	5.8484	–2.4177	0.4955
H21A	5.2281	–2.5414	1.3901
H21B	6.8372	–2.8384	0.6772
H21C	5.3818	–2.9313	–0.3523
F1	0.8203	1.8254	1.5261
F2	–0.7208	2.4402	0.1162
F3	–1.2286	1.1480	1.7944
N1	–0.9137	–0.7341	–0.3265
N2	–0.3261	–1.7622	–0.9664
N3	0.9563	–1.5258	–1.0263
O1	6.0643	–1.0335	0.2044

Table S16. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *dmso*

	Coordinates		
	x	*y*	*z*
C4	1.2364	–0.3267	–0.4325
C5	0.0320	0.1851	0.0386
C6	–0.2741	1.3930	0.8660
C7	2.6167	0.1924	–0.3903
C8	3.6616	–0.7020	–0.0914
H8	3.4211	–1.7335	0.1311
C9	4.9843	–0.2463	–0.0780
C10	5.2666	1.0997	–0.3648
H10	6.2986	1.4355	–0.3490
C11	4.2277	1.9748	–0.6674
H11	4.4519	3.0116	–0.8991
C12	2.9009	1.5315	–0.6854
H12	2.1030	2.2190	–0.9440
C13	–2.3414	–0.7321	–0.1489
C14	–3.1142	0.2475	–0.7748
H14	–2.6328	1.0033	–1.3876
C15	–4.5056	0.2542	–0.6265
C16	–5.1200	–0.7533	0.1551
C17	–4.3183	–1.7316	0.7597
H17	–4.7882	–2.5060	1.3591
C18	–2.9298	–1.7332	0.6194
H18	–2.3179	–2.4888	1.1000
C19	–5.3296	1.3216	–1.3059
H19A	–4.6950	2.0106	–1.8685
H19B	–5.9017	1.9070	–0.5766
H19C	–6.0555	0.8843	–2.0013
C20	–6.6180	–0.7827	0.3362
H20A	–6.9207	–1.6183	0.9718
H20B	–7.1346	–0.8837	–0.6256
H20C	–6.9835	0.1433	0.7955
C21	5.8478	–2.4174	0.4975
H21A	5.2268	–2.5404	1.3916
H21B	6.8364	–2.8380	0.6802
H21C	5.3818	–2.9315	–0.3504
F1	0.8213	1.8241	1.5263
F2	–0.7219	2.4394	0.1190
F3	–1.2269	1.1452	1.7964
N1	–0.9138	–0.7337	–0.3280
N2	–0.3266	–1.7608	–0.9696
N3	0.9559	–1.5245	–1.0295
O1	6.0639	–1.0333	0.2056

Table S17. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Formicacid*

	Coordinates		
	x	y	z
C4	1.2363	–0.3266	–0.4330
C5	0.0320	0.1850	0.0384
C6	–0.2740	1.3926	0.8663
C7	2.6168	0.1924	–0.3906
C8	3.6616	–0.7019	–0.0914
H8	3.4209	–1.7334	0.1312
C9	4.9842	–0.2463	–0.0778
C10	5.2667	1.0997	–0.3647
H10	6.2986	1.4355	–0.3489
C11	4.2278	1.9748	–0.6676
H11	4.4520	3.0116	–0.8994
C12	2.9009	1.5315	–0.6858
H12	2.1031	2.2190	–0.9446
C13	–2.3414	–0.7320	–0.1492
C14	–3.1143	0.2477	–0.7750
H14	–2.6331	1.0034	–1.3878
C15	–4.5057	0.2543	–0.6264
C16	–5.1199	–0.7532	0.1553
C17	–4.3181	–1.7314	0.7598
H17	–4.7879	–2.5059	1.3593
C18	–2.9296	–1.7331	0.6193
H18	–2.3176	–2.4886	1.0998
C19	–5.3298	1.3216	–1.3058
H19A	–4.6953	2.0107	–1.8684
H19B	–5.9019	1.9070	–0.5764
H19C	–6.0558	0.8843	–2.0010
C20	–6.6179	–0.7826	0.3367
H20A	–6.9205	–1.6182	0.9723
H20B	–7.1346	–0.8837	–0.6251
H20C	–6.9833	0.1434	0.7960
C21	5.8475	–2.4174	0.4981
H21A	5.2263	–2.5402	1.3921
H21B	6.8361	–2.8379	0.6811
H21C	5.3817	–2.9316	–0.3498
F1	0.8215	1.8236	1.5264
F2	–0.7222	2.4392	0.1198
F3	–1.2265	1.1444	1.7970
N1	–0.9138	–0.7335	–0.3285
N2	–0.3267	–1.7604	–0.9706
N3	0.9558	–1.5241	–1.0305
O1	6.0638	–1.0333	0.2060

Table S18. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Water*

	Coordinates		
	x	*y*	*z*
C4	1.2362	–0.3261	–0.4349
C5	0.0322	0.1849	0.0377
C6	–0.2735	1.3913	0.8676
C7	2.6168	0.1927	–0.3918
C8	3.6612	–0.7018	–0.0916
H8	3.4203	–1.7331	0.1315
C9	4.9840	–0.2463	–0.0774
C10	5.2668	1.0996	–0.3647
H10	6.2988	1.4353	–0.3484
C11	4.2282	1.9748	–0.6686
H11	4.4527	3.0114	–0.9007
C12	2.9013	1.5316	–0.6874
H12	2.1037	2.2191	–0.9469
C13	–2.3415	–0.7315	–0.1502
C14	–3.1148	0.2481	–0.7756
H14	–2.6339	1.0039	–1.3888
C15	–4.5061	0.2546	–0.6261
C16	–5.1197	–0.7528	0.1561
C17	–4.3175	–1.7310	0.7601
H17	–4.7869	–2.5054	1.3600
C18	–2.9291	–1.7325	0.6187
H18	–2.3167	–2.4879	1.0990
C19	–5.3307	1.3219	–1.3050
H19A	–4.6967	2.0110	–1.8680
H19B	–5.9025	1.9071	–0.5753
H19C	–6.0570	0.8844	–1.9998
C20	–6.6176	–0.7824	0.3383
H20A	–6.9197	–1.6180	0.9742
H20B	–7.1348	–0.8835	–0.6231
H20C	–6.9828	0.1437	0.7977
C21	5.8466	–2.4172	0.5005
H21A	5.2247	–2.5392	1.3941
H21B	6.8350	–2.8376	0.6846
H21C	5.3815	–2.9320	–0.3474
F1	0.8226	1.8220	1.5269
F2	–0.7232	2.4385	0.1230
F3	–1.2247	1.1413	1.7990
N1	–0.9139	–0.7328	–0.3305
N2	–0.3273	–1.7586	–0.9746
N3	0.9553	–1.5224	–1.0345
O1	6.0632	–1.0333	0.2076

Table S19. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *Formamide*

	Coordinates		
	x	y	z
C4	1.2362	–0.3254	–0.4365
C5	0.0323	0.1851	0.0371
C6	–0.2732	1.3905	0.8684
C7	2.6169	0.1930	–0.3929
C8	3.6609	–0.7017	–0.0920
H8	3.4197	–1.7329	0.1312
C9	4.9838	–0.2465	–0.0770
C10	5.2671	1.0993	–0.3642
H10	6.2991	1.4348	–0.3472
C11	4.2289	1.9747	–0.6687
H11	4.4538	3.0113	–0.9005
C12	2.9019	1.5319	–0.6882
H12	2.1046	2.2196	–0.9481
C13	–2.3415	–0.7309	–0.1510
C14	–3.1153	0.2480	–0.7768
H14	–2.6350	1.0034	–1.3908
C15	–4.5066	0.2543	–0.6265
C16	–5.1195	–0.7526	0.1571
C17	–4.3166	–1.7300	0.7615
H17	–4.7854	–2.5040	1.3625
C18	–2.9283	–1.7313	0.6193
H18	–2.3155	–2.4861	1.1000
C19	–5.3319	1.3207	–1.3058
H19A	–4.6984	2.0098	–1.8694
H19B	–5.9040	1.9060	–0.5764
H19C	–6.0581	0.8823	–2.0002
C20	–6.6172	–0.7823	0.3404
H20A	–6.9188	–1.6178	0.9766
H20B	–7.1352	–0.8835	–0.6206
H20C	–6.9821	0.1439	0.8000
C21	5.8456	–2.4176	0.5018
H21A	5.2231	–2.5393	1.3951
H21B	6.8339	–2.8382	0.6866
H21C	5.3810	–2.9323	–0.3463
F1	0.8233	1.8210	1.5272
F2	–0.7240	2.4382	0.1252
F3	–1.2235	1.1392	1.8004
N1	–0.9140	–0.7321	–0.3321
N2	–0.3276	–1.7570	–0.9778
N3	0.9550	–1.5208	–1.0378
O1	6.0627	–1.0337	0.2088

Table S20. DFT-B3LYP/6-311+G(d) of the optimized DMTT molecule in *n-Methylformamide-Mixture*

	Coordinates		
	x	*y*	*z*
C4	1.2361	–0.3249	–0.4381
C5	0.0324	0.1850	0.0366
C6	–0.2727	1.3894	0.8694
C7	2.6169	0.1933	–0.3941
C8	3.6606	–0.7015	–0.0923
H8	3.4191	–1.7327	0.1311
C9	4.9835	–0.2465	–0.0766
C10	5.2672	1.0992	–0.3639
H10	6.2992	1.4346	–0.3464
C11	4.2293	1.9747	–0.6692
H11	4.4545	3.0112	–0.9011
C12	2.9022	1.5321	–0.6895
H12	2.1051	2.2198	–0.9499
C13	–2.3415	–0.7304	–0.1518
C14	–3.1158	0.2480	–0.7779
H14	–2.6359	1.0030	–1.3927
C15	–4.5070	0.2542	–0.6268
C16	–5.1193	–0.7521	0.1580
C17	–4.3160	–1.7290	0.7627
H17	–4.7843	–2.5025	1.3645
C18	–2.9277	–1.7302	0.6197
H18	–2.3145	–2.4845	1.1007
C19	–5.3329	1.3199	–1.3065
H19A	–4.6998	2.0087	–1.8711
H19B	–5.9045	1.9057	–0.5772
H19C	–6.0595	0.8809	–2.0001
C20	–6.6169	–0.7819	0.3422
H20A	–6.9179	–1.6168	0.9794
H20B	–7.1354	–0.8842	–0.6185
H20C	–6.9817	0.1447	0.8010
C21	5.8449	–2.4176	0.5033
H21A	5.2218	–2.5391	1.3961
H21B	6.8330	–2.8382	0.6888
H21C	5.3808	–2.9325	–0.3450
F1	0.8242	1.8196	1.5277
F2	–0.7246	2.4378	0.1279
F3	–1.2222	1.1368	1.8021
N1	–0.9141	–0.7315	–0.3336
N2	–0.3281	–1.7555	–0.9811
N3	0.9545	–1.5194	–1.0411
O1	6.0622	–1.0338	0.2101

Table S21. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Gas Phase

	Coordinates		
	x	y	z
C20	6.4573	–1.7194	–0.2711
H20A	7.5329	–1.5767	–0.1618
H20B	6.1061	–2.4374	0.4808
H20C	6.2409	–2.1052	–1.2753
C19	4.4671	3.2880	0.5019
H19A	5.3635	3.8872	0.6656
H19B	3.9336	3.6605	–0.3813
H19C	3.8139	3.3610	1.3806
F1	–1.1078	–2.6872	–0.1766
F3	–2.0702	–1.6612	1.4901
F2	0.0890	–1.9055	1.4653
N1	–1.8883	0.4745	–0.3638
N3	–0.1316	1.6239	–0.8164
O3	–6.3743	1.9212	0.7572
H3	–5.8922	2.6821	1.1071
O2	5.8774	–0.4361	–0.0729
N2	–1.4304	1.6549	–0.8364
O1	4.9269	1.9560	0.3068
C9	4.0038	0.9854	0.0607
C5	–0.8284	–0.3280	–0.0163
C11	3.6454	–1.3686	–0.4158
H11	4.0261	–2.3670	–0.5935
C15	–5.5066	1.0167	0.2119
C10	4.5248	–0.3196	–0.1484
C7	1.7429	0.1264	–0.2513
C14	–4.1224	1.2052	0.2284
H14	–3.6777	2.0881	0.6766
C12	2.2642	–1.1488	–0.4710
H12	1.6108	–1.9817	–0.7049
C8	2.6303	1.1934	0.0057
H8	2.2172	2.1828	0.1527
C18	–3.8293	–0.9061	–0.9534
H18	–3.1788	–1.6354	–1.4216
C16	–6.0575	–0.1326	–0.3679
H16	–7.1346	–0.2599	–0.3629
C4	0.3043	0.4165	–0.3349
C6	–0.9797	–1.6379	0.6880
C13	–3.3014	0.2367	–0.3536
C17	–5.2159	–1.0818	–0.9433
H17	–5.6441	–1.9674	–1.4020

Table S22. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Argon

	Coordinates		
	x	*y*	*z*
C20	6.4531	–1.7299	–0.2686
H20A	7.5283	–1.5902	–0.1534
H20B	6.0960	–2.4494	0.4785
H20C	6.2400	–2.1092	–1.2755
C19	4.4679	3.2818	0.5217
H19A	5.3643	3.8779	0.6955
H19B	3.9412	3.6610	–0.3623
H19C	3.8097	3.3484	1.3969
F1	–1.1107	–2.6804	–0.1437
F3	–2.0664	–1.6269	1.5092
F2	0.0929	–1.8734	1.4810
N1	–1.8883	0.4755	–0.3843
N3	–0.1322	1.6162	–0.8602
O3	–6.3707	1.9016	0.7817
H3	–5.8899	2.6640	1.1314
O2	5.8747	–0.4444	–0.0667
N2	–1.4321	1.6457	–0.8799
O1	4.9269	1.9489	0.3194
C9	4.0033	0.9811	0.0632
C5	–0.8282	–0.3194	–0.0229
C11	3.6427	–1.3708	–0.4245
H11	4.0222	–2.3692	–0.6039
C15	–5.5043	1.0040	0.2237
C10	4.5227	–0.3243	–0.1486
C7	1.7426	0.1283	–0.2650
C14	–4.1202	1.1966	0.2320
H14	–3.6759	2.0761	0.6869
C12	2.2622	–1.1475	–0.4860
H12	1.6079	–1.9780	–0.7268
C8	2.6304	1.1925	0.0013
H8	2.2198	2.1823	0.1521
C18	–3.8297	–0.9052	–0.9693
H18	–3.1800	–1.6280	–1.4486
C16	–6.0555	–0.1428	–0.3612
H16	–7.1321	–0.2742	–0.3502
C4	0.3043	0.4191	–0.3556
C6	–0.9786	–1.6176	0.7028
C13	–3.3019	0.2351	–0.3645
C17	–5.2156	–1.0854	–0.9503
H17	–5.6449	–1.9685	–1.4128

Table S23. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Heptane

	Coordinates		
	x	*y*	*z*
C20	6.4515	–1.7347	–0.2656
H20A	7.5262	–1.5962	–0.1457
H20B	6.0906	–2.4561	0.4773
H20C	6.2415	–2.1088	–1.2748
C19	4.4646	3.2779	0.5388
H19A	5.3602	3.8725	0.7212
H19B	3.9431	3.6624	–0.3457
H19C	3.8020	3.3382	1.4108
F1	–1.1113	–2.6768	–0.1188
F3	–2.0628	–1.6023	1.5226
F2	0.0965	–1.8492	1.4923
N1	–1.8885	0.4736	–0.4015
N3	–0.1331	1.6074	–0.8968
O3	–6.3649	1.8917	0.7993
H3	–5.8835	2.6544	1.1485
O2	5.8729	–0.4483	–0.0604
N2	–1.4339	1.6355	–0.9158
O1	4.9247	1.9450	0.3301
C9	4.0019	0.9786	0.0654
C5	–0.8279	–0.3147	–0.0291
C11	3.6419	–1.3718	–0.4315
H11	4.0216	–2.3699	–0.6118
C15	–5.5012	0.9971	0.2327
C10	4.5213	–0.3266	–0.1483
C7	1.7424	0.1286	–0.2770
C14	–4.1171	1.1914	0.2325
H14	–3.6716	2.0692	0.6892
C12	2.2619	–1.1472	–0.4988
H12	1.6079	–1.9764	–0.7451
C8	2.6293	1.1914	–0.0028
H8	2.2195	2.1811	0.1510
C18	–3.8321	–0.9069	–0.9776
H18	–3.1845	–1.6271	–1.4636
C16	–6.0546	–0.1487	–0.3525
H16	–7.1310	–0.2820	–0.3354
C4	0.3041	0.4189	–0.3735
C6	–0.9771	–1.6034	0.7134
C13	–3.3024	0.2325	–0.3729
C17	–5.2178	–1.0888	–0.9501
H17	–5.6492	–1.9708	–1.4126

Table S24. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Toluene

	Coordinates		
	x	*y*	*z*
C20	6.4508	–1.7391	–0.2544
H20A	7.5250	–1.6013	–0.1296
H20B	6.0858	–2.4602	0.4865
H20C	6.2449	–2.1122	–1.2647
C19	4.4618	3.2757	0.5462
H19A	5.3566	3.8696	0.7341
H19B	3.9449	3.6618	–0.3402
H19C	3.7952	3.3339	1.4150
F1	–1.1196	–2.6727	–0.1032
F3	–2.0609	–1.5804	1.5320
F2	0.0976	–1.8346	1.4954
N1	–1.8879	0.4726	–0.4182
N3	–0.1322	1.5995	–0.9274
O3	–6.3561	1.8806	0.8263
H3	–5.8728	2.6401	1.1804
O2	5.8718	–0.4517	–0.0512
N2	–1.4335	1.6274	–0.9468
O1	4.9227	1.9424	0.3368
C9	4.0008	0.9763	0.0668
C5	–0.8279	–0.3112	–0.0365
C11	3.6420	–1.3739	–0.4327
H11	4.0220	–2.3721	–0.6116
C15	–5.4964	0.9910	0.2461
C10	4.5206	–0.3291	–0.1452
C7	1.7426	0.1276	–0.2865
C14	–4.1124	1.1862	0.2367
H14	–3.6642	2.0605	0.6974
C12	2.2624	–1.1485	–0.5062
H12	1.6090	–1.9773	–0.7554
C8	2.6286	1.1900	–0.0077
H8	2.2190	2.1798	0.1460
C18	–3.8353	–0.9036	–0.9909
H18	–3.1907	–1.6198	–1.4868
C16	–6.0534	–0.1506	–0.3440
H16	–7.1295	–0.2851	–0.3203
C4	0.3046	0.4177	–0.3891
C6	–0.9784	–1.5927	0.7183
C13	–3.3023	0.2319	–0.3818
C17	–5.2208	–1.0862	–0.9549
H17	–5.6554	–1.9647	–1.4207

Table S25. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Chloroform

	Coordinates		
	x	y	z
C20	6.4504	–1.7475	–0.2211
H20A	7.5227	–1.6104	–0.0822
H20B	6.0745	–2.4670	0.5153
H20C	6.2568	–2.1194	–1.2337
C19	4.4502	3.2711	0.5658
H19A	5.3421	3.8641	0.7688
H19B	3.9453	3.6616	–0.3252
H19C	3.7726	3.3226	1.4260
F1	–1.1406	–2.6637	–0.0641
F3	–2.0562	–1.5252	1.5530
F2	0.1001	–1.7983	1.5017
N1	–1.8865	0.4669	–0.4633
N3	–0.1300	1.5748	–1.0090
O3	–6.3273	1.8566	0.8978
H3	–5.8351	2.6029	1.2687
O2	5.8689	–0.4576	–0.0253
N2	–1.4326	1.6027	–1.0290
O1	4.9149	1.9376	0.3538
C9	3.9967	0.9713	0.0697
C5	–0.8279	–0.3045	–0.0575
C11	3.6438	–1.3790	–0.4354
H11	4.0257	–2.3773	–0.6093
C15	–5.4811	0.9784	0.2820
C10	4.5187	–0.3341	–0.1366
C7	1.7432	0.1235	–0.3131
C14	–4.0975	1.1746	0.2455
H14	–3.6403	2.0404	0.7128
C12	2.2651	–1.1531	–0.5260
H12	1.6142	–1.9816	–0.7829
C8	2.6253	1.1858	–0.0224
H8	2.2149	2.1755	0.1306
C18	–3.8464	–0.8959	–1.0223
H18	–3.2115	–1.6038	–1.5422
C16	–6.0503	–0.1526	–0.3177
H16	–7.1257	–0.2889	–0.2746
C4	0.3055	0.4116	–0.4318
C6	–0.9817	–1.5665	0.7292
C13	–3.3021	0.2298	–0.4052
C17	–5.2314	–1.0780	–0.9623
H17	–5.6765	–1.9479	–1.4343

Table S26. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Chlorobenzene

	Coordinates		
	x	*y*	*z*
C20	6.4501	–1.7493	–0.2187
H20A	7.5223	–1.6124	–0.0781
H20B	6.0729	–2.4690	0.5167
H20C	6.2579	–2.1203	–1.2318
C19	4.4486	3.2696	0.5713
H19A	5.3400	3.8621	0.7774
H19B	3.9454	3.6619	–0.3197
H19C	3.7694	3.3187	1.4303
F1	–1.1447	–2.6612	–0.0537
F3	–2.0549	–1.5130	1.5595
F2	0.1009	–1.7902	1.5050
N1	–1.8863	0.4660	–0.4705
N3	–0.1297	1.5699	–1.0237
O3	–6.3235	1.8514	0.9074
H3	–5.8303	2.5960	1.2807
O2	5.8684	–0.4590	–0.0229
N2	–1.4326	1.5977	–1.0438
O1	4.9139	1.9362	0.3570
C9	3.9961	0.9702	0.0702
C5	–0.8279	–0.3027	–0.0598
C11	3.6438	–1.3799	–0.4371
H11	4.0260	–2.3782	–0.6108
C15	–5.4789	0.9754	0.2865
C10	4.5183	–0.3352	–0.1363
C7	1.7433	0.1229	–0.3173
C14	–4.0954	1.1722	0.2464
H14	–3.6371	2.0364	0.7155
C12	2.2653	–1.1537	–0.5298
H12	1.6145	–1.9820	–0.7881
C8	2.6248	1.1850	–0.0243
H8	2.2145	2.1746	0.1294
C18	–3.8475	–0.8950	–1.0280
H18	–3.2139	–1.6013	–1.5516
C16	–6.0496	–0.1539	–0.3151
H16	–7.1248	–0.2907	–0.2695
C4	0.3056	0.4107	–0.4386
C6	–0.9822	–1.5604	0.7335
C13	–3.3020	0.2291	–0.4093
C17	–5.2325	–1.0774	–0.9647
H17	–5.6788	–1.9460	–1.4380

Table S27. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Tetrahydrofuran

	Coordinates		
	x	*y*	*z*
C20	6.4497	–1.7516	–0.2173
H20A	7.5216	–1.6151	–0.0746
H20B	6.0707	–2.4718	0.5165
H20C	6.2590	–2.1210	–1.2311
C19	4.4470	3.2673	0.5790
H19A	5.3379	3.8591	0.7888
H19B	3.9457	3.6623	–0.3118
H19C	3.7662	3.3134	1.4368
F1	–1.1507	–2.6579	–0.0396
F3	–2.0525	–1.4969	1.5690
F2	0.1025	–1.7799	1.5091
N1	–1.8860	0.4649	–0.4789
N3	–0.1294	1.5640	–1.0414
O3	–6.3198	1.8453	0.9169
H3	–5.8259	2.5884	1.2926
O2	5.8677	–0.4608	–0.0209
N2	–1.4326	1.5916	–1.0616
O1	4.9128	1.9341	0.3613
C9	3.9954	0.9686	0.0709
C5	–0.8278	–0.3004	–0.0622
C11	3.6437	–1.3809	–0.4400
H11	4.0260	–2.3791	–0.6141
C15	–5.4766	0.9716	0.2908
C10	4.5178	–0.3365	–0.1365
C7	1.7433	0.1223	–0.3223
C14	–4.0932	1.1693	0.2469
H14	–3.6338	2.0320	0.7177
C12	2.2655	–1.1543	–0.5350
H12	1.6148	–1.9821	–0.7951
C8	2.6243	1.1840	–0.0262
H8	2.2140	2.1734	0.1289
C18	–3.8485	–0.8946	–1.0342
H18	–3.2159	–1.5990	–1.5616
C16	–6.0485	–0.1563	–0.3125
H16	–7.1235	–0.2939	–0.2640
C4	0.3058	0.4099	–0.4466
C6	–0.9827	–1.5526	0.7397
C13	–3.3019	0.2282	–0.4140
C17	–5.2332	–1.0777	–0.9672
H17	–5.6808	–1.9451	–1.4416

Table S28. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Dichloromethane

	Coordinates		
	x	*y*	*z*
C20	6.4494	–1.7528	–0.2168
H20A	7.5210	–1.6166	–0.0724
H20B	6.0692	–2.4736	0.5156
H20C	6.2598	–2.1207	–1.2313
C19	4.4454	3.2655	0.5851
H19A	5.3360	3.8570	0.7975
H19B	3.9455	3.6625	–0.3056
H19C	3.7634	3.3093	1.4419
F1	–1.1552	–2.6555	–0.0294
F3	–2.0500	–1.4854	1.5762
F2	0.1044	–1.7730	1.5114
N1	–1.8859	0.4640	–0.4846
N3	–0.1294	1.5598	–1.0537
O3	–6.3174	1.8422	0.9215
H3	–5.8231	2.5847	1.2979
O2	5.8672	–0.4619	–0.0195
N2	–1.4328	1.5872	–1.0738
O1	4.9119	1.9327	0.3648
C9	3.9948	0.9676	0.0715
C5	–0.8277	–0.2989	–0.0640
C11	3.6437	–1.3814	–0.4427
H11	4.0262	–2.3794	–0.6172
C15	–5.4752	0.9694	0.2930
C10	4.5174	–0.3373	–0.1368
C7	1.7434	0.1220	–0.3261
C14	–4.0919	1.1678	0.2462
H14	–3.6318	2.0302	0.7168
C12	2.2656	–1.1545	–0.5393
H12	1.6150	–1.9818	–0.8012
C8	2.6238	1.1833	–0.0274
H8	2.2135	2.1725	0.1289
C18	–3.8491	–0.8955	–1.0366
H18	–3.2172	–1.5993	–1.5657
C16	–6.0478	–0.1583	–0.3099
H16	–7.1227	–0.2966	–0.2593
C4	0.3058	0.4092	–0.4523
C6	–0.9827	–1.5472	0.7441
C13	–3.3018	0.2272	–0.4170
C17	–5.2336	–1.0792	–0.9670
H17	–5.6820	–1.9463	–1.4409

Table S29. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Dichloroethane

	Coordinates		
	x	*y*	*z*
C20	6.4495	–1.7531	–0.2170
H20A	7.5210	–1.6170	–0.0717
H20B	6.0687	–2.4745	0.5145
H20C	6.2607	–2.1202	–1.2320
C19	4.4442	3.2645	0.5893
H19A	5.3345	3.8557	0.8035
H19B	3.9450	3.6629	–0.3011
H19C	3.7615	3.3065	1.4456
F1	–1.1588	–2.6542	–0.0227
F3	–2.0481	–1.4780	1.5815
F2	0.1058	–1.7692	1.5126
N1	–1.8858	0.4631	–0.4880
N3	–0.1294	1.5569	–1.0613
O3	–6.3160	1.8410	0.9233
H3	–5.8214	2.5833	1.2997
O2	5.8671	–0.4622	–0.0191
N2	–1.4329	1.5841	–1.0814
O1	4.9111	1.9320	0.3670
C9	3.9944	0.9670	0.0719
C5	–0.8276	–0.2982	–0.0649
C11	3.6439	–1.3816	–0.4446
H11	4.0266	–2.3794	–0.6197
C15	–5.4742	0.9684	0.2939
C10	4.5172	–0.3377	–0.1372
C7	1.7434	0.1216	–0.3284
C14	–4.0910	1.1671	0.2454
H14	–3.6305	2.0294	0.7158
C12	2.2659	–1.1547	–0.5421
H12	1.6154	–1.9818	–0.8050
C8	2.6235	1.1828	–0.0281
H8	2.2130	2.1718	0.1291
C18	–3.8495	–0.8965	–1.0377
H18	–3.2181	–1.6002	–1.5675
C16	–6.0474	–0.1595	–0.3085
H16	–7.1222	–0.2979	–0.2567
C4	0.3058	0.4085	–0.4557
C6	–0.9827	–1.5439	0.7471
C13	–3.3017	0.2265	–0.4187
C17	–5.2340	–1.0802	–0.9665
H17	–5.6828	–1.9475	–1.4399

Table S30. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in 2-Methyl-2-Propanol

	Coordinates		
	x	*y*	*z*
C20	6.4498	–1.7532	–0.2180
H20A	7.5212	–1.6171	–0.0713
H20B	6.0683	–2.4758	0.5119
H20C	6.2622	–2.1184	–1.2338
C19	4.4420	3.2627	0.5966
H19A	5.3317	3.8536	0.8139
H19B	3.9439	3.6635	–0.2932
H19C	3.7581	3.3017	1.4521
F1	–1.1659	–2.6519	–0.0114
F3	–2.0440	–1.4653	1.5912
F2	0.1086	–1.7638	1.5137
N1	–1.8857	0.4614	–0.4936
N3	–0.1295	1.5519	–1.0736
O3	–6.3137	1.8400	0.9248
H3	–5.8188	2.5825	1.3005
O2	5.8668	–0.4625	–0.0185
N2	–1.4332	1.5788	–1.0936
O1	4.9098	1.9308	0.3709
C9	3.9936	0.9661	0.0726
C5	–0.8274	–0.2972	–0.0663
C11	3.6444	–1.3818	–0.4481
H11	4.0276	–2.3792	–0.6241
C15	–5.4728	0.9672	0.2946
C10	4.5170	–0.3380	–0.1381
C7	1.7435	0.1209	–0.3322
C14	–4.0897	1.1661	0.2434
H14	–3.6283	2.0286	0.7126
C12	2.2664	–1.1550	–0.5469
H12	1.6162	–1.9818	–0.8116
C8	2.6228	1.1819	–0.0290
H8	2.2119	2.1706	0.1298
C18	–3.8502	–0.8987	–1.0383
H18	–3.2196	–1.6027	–1.5687
C16	–6.0469	–0.1613	–0.3058
H16	–7.1215	–0.3001	–0.2520
C4	0.3058	0.4072	–0.4613
C6	–0.9826	–1.5387	0.7522
C13	–3.3016	0.2249	–0.4214
C17	–5.2345	–1.0826	–0.9645
H17	–5.6841	–1.9503	–1.4363

Table S31. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in 1-Butanol

	Coordinates		
	x	y	z
C20	6.4507	–1.7525	–0.2196
H20A	7.5217	–1.6162	–0.0707
H20B	6.0683	–2.4771	0.5077
H20C	6.2648	–2.1150	–1.2366
C19	4.4380	3.2602	0.6078
H19A	5.3268	3.8508	0.8297
H19B	3.9415	3.6648	–0.2812
H19C	3.7524	3.2944	1.4620
F1	–1.1777	–2.6488	0.0050
F3	–2.0369	–1.4466	1.6061
F2	0.1135	–1.7573	1.5140
N1	–1.8856	0.4584	–0.5015
N3	–0.1298	1.5442	–1.0914
O3	–6.3102	1.8402	0.9253
H3	–5.8146	2.5832	1.2993
O2	5.8666	–0.4624	–0.0176
N2	–1.4337	1.5707	–1.1111
O1	4.9074	1.9295	0.3767
C9	3.9924	0.9651	0.0736
C5	–0.8271	–0.2964	–0.0686
C11	3.6455	–1.3819	–0.4534
H11	4.0295	–2.3787	–0.6309
C15	–5.4707	0.9662	0.2951
C10	4.5169	–0.3383	–0.1394
C7	1.7436	0.1197	–0.3378
C14	–4.0876	1.1652	0.2398
H14	–3.6250	2.0286	0.7063
C12	2.2675	–1.1556	–0.5543
H12	1.6179	–1.9820	–0.8215
C8	2.6216	1.1805	–0.0304
H8	2.2100	2.1685	0.1306
C18	–3.8514	–0.9029	–1.0378
H18	–3.2220	–1.6080	–1.5681
C16	–6.0461	–0.1638	–0.3012
H16	–7.1206	–0.3027	–0.2444
C4	0.3059	0.4050	–0.4695
C6	–0.9824	–1.5316	0.7594
C13	–3.3015	0.2224	–0.4250
C17	–5.2355	–1.0867	–0.9600
H17	–5.6864	–1.9555	–1.4285

Table S32. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Acetone

	Coordinates		
	x	*y*	*z*
C20	6.4511	–1.7522	–0.2203
H20A	7.5219	–1.6159	–0.0701
H20B	6.0680	–2.4776	0.5059
H20C	6.2663	–2.1135	–1.2378
C19	4.4363	3.2591	0.6126
H19A	5.3247	3.8495	0.8364
H19B	3.9403	3.6652	–0.2759
H19C	3.7500	3.2912	1.4663
F1	–1.1826	–2.6476	0.0126
F3	–2.0336	–1.4384	1.6128
F2	0.1159	–1.7542	1.5141
N1	–1.8855	0.4570	–0.5047
N3	–0.1301	1.5411	–1.0985
O3	–6.3090	1.8404	0.9249
H3	–5.8132	2.5838	1.2978
O2	5.8665	–0.4622	–0.0174
N2	–1.4340	1.5673	–1.1181
O1	4.9064	1.9289	0.3792
C9	3.9918	0.9646	0.0740
C5	–0.8269	–0.2962	–0.0696
C11	3.6459	–1.3818	–0.4562
H11	4.0303	–2.3784	–0.6345
C15	–5.4699	0.9657	0.2950
C10	4.5168	–0.3383	–0.1402
C7	1.7437	0.1192	–0.3404
C14	–4.0869	1.1649	0.2379
H14	–3.6239	2.0287	0.7031
C12	2.2680	–1.1557	–0.5579
H12	1.6187	–1.9820	–0.8266
C8	2.6210	1.1799	–0.0309
H8	2.2091	2.1676	0.1313
C18	–3.8518	–0.9050	–1.0372
H18	–3.2229	–1.6107	–1.5672
C16	–6.0458	–0.1651	–0.2994
H16	–7.1202	–0.3041	–0.2412
C4	0.3058	0.4040	–0.4730
C6	–0.9821	–1.5286	0.7626
C13	–3.3015	0.2212	–0.4265
C17	–5.2359	–1.0888	–0.9578
H17	–5.6871	–1.9583	–1.4247

Table S33. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Ethanol

	Coordinates		
	x	*y*	*z*
C20	6.4518	–1.7516	–0.2204
H20A	7.5224	–1.6150	–0.0692
H20B	6.0682	–2.4776	0.5048
H20C	6.2679	–2.1121	–1.2384
C19	4.4343	3.2584	0.6166
H19A	5.3223	3.8488	0.8420
H19B	3.9389	3.6657	–0.2717
H19C	3.7474	3.2887	1.4698
F1	–1.1884	–2.6465	0.0187
F3	–2.0304	–1.4311	1.6189
F2	0.1179	–1.7529	1.5133
N1	–1.8854	0.4556	–0.5077
N3	–0.1301	1.5379	–1.1052
O3	–6.3074	1.8409	0.9252
H3	–5.8113	2.5848	1.2969
O2	5.8666	–0.4618	–0.0169
N2	–1.4341	1.5639	–1.1246
O1	4.9052	1.9287	0.3813
C9	3.9913	0.9643	0.0744
C5	–0.8268	–0.2962	–0.0705
C11	3.6466	–1.3818	–0.4582
H11	4.0315	–2.3780	–0.6370
C15	–5.4689	0.9657	0.2952
C10	4.5168	–0.3382	–0.1407
C7	1.7438	0.1185	–0.3426
C14	–4.0860	1.1646	0.2367
H14	–3.6223	2.0286	0.7009
C12	2.2687	–1.1561	–0.5607
H12	1.6199	–1.9823	–0.8305
C8	2.6204	1.1792	–0.0314
H8	2.2081	2.1666	0.1316
C18	–3.8524	–0.9065	–1.0370
H18	–3.2241	–1.6127	–1.5670
C16	–6.0456	–0.1656	–0.2976
H16	–7.1199	–0.3044	–0.2384
C4	0.3059	0.4028	–0.4761
C6	–0.9822	–1.5262	0.7652
C13	–3.3014	0.2202	–0.4277
C17	–5.2364	–1.0901	–0.9560
H17	–5.6883	–1.9598	–1.4217

Table S34. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Methanol

	Coordinates		
	x	*y*	*z*
C20	6.4525	–1.7509	–0.2206
H20A	7.5229	–1.6141	–0.0684
H20B	6.0685	–2.4777	0.5034
H20C	6.2695	–2.1102	–1.2392
C19	4.4321	3.2576	0.6210
H19A	5.3195	3.8481	0.8483
H19B	3.9373	3.6660	–0.2671
H19C	3.7443	3.2861	1.4736
F1	–1.1944	–2.6452	0.0256
F3	–2.0268	–1.4230	1.6255
F2	0.1202	–1.7511	1.5125
N1	–1.8854	0.4541	–0.5111
N3	–0.1302	1.5342	–1.1129
O3	–6.3056	1.8416	0.9253
H3	–5.8092	2.5857	1.2961
O2	5.8666	–0.4614	–0.0162
N2	–1.4343	1.5601	–1.1321
O1	4.9039	1.9284	0.3840
C9	3.9906	0.9640	0.0749
C5	–0.8266	–0.2962	–0.0717
C11	3.6474	–1.3817	–0.4606
H11	4.0328	–2.3776	–0.6400
C15	–5.4679	0.9656	0.2955
C10	4.5169	–0.3381	–0.1411
C7	1.7439	0.1178	–0.3451
C14	–4.0849	1.1644	0.2351
H14	–3.6205	2.0287	0.6980
C12	2.2695	–1.1564	–0.5641
H12	1.6210	–1.9825	–0.8352
C8	2.6198	1.1786	–0.0320
H8	2.2069	2.1656	0.1321
C18	–3.8531	–0.9084	–1.0364
H18	–3.2254	–1.6152	–1.5663
C16	–6.0453	–0.1664	–0.2953
H16	–7.1196	–0.3050	–0.2347
C4	0.3059	0.4015	–0.4797
C6	–0.9821	–1.5235	0.7680
C13	–3.3013	0.2190	–0.4292
C17	–5.2371	–1.0917	–0.9536
H17	–5.6896	–1.9620	–1.4177

Table S35. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Acetonitrile

	Coordinates		
	x	y	z
C20	6.4530	–1.7503	–0.2207
H20A	7.5234	–1.6133	–0.0683
H20B	6.0691	–2.4774	0.5032
H20C	6.2701	–2.1094	–1.2393
C19	4.4313	3.2576	0.6219
H19A	5.3186	3.8481	0.8495
H19B	3.9368	3.6662	–0.2662
H19C	3.7433	3.2857	1.4743
F1	–1.1969	–2.6451	0.0273
F3	–2.0259	–1.4209	1.6275
F2	0.1206	–1.7514	1.5119
N1	–1.8853	0.4535	–0.5120
N3	–0.1301	1.5331	–1.1147
O3	–6.3048	1.8420	0.9257
H3	–5.8082	2.5864	1.2960
O2	5.8667	–0.4610	–0.0159
N2	–1.4342	1.5590	–1.1339
O1	4.9034	1.9285	0.3845
C9	3.9904	0.9639	0.0751
C5	–0.8266	–0.2965	–0.0720
C11	3.6478	–1.3817	–0.4609
H11	4.0335	–2.3776	–0.6404
C15	–5.4674	0.9659	0.2957
C10	4.5170	–0.3380	–0.1411
C7	1.7440	0.1173	–0.3456
C14	–4.0844	1.1643	0.2349
H14	–3.6196	2.0285	0.6978
C12	2.2699	–1.1568	–0.5646
H12	1.6217	–1.9831	–0.8359
C8	2.6196	1.1782	–0.0321
H8	2.2064	2.1651	0.1321
C18	–3.8535	–0.9086	–1.0366
H18	–3.2261	–1.6156	–1.5667
C16	–6.0452	–0.1660	–0.2949
H16	–7.1196	–0.3044	–0.2340
C4	0.3060	0.4008	–0.4806
C6	–0.9824	–1.5231	0.7687
C13	–3.3013	0.2187	–0.4296
C17	–5.2375	–1.0916	–0.9533
H17	–5.6903	–1.9618	–1.4173

Table S36. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in dmso

	Coordinates		
	x	*y*	*z*
C20	6.4532	–1.7502	–0.2202
H20A	7.5234	–1.6133	–0.0667
H20B	6.0685	–2.4775	0.5031
H20C	6.2713	–2.1090	–1.2391
C19	4.4301	3.2570	0.6245
H19A	5.3171	3.8476	0.8532
H19B	3.9359	3.6664	–0.2635
H19C	3.7417	3.2840	1.4765
F1	–1.1998	–2.6441	0.0312
F3	–2.0239	–1.4163	1.6310
F2	0.1220	–1.7499	1.5117
N1	–1.8853	0.4527	–0.5141
N3	–0.1302	1.5310	–1.1194
O3	–6.3039	1.8421	0.9260
H3	–5.8072	2.5866	1.2956
O2	5.8667	–0.4609	–0.0157
N2	–1.4344	1.5568	–1.1385
O1	4.9028	1.9282	0.3861
C9	3.9901	0.9637	0.0753
C5	–0.8265	–0.2962	–0.0726
C11	3.6482	–1.3817	–0.4624
H11	4.0341	–2.3773	–0.6424
C15	–5.4668	0.9656	0.2960
C10	4.5170	–0.3380	–0.1415
C7	1.7440	0.1170	–0.3472
C14	–4.0839	1.1641	0.2341
H14	–3.6188	2.0285	0.6962
C12	2.2702	–1.1568	–0.5668
H12	1.6222	–1.9829	–0.8389
C8	2.6192	1.1779	–0.0325
H8	2.2059	2.1645	0.1325
C18	–3.8538	–0.9097	–1.0362
H18	–3.2267	–1.6170	–1.5663
C16	–6.0450	–0.1667	–0.2935
H16	–7.1193	–0.3052	–0.2317
C4	0.3060	0.4002	–0.4828
C6	–0.9822	–1.5213	0.7704
C13	–3.3013	0.2181	–0.4304
C17	–5.2377	–1.0927	–0.9519
H17	–5.6909	–1.9632	–1.4149

Table S37. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Formicacid

	Coordinates		
	x	*y*	*z*
C20	6.4533	–1.7501	–0.2205
H20A	7.5235	–1.6130	–0.0669
H20B	6.0687	–2.4776	0.5026
H20C	6.2715	–2.1086	–1.2395
C19	4.4296	3.2568	0.6256
H19A	5.3165	3.8474	0.8547
H19B	3.9355	3.6665	–0.2623
H19C	3.7410	3.2832	1.4774
F1	–1.2008	–2.6438	0.0327
F3	–2.0232	–1.4146	1.6324
F2	0.1224	–1.7493	1.5118
N1	–1.8852	0.4524	–0.5148
N3	–0.1303	1.5302	–1.1210
O3	–6.3036	1.8422	0.9259
H3	–5.8069	2.5869	1.2951
O2	5.8667	–0.4608	–0.0156
N2	–1.4344	1.5560	–1.1400
O1	4.9025	1.9282	0.3865
C9	3.9899	0.9636	0.0754
C5	–0.8265	–0.2962	–0.0727
C11	3.6483	–1.3817	–0.4629
H11	4.0344	–2.3773	–0.6430
C15	–5.4667	0.9655	0.2959
C10	4.5170	–0.3380	–0.1416
C7	1.7440	0.1169	–0.3477
C14	–4.0837	1.1641	0.2337
H14	–3.6185	2.0286	0.6955
C12	2.2704	–1.1569	–0.5674
H12	1.6225	–1.9830	–0.8398
C8	2.6191	1.1778	–0.0326
H8	2.2057	2.1643	0.1325
C18	–3.8539	–0.9102	–1.0361
H18	–3.2269	–1.6176	–1.5661
C16	–6.0449	–0.1670	–0.2931
H16	–7.1192	–0.3055	–0.2310
C4	0.3060	0.3999	–0.4836
C6	–0.9822	–1.5206	0.7710
C13	–3.3013	0.2178	–0.4307
C17	–5.2378	–1.0932	–0.9514
H17	–5.6910	–1.9638	–1.4140

Table S38. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Water

	Coordinates		
	x	*y*	*z*
C20	6.4540	–1.7495	–0.2203
H20A	7.5241	–1.6122	–0.0665
H20B	6.0694	–2.4773	0.5025
H20C	6.2724	–2.1077	–1.2394
C19	4.4284	3.2567	0.6270
H19A	5.3150	3.8474	0.8569
H19B	3.9347	3.6668	–0.2609
H19C	3.7394	3.2824	1.4786
F1	–1.2041	–2.6433	0.0355
F3	–2.0220	–1.4112	1.6351
F2	0.1230	–1.7491	1.5113
N1	–1.8851	0.4516	–0.5164
N3	–0.1301	1.5283	–1.1244
O3	–6.3024	1.8424	0.9270
H3	–5.8055	2.5870	1.2961
O2	5.8669	–0.4604	–0.0151
N2	–1.4343	1.5541	–1.1434
O1	4.9018	1.9283	0.3874
C9	3.9897	0.9635	0.0756
C5	–0.8265	–0.2964	–0.0733
C11	3.6489	–1.3818	–0.4634
H11	4.0353	–2.3772	–0.6435
C15	–5.4659	0.9657	0.2965
C10	4.5171	–0.3379	–0.1416
C7	1.7442	0.1162	–0.3487
C14	–4.0829	1.1639	0.2336
H14	–3.6171	2.0280	0.6956
C12	2.2709	–1.1573	–0.5684
H12	1.6234	–1.9837	–0.8411
C8	2.6188	1.1773	–0.0329
H8	2.2050	2.1637	0.1325
C18	–3.8544	–0.9104	–1.0366
H18	–3.2279	–1.6179	–1.5670
C16	–6.0448	–0.1666	–0.2924
H16	–7.1191	–0.3049	–0.2298
C4	0.3061	0.3990	–0.4851
C6	–0.9825	–1.5197	0.7721
C13	–3.3012	0.2174	–0.4314
C17	–5.2383	–1.0931	–0.9512
H17	–5.6921	–1.9635	–1.4137

Table S39. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in Formamide

	Coordinates		
	x	*y*	*z*
C20	6.4540	–1.7496	–0.2199
H20A	7.5241	–1.6123	–0.0656
H20B	6.0691	–2.4774	0.5026
H20C	6.2729	–2.1077	–1.2392
C19	4.4280	3.2564	0.6282
H19A	5.3145	3.8470	0.8586
H19B	3.9344	3.6669	–0.2596
H19C	3.7388	3.2815	1.4796
F1	–1.2056	–2.6427	0.0374
F3	–2.0211	–1.4088	1.6369
F2	0.1235	–1.7484	1.5112
N1	–1.8851	0.4513	–0.5173
N3	–0.1301	1.5273	–1.1267
O3	–6.3021	1.8421	0.9273
H3	–5.8051	2.5867	1.2965
O2	5.8668	–0.4604	–0.0150
N2	–1.4344	1.5530	–1.1457
O1	4.9016	1.9281	0.3880
C9	3.9895	0.9634	0.0756
C5	–0.8264	–0.2961	–0.0735
C11	3.6490	–1.3818	–0.4641
H11	4.0355	–2.3772	–0.6444
C15	–5.4657	0.9654	0.2968
C10	4.5171	–0.3380	–0.1417
C7	1.7442	0.1161	–0.3494
C14	–4.0827	1.1637	0.2334
H14	–3.6168	2.0279	0.6951
C12	2.2710	–1.1574	–0.5693
H12	1.6235	–1.9836	–0.8424
C8	2.6186	1.1772	–0.0331
H8	2.2049	2.1635	0.1327
C18	–3.8545	–0.9107	–1.0367
H18	–3.2281	–1.6182	–1.5673
C16	–6.0447	–0.1670	–0.2918
H16	–7.1190	–0.3053	–0.2289
C4	0.3061	0.3988	–0.4861
C6	–0.9825	–1.5187	0.7730
C13	–3.3012	0.2172	–0.4318
C17	–5.2384	–1.0935	–0.9508
H17	–5.6923	–1.9640	–1.4131

Table S40. DFT-B3LYP/6-311+G(d) of the optimized DTTP molecule in n-Methylformamide-Mixture

	Coordinates		
	x	*y*	*z*
C20	6.4544	–1.7492	–0.2199
H20A	7.5244	–1.6118	–0.0651
H20B	6.0693	–2.4772	0.5022
H20C	6.2738	–2.1069	–1.2394
C19	4.4271	3.2563	0.6295
H19A	5.3134	3.8470	0.8603
H19B	3.9337	3.6669	–0.2583
H19C	3.7376	3.2811	1.4807
F1	–1.2078	–2.6424	0.0397
F3	–2.0199	–1.4061	1.6391
F2	0.1242	–1.7480	1.5109
N1	–1.8851	0.4507	–0.5185
N3	–0.1301	1.5258	–1.1293
O3	–6.3014	1.8426	0.9273
H3	–5.8042	2.5871	1.2963
O2	5.8669	–0.4601	–0.0147
N2	–1.4344	1.5516	–1.1482
O1	4.9010	1.9280	0.3891
C9	3.9892	0.9633	0.0759
C5	–0.8264	–0.2963	–0.0739
C11	3.6494	–1.3817	–0.4650
H11	4.0361	–2.3769	–0.6456
C15	–5.4653	0.9655	0.2969
C10	4.5172	–0.3378	–0.1419
C7	1.7442	0.1157	–0.3502
C14	–4.0823	1.1637	0.2328
H14	–3.6160	2.0279	0.6942
C12	2.2714	–1.1576	–0.5706
H12	1.6242	–1.9838	–0.8443
C8	2.6183	1.1768	–0.0332
H8	2.2043	2.1630	0.1331
C18	–3.8548	–0.9114	–1.0365
H18	–3.2287	–1.6191	–1.5670
C16	–6.0446	–0.1671	–0.2911
H16	–7.1188	–0.3053	–0.2276
C4	0.3061	0.3981	–0.4874
C6	–0.9825	–1.5179	0.7739
C13	–3.3012	0.2168	–0.4323
C17	–5.2387	–1.0939	–0.9500
H17	–5.6928	–1.9646	–1.4117

Table S41. Results for the angles and torsions for the triazole derivatives molecules immersed in several solvent media

	Angles							Torsions					
	DMTT			DTTP				DMTT			DTTP		
	C5-C6-F1	C13-N1-C5	C9-O1-C21	C13-N1-C5	C5-C6-F1	C9-O1-C19	C15-O3-H13	C7-C4-C5-C6	N2-N1-C13-C18	C9-O1-C21-H21A	C7-C4-C5-C6	N2-N1-C13-C14	C9-O1-C19-H19B
X-ray	111.49	130.09	117.86	132.20	112.86	117.41	109.47	–7.73	73.90	59.95	3.78	48.92	60.02
1.000	111.39	131.23	118.59	131.44	112.61	118.23	110.41	–7.71	53.96	62.18	8.73	51.16	60.36
1.430	111.36	131.08	118.61	131.32	112.63	118.24	110.51	–7.51	55.87	62.18	8.51	52.75	60.52
1.911	111.35	130.98	118.62	131.25	112.64	118.25	110.57	–7.31	57.29	62.18	8.26	53.83	60.67
2.374	111.33	130.93	118.63	131.17	112.64	118.26	110.62	–7.16	58.17	62.17	7.99	54.95	60.73
4.711	111.30	130.80	118.66	131.00	112.65	118.28	110.69	–6.79	60.57	62.08	7.24	57.74	60.94
5.697	111.29	130.77	118.67	130.96	112.66	118.28	110.71	–6.71	61.08	62.04	7.13	58.29	61.01
7.426	111.28	130.74	118.68	130.91	112.67	118.29	110.73	–6.62	61.66	61.99	7.03	58.94	61.08
8.930	111.28	130.73	118.68	130.88	112.67	118.28	110.74	–6.56	61.99	61.96	6.97	59.30	61.12
10.125	111.28	130.72	118.69	130.87	112.68	118.28	110.74	–6.53	62.18	61.94	6.94	59.51	61.15
12.470	111.27	130.70	118.69	130.85	112.68	118.29	110.76	–6.48	62.45	61.91	6.90	59.79	61.20
17.332	111.26	130.69	118.70	130.82	112.69	118.29	110.77	–6.41	62.78	61.86	6.84	60.13	61.29
20.493	111.26	130.68	118.70	130.81	112.70	118.29	110.78	–6.38	62.99	61.84	6.85	60.24	61.31
24.852	111.26	130.68	118.70	130.80	112.71	118.29	110.78	–6.35	63.03	61.82	6.83	60.36	61.34
32.613	111.26	130.67	118.70	130.79	112.71	118.28	110.79	–6.31	63.17	61.79	6.80	60.49	61.36
35.688	111.26	130.67	118.70	130.79	112.72	118.29	110.80	–6.31	63.21	61.79	6.80	60.53	61.37
46.826	111.25	130.66	118.70	130.78	112.72	118.29	110.80	–6.29	63.29	61.76	6.76	60.62	61.38
51.100	111.25	130.66	118.70	130.78	112.72	118.28	110.80	–6.28	63.31	61.75	6.75	60.65	61.39
78.355	111.25	130.66	118.71	130.78	112.72	118.29	110.81	–6.25	63.42	61.73	6.73	60.74	61.41
108.940	111.25	130.65	118.71	130.77	112.72	118.29	110.81	–6.23	63.55	61.74	6.70	60.80	61.42
181.560	111.25	130.64	118.71	130.77	112.72	118.29	110.81	–6.21	63.68	61.73	6.69	60.84	61.40

Table S42. CAM-B3LYP/6-311+G(d) charges ChelpG of the DMTT structure

	Charge (e)																			
	ε																			
Atom	**1.00**	**1.43**	**1.91**	**2.37**	**4.71**	**5.70**	**7.43**	**8.93**	**10.13**	**12.47**	**17.33**	**20.49**	**24.85**	**32.61**	**35.69**	**46.83**	**51.10**	**78.36**	**108.94**	**181.56**
C4	0.42	0.44	0.43	0.43	0.44	0.45	0.45	0.46	0.47	0.47	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46
C5	–0.43	–0.43	–0.43	–0.43	–0.41	–0.41	–0.41	–0.42	–0.42	–0.41	–0.40	–0.40	–0.40	–0.41	–0.40	–0.40	–0.40	–0.40	–0.40	–0.40
C6	0.91	0.92	0.93	0.93	0.93	0.92	0.92	0.93	0.93	0.91	0.90	0.91	0.91	0.92	0.92	0.92	0.92	0.92	0.92	0.92
C7	–0.06	–0.07	–0.05	–0.05	–0.05	–0.07	–0.07	–0.08	–0.08	–0.08	–0.07	–0.07	–0.07	–0.07	–0.06	–0.06	–0.06	–0.06	–0.06	–0.06
C8	–0.25	–0.25	–0.28	–0.28	–0.29	–0.29	–0.29	–0.28	–0.28	–0.28	–0.29	–0.30	–0.30	–0.30	–0.31	–0.31	–0.31	–0.31	–0.31	–0.32
H8	0.12	0.12	0.13	0.14	0.15	0.14	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.16	0.16	0.16	0.16	0.16	0.16
C9	0.46	0.47	0.49	0.49	0.50	0.50	0.50	0.49	0.49	0.49	0.50	0.50	0.50	0.51	0.51	0.51	0.51	0.51	0.51	0.51
C10	–0.30	–0.31	–0.32	–0.32	–0.33	–0.33	–0.33	–0.32	–0.33	–0.33	–0.33	–0.33	–0.34	–0.34	–0.34	–0.34	–0.34	–0.34	–0.34	–0.34
H10	0.14	0.15	0.15	0.15	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
C11	–0.02	–0.03	–0.02	–0.02	–0.02	–0.02	–0.02	–0.02	–0.02	–0.02	–0.02	–0.01	–0.01	–0.01	–0.01	–0.01	–0.01	–0.01	–0.01	–0.01
H11	0.10	0.11	0.10	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11
C12	–0.12	–0.12	–0.13	–0.13	–0.14	–0.13	–0.13	–0.13	–0.13	–0.13	–0.14	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15
H12	0.07	0.07	0.07	0.07	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09
C13	–0.04	–0.06	–0.07	–0.06	–0.07	–0.09	–0.10	–0.11	–0.13	–0.13	–0.13	–0.13	–0.12	–0.12	–0.12	–0.12	–0.12	–0.11	–0.11	–0.11
C14	–0.16	–0.17	–0.17	–0.17	–0.18	–0.17	–0.16	–0.16	–0.14	–0.14	–0.14	–0.14	–0.14	–0.15	–0.14	–0.14	–0.14	–0.15	–0.15	–0.15
H14	0.10	0.10	0.10	0.11	0.11	0.11	0.11	0.11	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.11	0.11	0.11
C15	0.14	0.15	0.14	0.14	0.14	0.14	0.14	0.14	0.12	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.14
C16	0.09	0.10	0.10	0.10	0.11	0.11	0.10	0.11	0.12	0.12	0.12	0.12	0.12	0.11	0.12	0.12	0.12	0.12	0.12	0.12
C17	–0.15	–0.16	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16	–0.16
H17	0.12	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14
C18	–0.15	–0.14	–0.15	–0.16	–0.16	–0.15	–0.15	–0.14	–0.13	–0.13	–0.14	–0.14	–0.14	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15	–0.15
H18	0.14	0.14	0.14	0.14	0.15	0.14	0.14	0.14	0.14	0.14	0.14	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
C19	–0.30	–0.32	–0.30	–0.30	–0.29	–0.29	–0.30	–0.31	–0.31	–0.31	–0.33	–0.33	–0.33	–0.33	–0.33	–0.33	–0.33	–0.33	–0.33	–0.33
H19A	0.10	0.11	0.11	0.11	0.10	0.10	0.11	0.11	0.11	0.11	0.11	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12
H19B	0.09	0.10	0.10	0.10	0.09	0.09	0.10	0.10	0.10	0.10	0.10	0.11	0.11	0.11	0.11	0.11	0.11	0.10	0.10	0.11
H19C	0.08	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
C20	–0.22	–0.26	–0.26	–0.26	–0.28	–0.28	–0.27	–0.27	–0.28	–0.28	–0.29	–0.28	–0.29	–0.28	–0.28	–0.29	–0.29	–0.30	–0.30	–0.29
H20A	0.07	0.08	0.08	0.08	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09
H20B	0.07	0.08	0.08	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.10	0.10	0.10
H20C	0.08	0.08	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
C21	0.15	0.15	0.15	0.15	0.17	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.19	0.19	0.19	0.18	0.18	0.18	0.19	0.19
H21A	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
H21B	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06
H21C	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
F1	–0.27	–0.28	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.28	–0.28	–0.28	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29
F2	–0.25	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26
F3	–0.30	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31	–0.31
N1	0.54	0.56	0.58	0.57	0.57	0.59	0.60	0.61	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62
N2	–0.33	–0.34	–0.35	–0.35	–0.36	–0.37	–0.37	–0.37	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.39	–0.39
N3	–0.28	–0.30	–0.31	–0.31	–0.33	–0.34	–0.34	–0.34	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35	–0.35
O1	–0.43	–0.44	–0.45	–0.46	–0.47	–0.47	–0.48	–0.48	–0.48	–0.48	–0.48	–0.48	–0.48	–0.49	–0.49	–0.49	–0.49	–0.49	–0.49	–0.49

Table S43. CAM-B3LYP/6-311+G(d) charges ChelpG of the DTTP structure

	Charge (e)																			
	ε																			
Atom	**1.00**	**1.43**	**1.91**	**2.37**	**4.71**	**5.70**	**7.43**	**8.93**	**10.13**	**12.47**	**17.33**	**20.49**	**24.85**	**32.61**	**35.69**	**46.83**	**51.10**	**78.36**	**108.94**	**181.56**
C20	0.19	0.19	0.19	0.18	0.17	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.18	0.17	0.18
H20A	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.06	0.06
H20B	0.01	0.01	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
H20C	0.00	0.00	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
C19	0.17	0.18	0.19	0.18	0.19	0.19	0.19	0.19	0.21	0.21	0.21	0.22	0.21	0.21	0.21	0.22	0.22	0.22	0.22	0.23
H19A	0.05	0.05	0.04	0.05	0.05	0.05	0.05	0.05	0.04	0.04	0.05	0.04	0.05	0.05	0.05	0.04	0.04	0.04	0.04	0.04
H19B	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H19C	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02
F1	–0.25	–0.25	–0.25	–0.26	–0.25	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26	–0.26
F3	–0.29	–0.30	–0.29	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30	–0.30
F2	–0.26	–0.27	–0.27	–0.28	–0.27	–0.27	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28
N1	0.51	0.51	0.52	0.50	0.53	0.55	0.56	0.57	0.57	0.57	0.56	0.56	0.57	0.56	0.57	0.56	0.56	0.57	0.56	0.56
N3	–0.29	–0.29	–0.31	–0.31	–0.34	–0.34	–0.35	–0.35	–0.35	–0.35	–0.36	–0.36	–0.36	–0.36	–0.36	–0.36	–0.36	–0.36	–0.36	–0.36
O3	–0.68	–0.69	–0.69	–0.70	–0.71	–0.71	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.72	–0.73	–0.73	–0.73
H3	0.46	0.46	0.47	0.48	0.48	0.48	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.50	0.50	0.50
O2	–0.38	–0.39	–0.40	–0.40	–0.41	–0.41	–0.41	–0.42	–0.42	–0.42	–0.42	–0.42	–0.43	–0.43	–0.43	–0.43	–0.43	–0.42	–0.42	–0.43
N2	–0.33	–0.34	–0.35	–0.35	–0.37	–0.37	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.38	–0.39	–0.38	–0.38
O1	–0.38	–0.39	–0.40	–0.40	–0.43	–0.43	–0.44	–0.44	–0.44	–0.44	–0.45	–0.45	–0.45	–0.45	–0.45	–0.45	–0.45	–0.45	–0.46	–0.46
C9	0.24	0.25	0.25	0.26	0.29	0.29	0.30	0.30	0.29	0.29	0.29	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30
C5	–0.42	–0.42	–0.43	–0.41	–0.42	–0.42	–0.42	–0.42	–0.42	–0.42	–0.41	–0.41	–0.41	–0.41	–0.41	–0.40	–0.40	–0.40	–0.40	–0.39
C11	–0.22	–0.21	–0.22	–0.22	–0.21	–0.21	–0.22	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21	–0.21
H11	0.15	0.15	0.15	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.17	0.17	0.17
C15	0.53	0.54	0.54	0.54	0.55	0.55	0.55	0.56	0.56	0.56	0.56	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55
C10	0.28	0.27	0.28	0.27	0.26	0.26	0.26	0.26	0.26	0.27	0.27	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26
C7	–0.18	–0.18	–0.20	–0.17	–0.19	–0.17	–0.17	–0.17	–0.17	–0.18	–0.19	–0.19	–0.18	–0.18	–0.18	–0.17	–0.17	–0.17	–0.17	–0.17
C14	–0.38	–0.39	–0.40	–0.40	–0.41	–0.40	–0.40	–0.41	–0.41	–0.41	–0.41	–0.41	–0.40	–0.40	–0.40	–0.40	–0.40	–0.40	–0.41	–0.41
H14	0.17	0.17	0.18	0.18	0.20	0.19	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20
C12	–0.09	–0.10	–0.10	–0.12	–0.11	–0.11	–0.11	–0.11	–0.11	–0.11	–0.11	–0.11	–0.11	–0.12	–0.12	–0.12	–0.12	–0.12	–0.12	–0.12
H12	0.09	0.09	0.09	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.11	0.11	0.11	0.10	0.10
C8	–0.14	–0.16	–0.17	–0.18	–0.21	–0.22	–0.23	–0.23	–0.23	–0.23	–0.23	–0.23	–0.24	–0.24	–0.24	–0.25	–0.25	–0.24	–0.25	–0.25
H8	0.10	0.11	0.11	0.12	0.13	0.14	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.16	0.16	0.16	0.16	0.16
C18	–0.13	–0.13	–0.15	–0.15	–0.16	–0.15	–0.15	–0.15	–0.15	–0.15	–0.16	–0.16	–0.16	–0.16	–0.16	–0.15	–0.16	–0.16	–0.16	–0.16
H18	0.09	0.09	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11
C16	–0.28	–0.28	–0.29	–0.28	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.29	–0.28	–0.28	–0.28	–0.28	–0.28	–0.28	–0.29	–0.28
H16	0.17	0.17	0.18	0.17	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18
C4	0.47	0.48	0.51	0.49	0.52	0.51	0.51	0.51	0.51	0.52	0.52	0.52	0.52	0.52	0.52	0.51	0.51	0.51	0.51	0.51
C6	0.13	0.13	0.13	0.14	0.14	0.14	0.15	0.15	0.15	0.15	0.15	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
C13	0.43	0.43	0.44	0.45	0.43	0.43	0.45	0.45	0.45	0.46	0.45	0.48	0.48	0.48	0.48	0.48	0.48	0.47	0.48	0.48
C17	0.01	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
H17	0.45	0.46	0.46	0.47	0.48	0.48	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.50	0.50	0.50

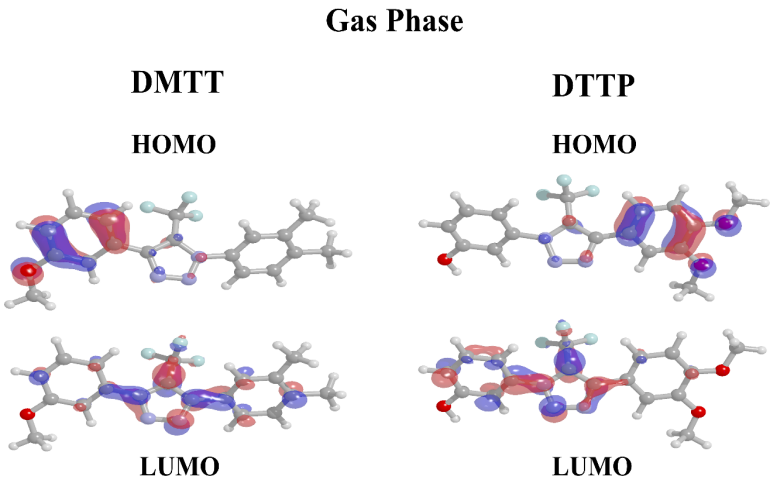

Figure S1. HOMO and LUMO of DMTT and DTTP structures in Gas Phase

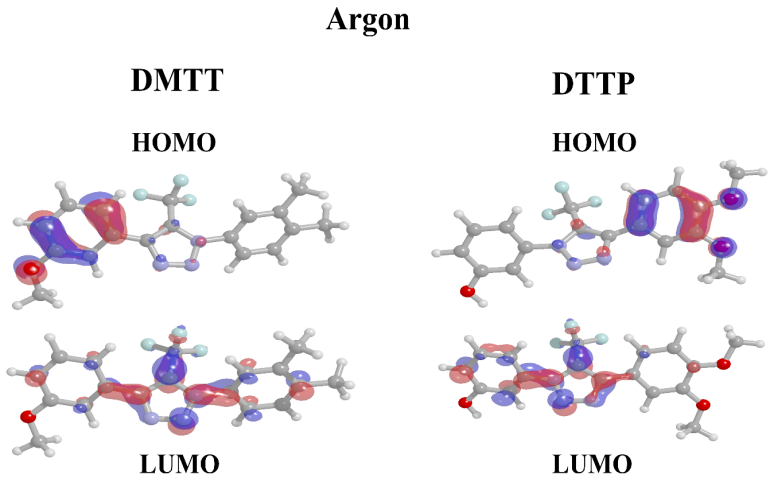

Figure S2. HOMO and LUMO of DMTT and DTTP structures in Argon

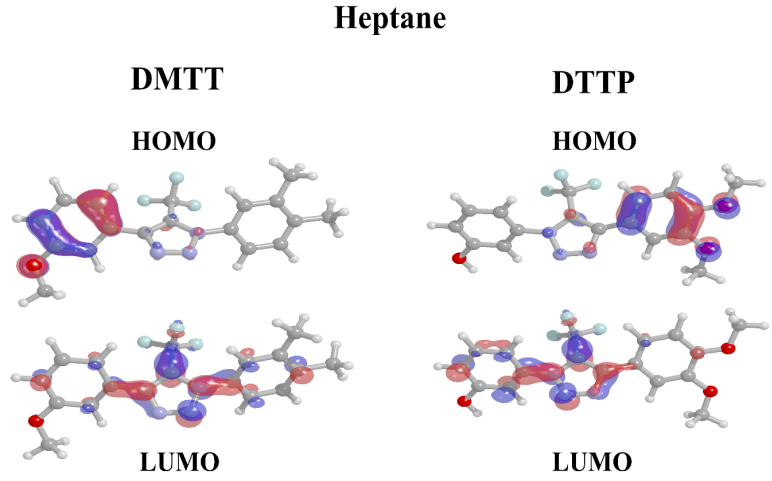

Figure S3. HOMO and LUMO of DMTT and DTTP structures in Heptane

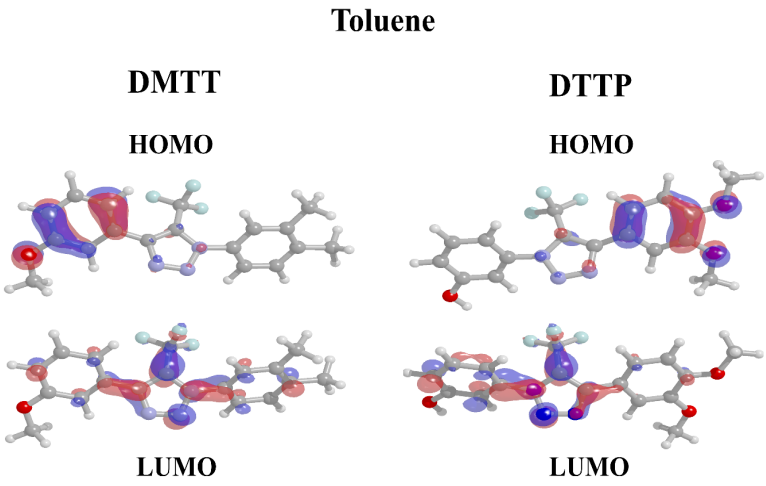

Figure S4. HOMO and LUMO of DMTT and DTTP structures in Toluene

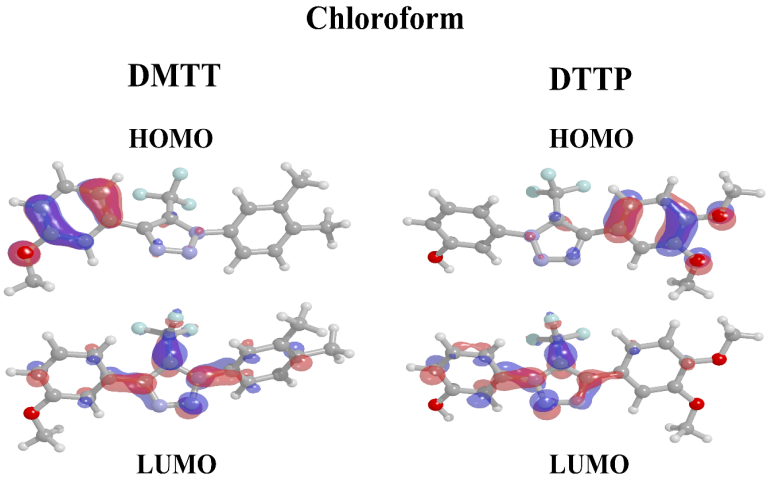

Figure S5. HOMO and LUMO of DMTT and DTTP structures in Chloroform

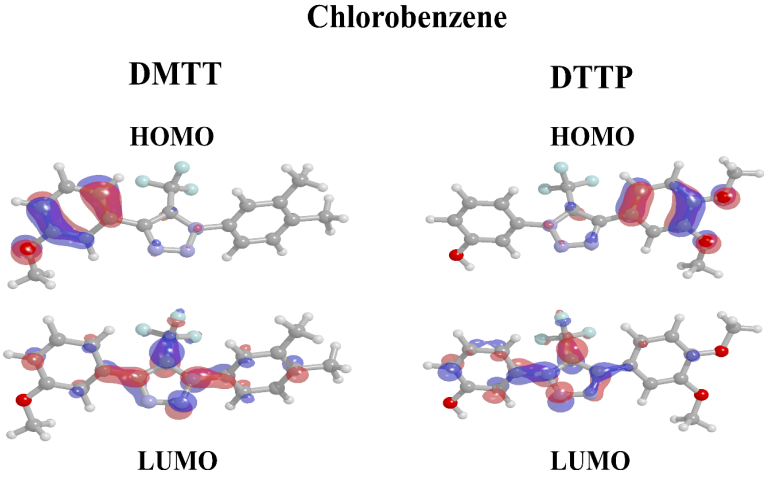

Figure S6. HOMO and LUMO of DMTT and DTTP structures in Chlorobenzene

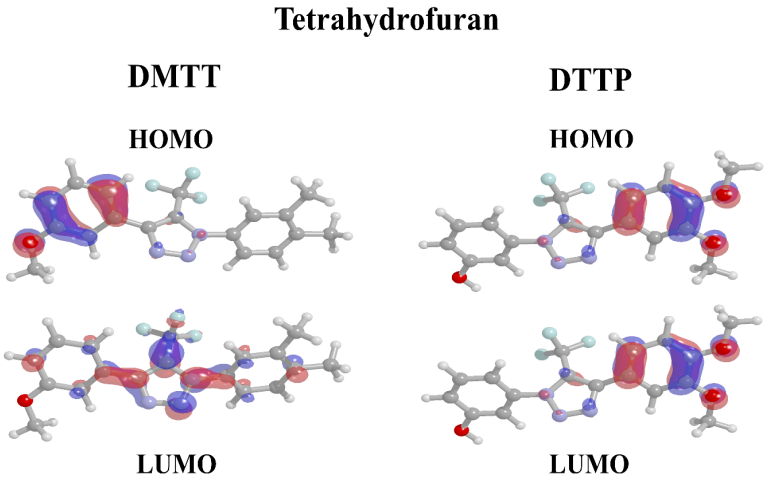

Figure S7. HOMO and LUMO of DMTT and DTTP structures in Tetrahydrofuran

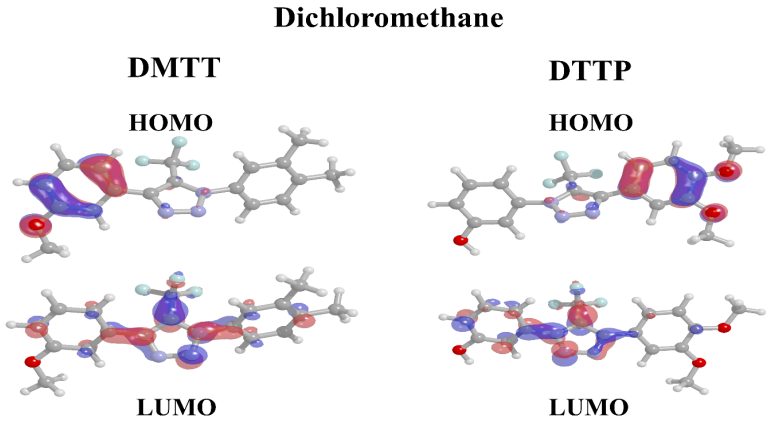

Figure S8. HOMO and LUMO of DMTT and DTTP structures in Dichloromethane

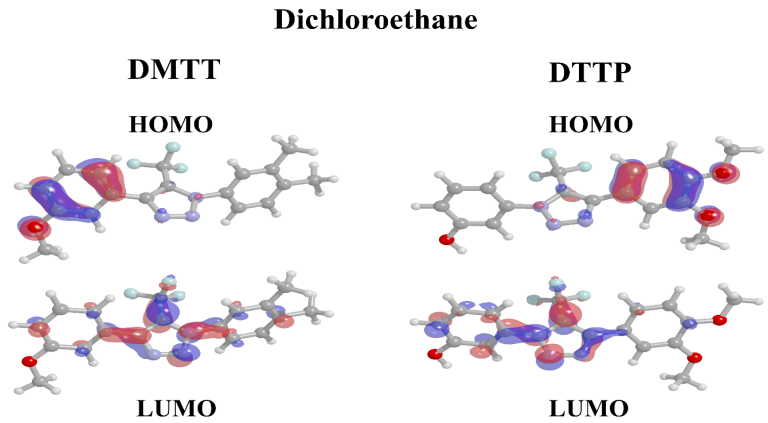

Figure S9. HOMO and LUMO of DMTT and DTTP structures in Dichloroethane

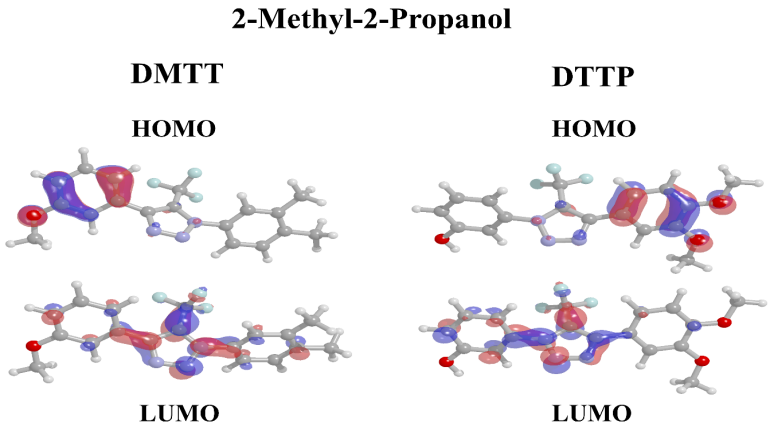

Figure S10. HOMO and LUMO of DMTT and DTTP structures in 2-Methyl-2-Propanol

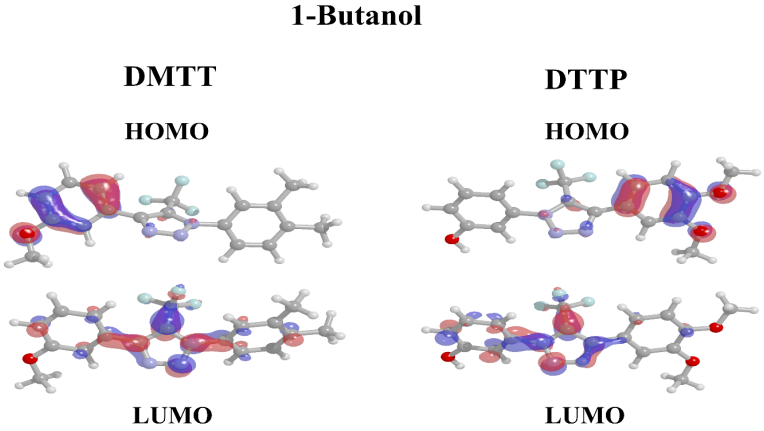

Figure S11. HOMO and LUMO of DMTT and DTTP structures in 1-Butanol

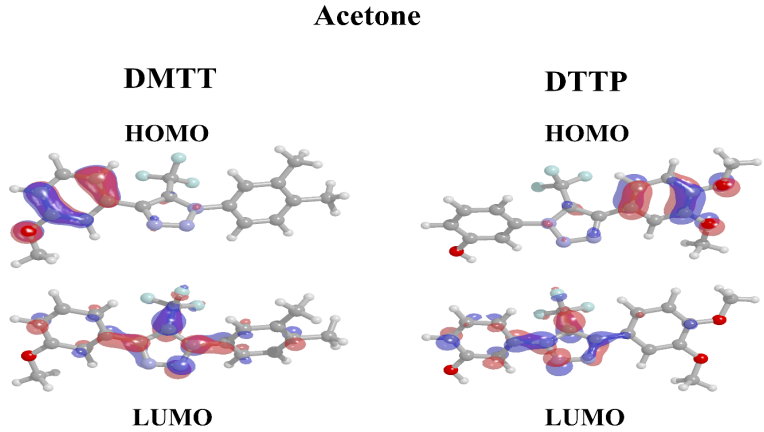

Figure S12. HOMO and LUMO of DMTT and DTTP structures in Acetone

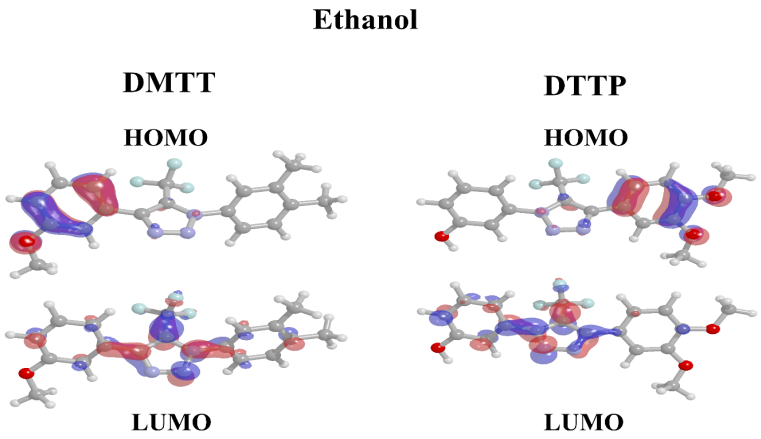

Figure S13. HOMO and LUMO of DMTT and DTTP structures in Ethanol

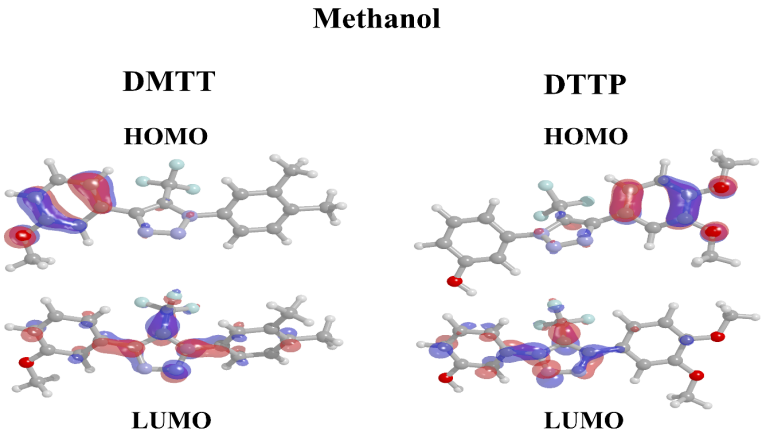

Figure S14. HOMO and LUMO of DMTT and DTTP structures in Methanol

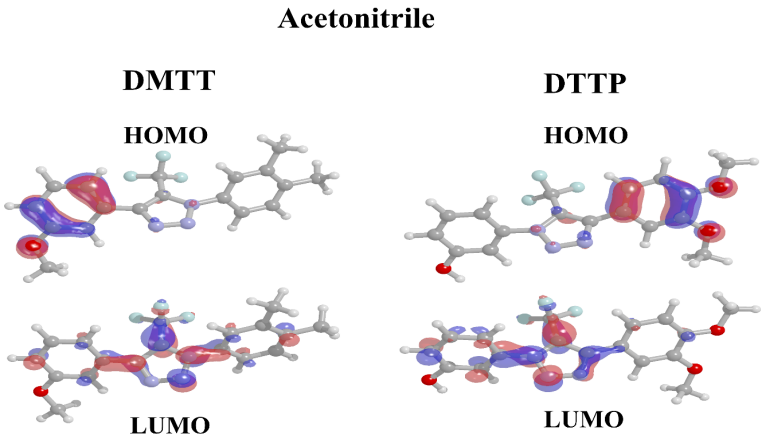

Figure S15. HOMO and LUMO of DMTT and DTTP structures in Acetonitrile

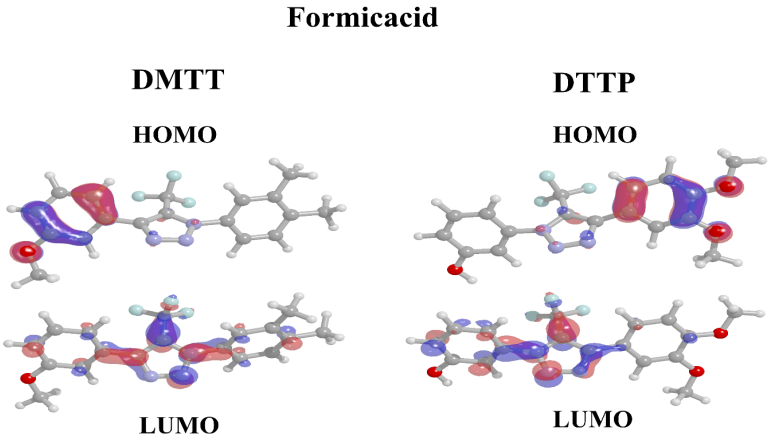

Figure S16. HOMO and LUMO of DMTT and DTTP structures in Formicacid

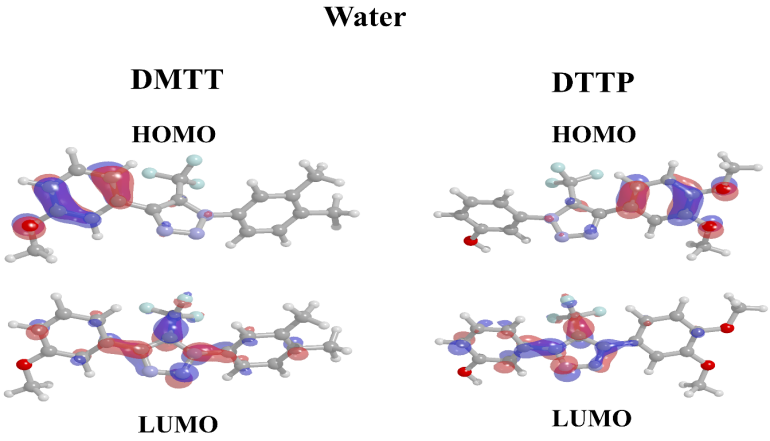

Figure S17. HOMO and LUMO of DMTT and DTTP structures in Water

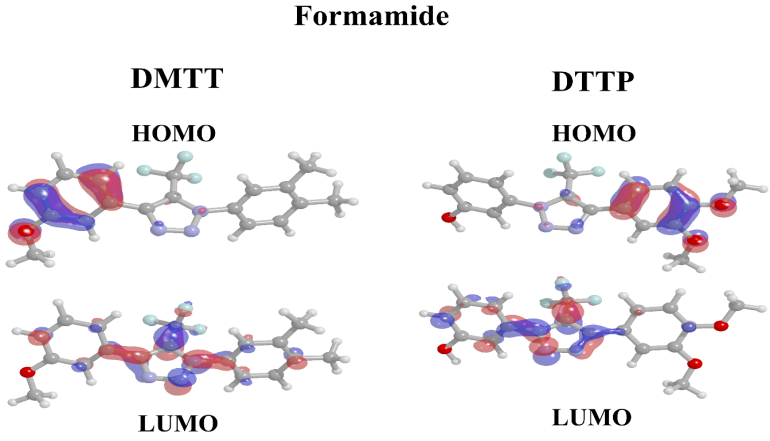

Figure S18. HOMO and LUMO of DMTT and DTTP structures in Formamide

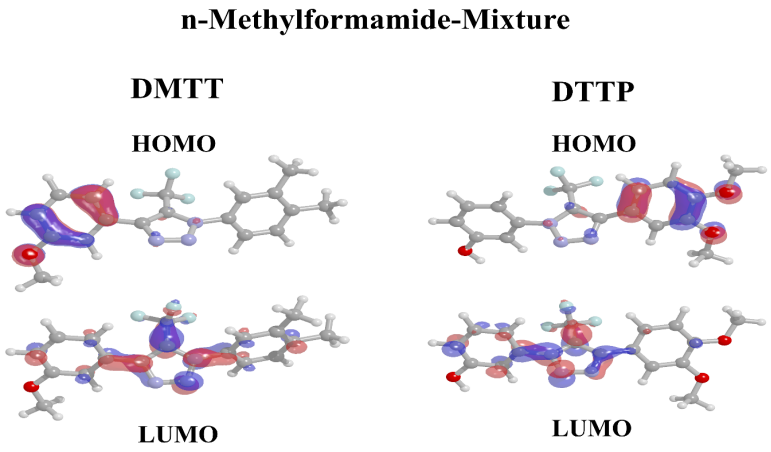

Figure S19. HOMO and LUMO of DMTT and DTTP structures in n-Methylformamide-Mixture

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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