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Developing Novel Charge Transfer Complexes: Synthesis, Characterization, and Optical Properties Examination

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ABSTRACT

In order to significantly enhance the applications of charge transfer complexes (CTCs) in electrical and optoelectronic fields, we have investigated the charge transfer (CT) interaction between organic donor molecules and molecular chloranil. Specifically, 1,1,4,4-Tetraphenyl-1,3-Butadiene (TPB) and 2,2,6,6-Tetramethylpiperidine-N-oxyl (TEMPO) were utilized as donor molecules and reacted with chloranil to form CTCs. The resulting compounds were analyzed using spectral techniques such as FT-IR, NMR and UV-Visible spectroscopy. These methods provided detailed insights into the structural and electronic properties of the CTCs. The CTCs obtained from these reactions were employed to measure band-gap and refractive index values, key parameters in determining the suitability of materials for optoelectronic devices. The observed values indicate that the studied CTCs exhibit promising characteristics for potential applications in optoelectronic technologies, such as in the development of advanced sensors, photovoltaic cells, and light-emitting diodes.

Keywords: Charge transfer complexes, chloranil, TEMPO, TPB, Optoelectronic

1. INTRODUCTION

The synthesis and characterization of novel charge-transfer complexes have been extensively explored in recent studies. Various methods have been employed to create these complexes, such as reacting quinones with specific compounds in defined mole ratios, resulting in unique charge-transfer complex compounds with good yields [1, 2]. Techniques like UV-Vis, FTIR, and NMR have been utilized to characterize these compounds, confirming their proposed chemical structures. Additionally, the molecular structures of these complexes have been investigated using density functional theory, providing insights into their stability and reactivity [3, 4]. Optical properties of charge-transfer complexes have been examined through UV-Vis spectroscopy, revealing interactions between electron donors and acceptors, as well as their potential applications in areas like medicinal chemistry and fluorescence labeling [5]. These studies collectively contribute to the understanding and potential utilization of charge-transfer complexes in various scientific fields.

The compound entitled, selenadiazobenzophenone in acetonitrile, was characterized using UV-Vis, FT-IR, ¹H-NMR and ¹³C-NMR spectroscopy, and their molecular structures were investigated using density functional theory (DFT) [1]. The study revealed that the donor-acceptor systems had higher reactivity and stability compared to other systems, as well as larger average polarizability, which is crucial for determining the physical characteristics of donor-bridge-acceptor systems [1].

In another study, Mohammed et al. have explored the synthesis of CTCs derived from N-phenyl-3,4-selenadiazobenzophenone imine [2]. The compounds were characterized by UV, IR, and NMR techniques, and their molecular geometries were optimized using DFT. The study found that the synthesized CTCs had lower electronegativity, ionization potential, electron affinity, and electrophilicity, indicating their potential application in various chemical processes.

Nampally et al. have investigated the interaction between O-phenylenediamine and 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ) using UV-vis spectroscopy [3].

The stoichiometry of the CTC was determined to be 1:1, and the formation constant and molar extinction coefficient was calculated. The stability of the synthesized CTC was confirmed through various spectroscopic parameters. The biological evaluation showed notable antibacterial activity, suggesting potential applications as bioactive drugs [3].

Yang et al. have synthesized two novel coumarin derivatives and corresponding europium complexes, which exhibited excellent aggregation-induced emission (AIE) properties [4]. The study highlighted the significant fluorescence enhancement due to electron-donating groups in the ligands. The complexes also demonstrated extreme thermal stability and suitable electrochemical properties, making them promising candidates for applications in fluorescence labeling and medicinal chemistry [4].

Issa et al. synthesized and characterized CT complexes of pyrazine Schiff bases with aromatic nitro compounds [5]. Theoretical studies using DFT and TD-DFT supported the experimental findings, showing the stability and existence of CT interactions within the

complexes. The study indicated that these complexes have potential applications in non-linear optical (NLO) materials due to their small energy gaps and significant intramolecular CT effects [5]. Basuroy et al. explored the photo-induced intramolecular charge transfer (ICT) processes in conformational polymorphic crystals of a donor-bridge-acceptor dyad [6]. Time-resolved X-ray diffraction measurements indicated different ICT state lifetimes for the thermodynamic and kinetic forms of the dyad, suggesting that these materials could be used in the design of solid-state optoelectronic materials [6].

Chen et al. developed high-performance small-molecular acceptors (SMAs) for polymer solar cells (PSCs) [7]. The study focused on a simple and eco-friendly device fabrication procedure that could be crucial for scalable production. The findings demonstrated the potential of these SMAs in enhancing the efficiency and scalability of PSCs. Dongala et al. employed a spectrophotometric method to study the CTC of chloranil with 6-(trifluoromethyl)furo[2,3-b]pyridine-2-carbohydrazide derivatives [8]. The formation of colored CTCs was confirmed by UV-Vis spectroscopy, ¹H-NMR, and IR spectral analysis, suggesting potential applications in photochemical processes [8].

Ashok et al. have studied the thermal degradation kinetics and temperature-dependent electrical conductivity of CTCs of phenothiazine with chloranil and picric acid [9]. The complexes exhibited semiconducting behavior, with activation energies indicating their potential use in electronic applications [9]. Buldurun synthesized and characterized Schiff base ligands and their Co(II) and Pd(II) complexes [10]. The optical properties of these complexes were studied in various solvents, revealing their suitability for use in diodes due to appropriate optical properties [10]. Takaki et al. synthesized and characterized stereoisomers of homoleptic dipyrinatoplatinum(II) complexes with arylborane charge-transfer substituents. The complexes exhibited intense absorption and broad emission spectra, indicating potential applications in photophysical studies [11].

Inspired by these research reports [1-16] demonstrating the formation of intriguing charge-transfer complexes (CTCs) between organic molecules and acceptors, this study focuses on exploring similar interactions. We aim to investigate CT interactions between organic donor molecules and the well-established acceptor molecule, chloranil.

Our research approach involves synthesizing CTCs using TEMPO and TPB as donor molecules and chloranil as the acceptor. We then employ various characterization techniques, including FT-IR, ¹H-NMR, and ¹³C-NMR spectroscopy, to confirm the formation and structure of the synthesized CTCs. Additionally; we analyze the band-gap of the prepared CTCs to gain further insights into their optoelectronic properties.

2. EXPERIMENTAL

2.1. Materials

The research prioritized the use of exceptionally pure chemicals (analytical grade) obtained from commercial sources. These chemicals, including TPB (1,1,4,4-tetraphenyl-1,3-butadiene, CAS No. 1450-63-1), TEMPO (2,2,6,6-tetramethylpiperidinoxy, CAS No. 2564-83-2), chloranil (CAS No. 118-75-2), DMSO (dimethyl sulfoxide, with a minimum purity of 99%), and DCM (dichloromethane, with a minimum purity of 99.8%), were used in the study without further purification. Loba Chemicals Pvt. Ltd. (Mumbai, India) is one example of a supplier that provided these high-purity chemicals.

2. 2. Preparation of CTCs

This research investigated the formation of charge-transfer complexes (CTCs) between solid donors and acceptors. The experiment involved grinding a mixture of a donor and chloranil (acceptor) on a clean, dry porcelain mortar. Two CTCs were synthesized: CTC1 with TPB (donor) and CTC2 with TEMPO (donor). The mass ratios used were 0.1 g of donor to 0.411 g of chloranil for CTC1 and 0.1 g of donor to 0.944 g of chloranil for CTC2.

In both cases, grinding the starting materials resulted in the formation of a new color, indicating a possible interaction. To verify this interaction, a small portion of the resulting product from each mixture was dissolved in dichloromethane (DCM) solvent. Ultraviolet-visible (UV-Vis) absorption spectroscopy was then performed on these solutions. The obtained spectra provided further evidence supporting the formation of complexes due to charge-transfer interactions.

2. 3. Instrumentation

The synthesized CTC samples underwent characterization using various instrumental methods. Ultraviolet-Visible (UV-Vis) absorption and diffuse reflectance spectroscopy (UV-DRS) were performed on a Shimadzu Spectrometer Model 2450 (UK) using 1 cm path length quartz cells within a wavelength range of 200-800 nm. Fourier-Transform Infrared (FT-IR) analysis was conducted using the KBr pellet method on a Shimadzu Model 8400S spectrometer (USA) to obtain spectra in the range of 400-4000 cm^{-1} . Finally, Proton-Nuclear Magnetic Resonance ($^1\text{H-NMR}$ and $^{13}\text{C-NMR}$) spectroscopy was carried out on a Bruker Avance IIITM HD 400 MHz spectrometer (Bruker Corporation, USA) using CDCl_3 solvent. Tetramethyl silane (TMS) was employed as the internal standard for the NMR measurements.

3. RESULTS & DISCUSSION

The solid-solid interaction between iodine and both donor molecules was achieved by grinding 3.83 mmol of chloranil with 0.27 mmol TPB and 1.67 mmol of chloranil with 0.64 mmol of TEMPO in a porcelain mortar. The resultant solid CTCs are seen in the **Figure 1**. The color change started even before the powders were ground together, likely when the iodine crystals first touched the surface of organic donors and thus, it reflects the strong donating property of TPB and TEMPO. As such, two CTCs were formed using the solid-solid approach and noted as CTC1 (TPB + chloranil) and CTC2 (TEMPO + chloranil).

3. 1. Analysis for structural elucidation

The prepared CTCs have been analyzed for spectral measurement using FT-ATR and ^1H - and $^{13}\text{C-NMR}$ spectroscopy. The obtained spectral information reveals the formation of CT interaction between used donors and acceptor molecules.

3. 1. 1. FT-ATR Infrared Spectra

In the charge transfer interaction, an electron from the HOMO of the electron-rich donor is excited and transferred to the LUMO of the electron-deficient acceptor, which produces optical adsorption band known as charge transfer band [17, 18]. Therefore, infrared

spectroscopy study of the CTCs led to an understanding of electronic conduction on the basis of the relation between the light absorption coefficient and electronic conductivity.

FT-ATR spectroscopy is a simple, surface sensitive and fast technique to confirm the formation CTC in the range 400-4000 cm^{-1} . The experimental data and theoretical information are assembled in **Tables 1** and **2**, and the spectral graphs are presented in Appendix.

3. 1. 2. NMR Spectra

The researchers examined the $^1\text{H-NMR}$ spectra of both CTCs in CDCl_3 solvent. The observed peaks differed significantly between the free molecules (individual starting materials) and the complexed samples (the synthesized CTCs). This suggests a change in electron density around the elements within the molecules due to complexation and the formation of charge-transfer (CT) interactions. Notably, the $^1\text{H-NMR}$ spectra of both CTCs exhibited a slight shift in the chemical shift (δ) values compared to the free molecules.

Spectral data (TPB + chloranil): $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 7.464, 7.447, 7.429, 7.409, 7.405 (m, 6H, a phenyl ring), 7.391, 7.383, 7.372, 7.357, 7.353 (m, 4H, b phenyl ring), 7.337, 7.285, 7.275, 7.262. $^{13}\text{C-NMR}$ (500 MHz, CDCl_3): 144.04, 142.50, 140.83, 139.88, 130.74, 128.27, 128.17, 127.76, 127.54, 127.40, 126.04, 77.37, 77.05, 76.74.

3. 1. 3. UV-Visible Spectra

Employing UV-Visible spectroscopy, researchers successfully confirmed the formation of charge-transfer (CT) interactions within the synthesized CTCs. A detailed analysis of the resulting spectra, presented in **Figures 4** and **5**, revealed a new, broader band for CTC1 (TPB + Chloranil) at a significantly lower wavelength ($\lambda = 327$ nm) compared to the free TPB molecule that shows a broad peak at ~ 348 nm. Similarly, for CTC2 (TEMPO + Chloranil), the characteristic peak at $\lambda = 283$ nm corresponding formation of CT and also found to be shifted compared to free TEMPO. These spectral changes strongly suggest that CT interactions altered the electronic environment of the molecules within the formation of complexes.

3. 1. 4. UV-diffuse reflectance spectra (UV-DRS)

Optical Properties and Band Gap Analysis:

UV-diffuse reflectance spectroscopy (UV-DRS) was employed to investigate the optical properties of the synthesized CTCs. The reflectance spectra were recorded across a wavelength range of 200-1400 nm. To determine the band gaps of the CTCs, Tauc plots were generated by plotting $(\alpha h\nu)^2$ versus photon energy ($h\nu$) (**Figures 6** and **7**). The band gap values were estimated by extrapolating the linear portion of the plots corresponding to the fundamental absorption edge. This analysis revealed a range of possible band gaps between 1.50 and 1.90 eV. The actual measured band gap values for CTC1 and CTC2 were approximately 2.42 eV and 2.36 eV, respectively.

3. 1. 5. Refractive index

By using the obtained band-gap values from the UV-DRS spectra, a theoretical refractive index determination has been performed. The optical efficiency these molecular systems depend on the efficiency of electronic communication between electron accepting and donating groups playing a key role in identifying the intramolecular charge. It could be determined that

the relation between α and refractive index which shows the polarization of the compounds through the electromagnetic field of the light.

The electronegativity is related to the refractive index; therefore the constants in Reddy's relation should be reshaped in the form of the electronegativity that gives a physical meaning of Raddy's constants [19-21].

The refractive index of the CTCs is obtained from the following different relations such as Moss and Ravindra equation (1 and 2), Modified Herve and Vandamme relation and Based on the oscillatory theory (3 and 4) [21]. Based on the oscillatory assumption, where the UV resonance energy occurs at a constant difference with band-gap energy, Herve et al. have proposed a relation for the static/optical refractive index as a function of the energy band-gap (See 3) [22].

(See 3) [31].

$$n^4 E_g = K \quad (1)$$

$$n = 4.084 - 0.62 (E_g) \quad (2)$$

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2} \quad (3)$$

$$n = \sqrt{1 + \left(\frac{A}{(\Delta\chi^*)(E_g) + B}\right)^2} \quad (4)$$

where, n = refractive index, and E_g = Band-gap, $\Delta\chi^*$ = optical electronegativity, A and B are constants ($A = 13.6$ and $B = 3.4$), K = constant = 95, it does not refer to any physical meaning or quantity, which is considered a disadvantage in the Moss' relation.

Refractive indices and their corresponding band-gaps were collected for the prepared CTCs, as shown in **Table 3**. It shows that Reddy's and Harve's relations have similar behavior indicates a perfect agreement for both CTCs can be used as optoelectronic materials.

Therefore, it was aim to correlate the optical refractive index to the energy band-gap using the mentioned relations.

4. CONCLUSION

In the present endeavor, we have demonstrated formation of charge transfer complexes (CTCs) by using organic donors and molecular iodine as effective acceptors. The formed both complexes, CTC1 (TPB + chloranil) and CTC2 (TEMPO + chloranil) were found to be stable. The spectral analysis supports the existing of charge transfer interaction between donors and acceptor molecules.

The measured band-gap values as lower range can be used as photo responding materials. Further, the theoretically calculated refractive index values also indicate the use of these CTCs in the fields of optoelectronics. However, additional investigation and characterization would reveal more interesting aspect of these CTCs.

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CRediT authorship contribution statement

Dhaval Khant: Investigation, Conceptualization, Methodology.

Tarun Parangi: Writing – original draft, review & editing.

Vishal Jain: Supervision, Project administration, Investigation

Salman Zabha: Resources

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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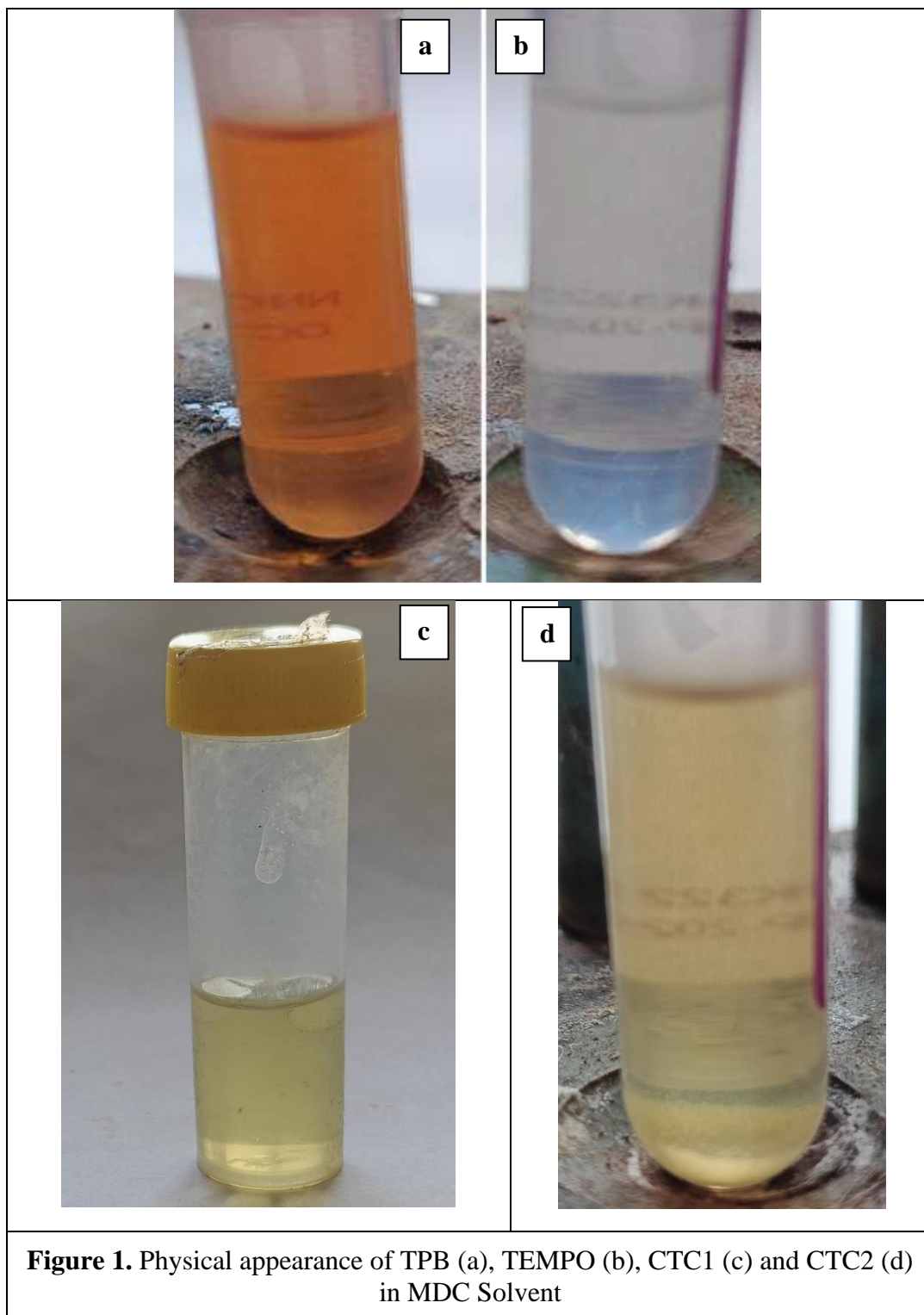
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Appendix

FIGURE CAPTIONS



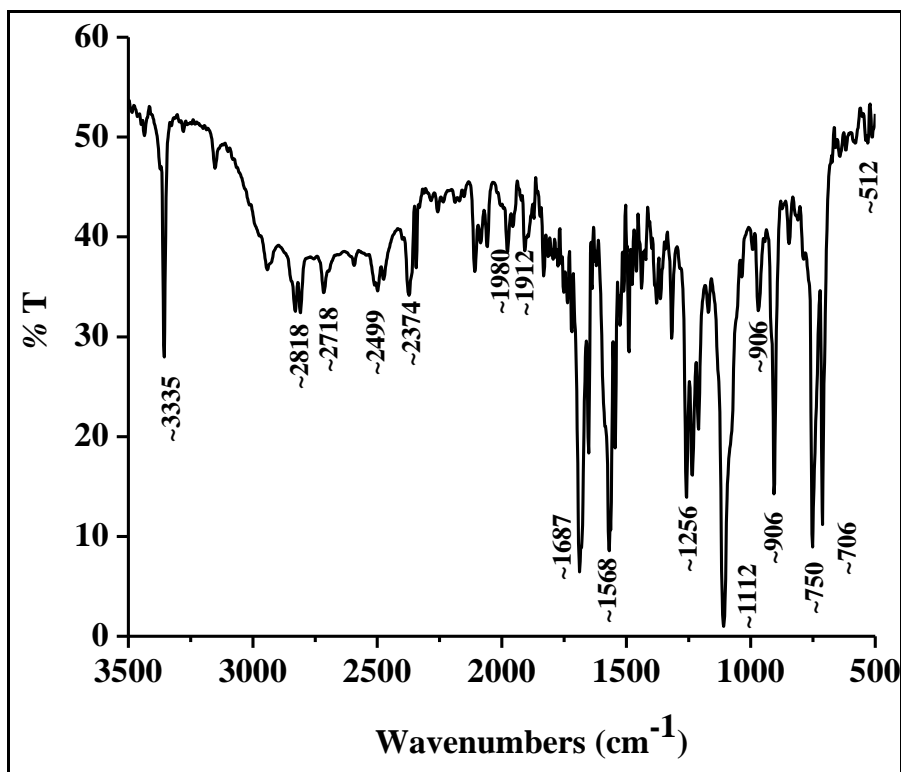


Figure 2. FT-IR spectrum of TPB + chloranil (CTC1)

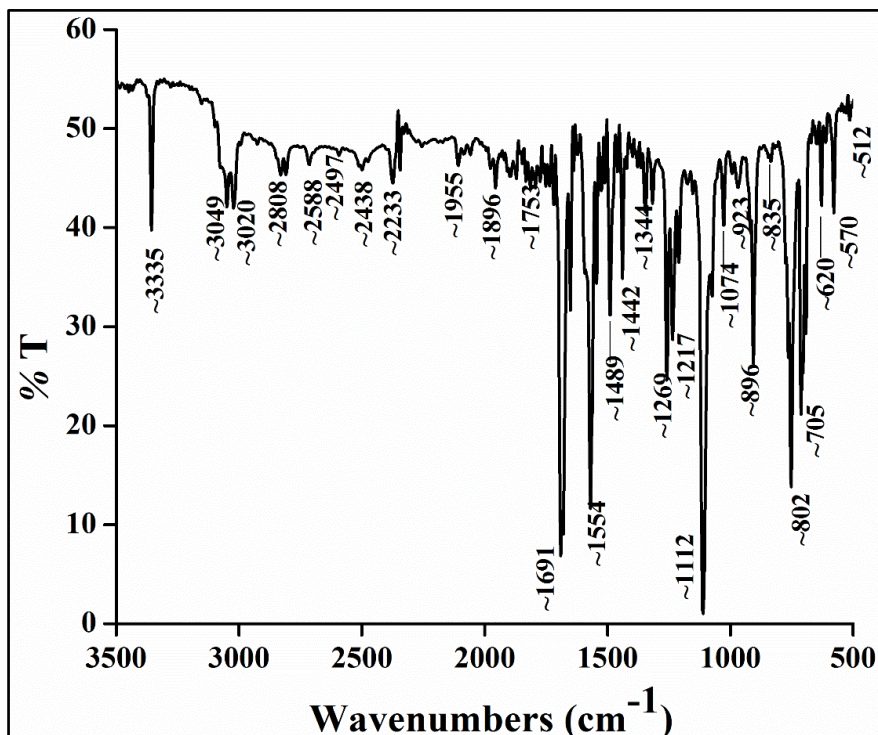


Figure 3. FT-IR spectrum of TEMPO + chloranil (CTC2)

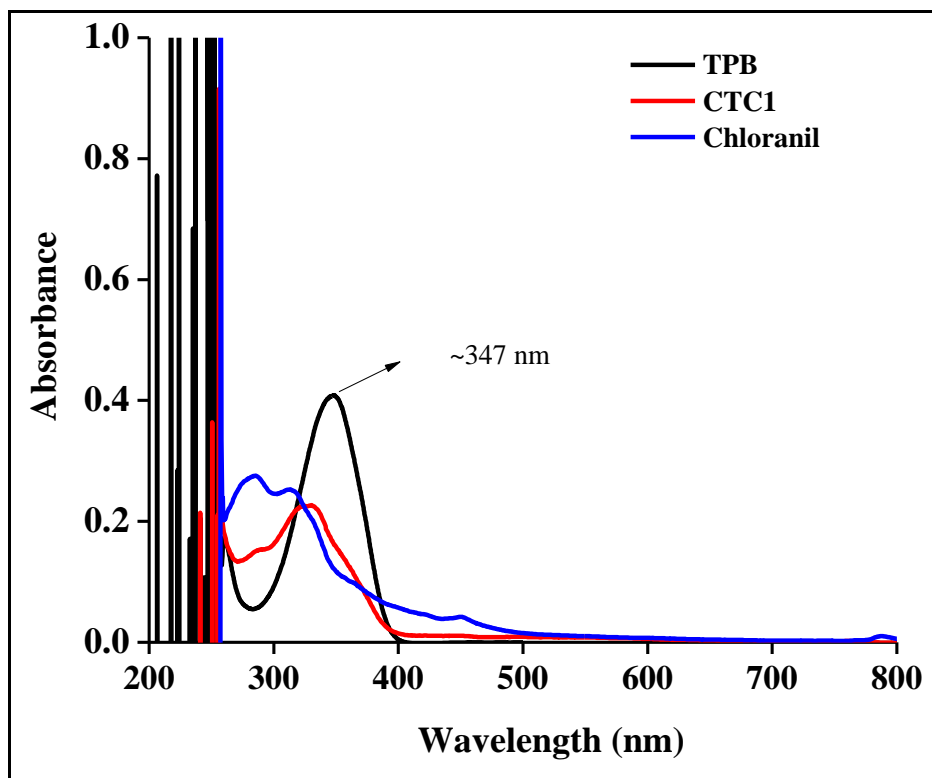


Figure 4. UV-visible spectra of TPB, chloranil and CTC1 complex in DMSO solvent

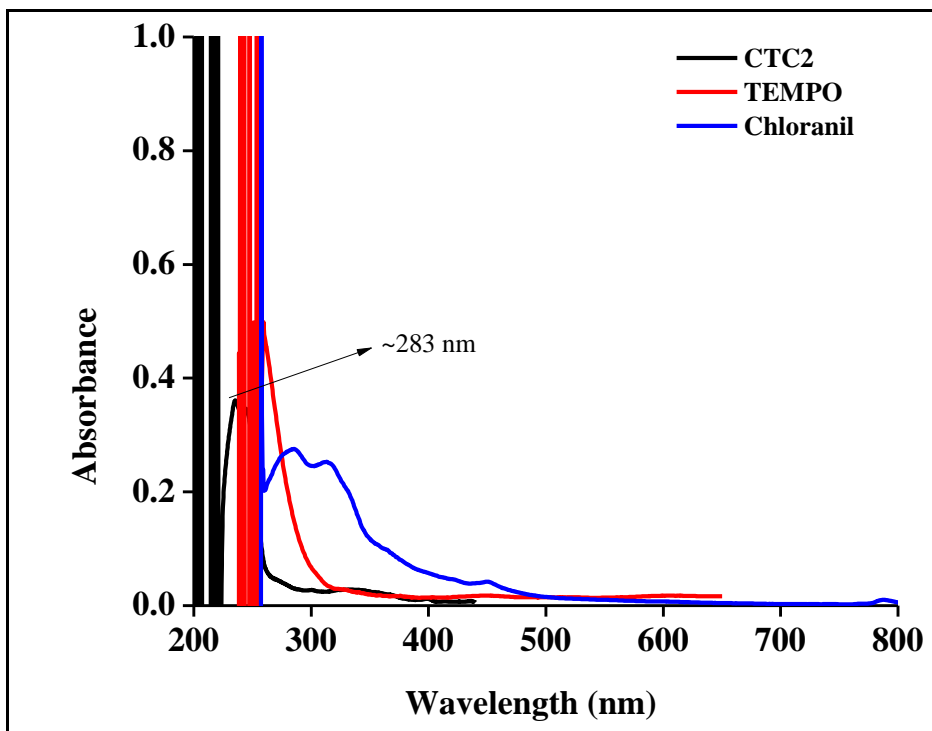


Figure 5. UV-visible spectra of TEMPO, chloranil and CTC2 complex in DMSO solvent

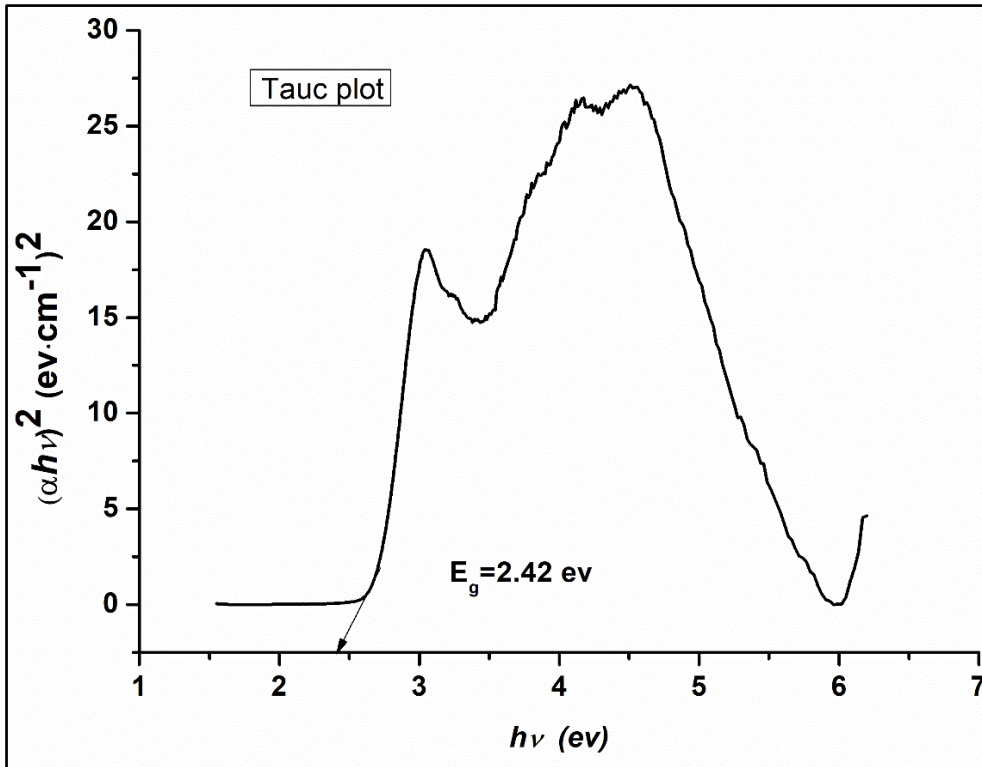


Figure 6. Tauc plot for CTC1

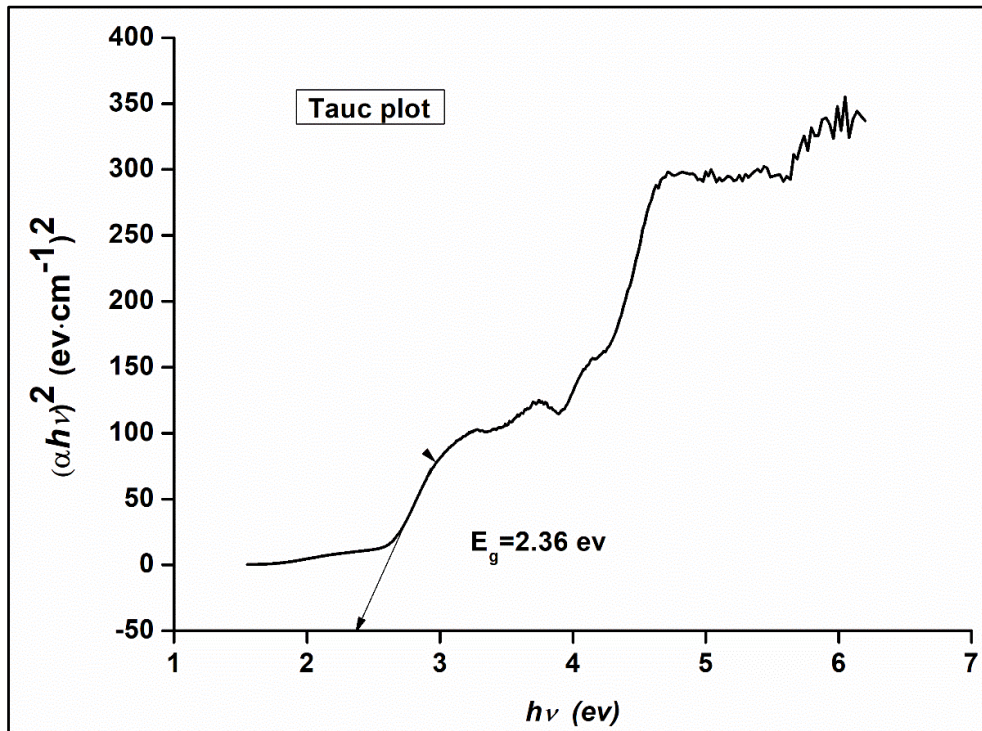


Figure 7. Tauc plot for CTC2

Captions to Table(s)

Table 1. FT-IR Spectral Information of TPB + chloranil (CTC1)

Peak value (cm ⁻¹)			Band Assignment
TPB	Chloranil	CTC1	
		802.39	C-H bending in phenyl ring
833.25		835.18	C-H bending in phenyl ring
		896.9	C-H bending in phenyl ring
902.69	907	923.9	C-Cl Stretching
1072.42		1074.35	C-H bending in phenyl ring
	1115	1114.86	C-H bending in phenyl ring
		1174.65	C-O stretching in tertiary alcohol
1230.58	1210	1217.08	C-H bending in alkenes
	1260	1269.16	C-O stretching in alkyl aryl ether
1344.38		1344.38	C=C stretching aromatic ring
		1554.63	C=C stretching aromatic ring
1595.13	1571	1595.13	C=C Stretching in Aromatic Ring
	1666	1674.21	C=O Stretching in Quinone Carbonyl
		1753.29	C=O Stretching in anhydride
		1896.03	C-H bending in aromatic compound
		1955.82	C=C=C stretching in allene
		2065.76	C=C=C stretching in allene
		2102.41	C≡C stretching in alkyne
		2164.13	S-C≡N stretching in thiocyanate
		2233.57	C≡N Stretching in nitrile
		2588.47	S-H stretching in thiol
		2692.63	C-H stretching in Aldehyde
		2723.49	C-H stretching in alkanes
		2750.49	C-H stretching in alkanes
		2939.52	C-H stretching in alkanes
3020.53		3020.53	C-H stretching aromatic ring
		3049.46	C-H stretching aromatic ring
		3327.21	N-H stretching in aliphatic primary amine
	3368	3342.64	N-H stretching in aliphatic primary amine

Table 2. FT-IR Spectral Information of TEMPO + chloranil (CTC2)

TEMPO	Peak value (cm ⁻¹)		Band assignment
	chloranil	CTC2	
532		514.99	C-H bending of CH ₂
722	713	719.45	C-Cl Stretching
859.4		894.97	C-Cl stretching
933.1	907	931.62	C-Cl Stretching
1060.2		1055.06	C-Cl stretching
1131.2		1174.65	C-O stretching
		1197.79	C-Cl stretching
1215.15	1210	1215.15	C-H bending
1242.1	1260	1267.23	C-H bending
1466.2		1460.11	N-O stretching
	1491	1479.4	NO ₂ stretching Nitro compound
		1525.69	NO ₂ stretching Nitro compound
	1571	1554.63	C=C Stretching in Aromatic Ring
1620	1666	1674.21	C=O Stretching in Quinone Carbonyl
		2166.06	C=C Stretching
		2223.92	C≡N stretching in nitriles
		2372.44	C-H bending
		2474.67	C-H bending
		2519.03	O-H stretching carboxylic Acids
		2584.61	O-H stretching carboxylic Acids
2721.2		2723.49	C-H stretching of aldehydes
		2767.85	C-H stretching of aldehydes
2855.6		2873.94	C-H Stretching
2958.4		2943.37	C-H stretching of Methyl
		3014.74	C-H stretching in Alkenes

Table 3. Values of Refractive index for CTC1 and CTC2

Methods	REFRACTIVE INDEX	
	CTC1	CTC2
Moss Equation	2.250	2.51
Ravindra Equation	2.58	2.61
Based on the oscillatory theory	2.54	2.56
Reddy et al. equation (Modified Herve and Vandamme relation)	2.54	2.56
Optical electronegativity	0.65	0.63
Band-gap	2.42	2.36