6-Alkyl Substituted Triazine-based Organic Molecules for Energy Harvesting Application

Vishnu Kanse[1], Vaijayanti Ghase[2], Vishwanath R. Patil[3], Rama S. Lokhande[4]

[1,4]Department of Chemistry, School of Basic Sciences, Jaipur National University, Jaipur-302017, India
[2]Department of Polymer Science, S K Somaiya College, Somaiya Vidyavihar University, Mumbai-400077, India
[3]Department of Chemistry, University of Mumbai, Santacruz (E), Mumbai-400 098, India

Abstract:

During the past 20 years, fluorescent materials have had a significant impact on modern cultures' technological advancements. Utilizing the advantageous qualities of these materials, a wide range of applications have been created, from organic photovoltaic to OLED TVs, from extremely sensitive early disease detection techniques to the sensing of environmental contaminants. For energy harvesting applications, the most crucial characteristic of organic molecules is their band gap. Differentially, we produced 4,4'-((6-alkyl-1,3,5-triazine-2,4-diyl)bis(azanediyl)) diphenol based organic molecule in this research. This molecule may be employed in organic electronics, such as solar cells and OLEDs, after further processing. UV-Visible spectroscopy was used to determine the energy gap of the synthesized new analogue.

Keywords: Triazine, Fluorescence, UV-Visible Spectroscopy, Thermal Study.

1. Introduction:

Over the past 20 years, organic materials have received a lot of interest for usage in electrical applications. Significant advancements in this area throughout time have made it possible for organic materials to be widely used in a variety of current applications, including xerographic and display technologies [1]. The development of potentially helpful technologies like field effect transistors and solar cells has been influenced by electronic organic materials.

They have also been used as emitting material for various LEDs, including OLEDs (Organic Lighting Emitting Diodes), PLEDs (Polymer Lighting Emitting Diodes), and inorganic based White LEDs [4, 5], as well as photovoltaics [6].

1,3,5-triazines, six-membered aromatic heterocyclic nitrogen derivatives, were among the first known organic compounds. Some of their derivative chemicals have been known for over 150 years. They are currently simply referred to as triazines. Originally, they were known as symmetrical triazines, abbreviated as s- or sym-triazines. Cyanuric chloride is one of the most important non-systematically named 1,3,5-triazines; it is the precursor of cyanuric acid, melamine, and triazines [7,8].

Because of their remarkable characteristics related to their high structural symmetry and strong electron-donor feature, 1,3,5 triazine derivatives—hereafter referred to as triazine—have emerged as one of the mo

st promising molecules among the many options found in organic compounds [9].

Additionally, they exhibit significant chemical stability in the face of high temperatures and light exposure—a quality that is essential for lighting applications [10]. Triazine-based materials have been used recently for CO_2 absorption as well as in several of the optoelectronic applications already described [11, 12].

The ability to adjust and modify the physical and chemical properties of these molecules based on the triazine core's decorative terminal structure is one of their most intriguing qualities [13]. In fact, the strength of the donor-acceptor interactions determines a lot of an organic compound's physical characteristics. Because organic compounds are π-electron-deficient aromatic systems, triazine reactivity is widely promoted, which makes it easier to form a variety of triazine-based compounds [14, 15].

In this study, we prepared different derivatives of 1,3,5-triazine by replacing one, chloride ions of cyanuric chloride with different alkyl chain (including methyl, ethyl, cyclohexyl) and evaluated their thermal, and optical study.

2. Experimental section
2.1 Material and Methods-
SD Fine and Sigma Aldrich were the suppliers of the necessary A.R. Grade chemicals. All synthetic activities were carried out in a nitrogen environment.

2.2 Instrumentation-
All the produced compounds were analyzed in ^1H and ^{13}C using a Bruker NMR (300 MHz) spectrometer. To ascertain the molecular weights of the substances, Shimadzu LCMS (Nexera UPLC+ LCMS-2020) were employed. Analysis using Thin Layer Chromatography was done to verify the compound's purity on plates covered with silica gel G (Merck). Bruker-XRD (2'nd Gen, D2, Phaser) was used to record the X-ray diffractograms. To capture UV spectra, the Shimadzu UV-2100 spectrophotometer was utilized. Using micro analytical methods, the elemental analysis of produced substances was carried out using EuroVector EA 3000 equipment. Instruments Perkin-Elmer LS55 The glow of light A spectrometer with a 200–800 nm wavelength range was utilized to examine the behavior of substances that exhibit photoluminescence. The SEM model Quanta (Make-FEI, Netherlands) was used to study morphology.

2.3 Synthesis of compounds
2.3.1. General procedure for Synthesis of compounds [2,4-dichloro-6-alkyl-1,3,5-triazine]
In a dried round-bottom flask under Nitrogen, Cyanuric chloride (5 g, 27.11 mmol, 1 eq.) was dissolved in 50 ml of anhydrous dichloromethane. The mixture was cooled to –10 °C with stirring. A solution of Grignard reagent alkyl-magnesium bromide in THF was added slowly. After addition, the reaction mixture was agitated for one hour at the same temperature (-10 °C). The temperature was gradually increased to room temperature and stirring maintained for another 5 hours. The completion of the reaction was monitored by TLC (Silica gel, DCM: Hexane system). The reaction was stopped by adding 50 mL of Sat. NH_4Cl solution. The separated organic phase was washed with 50 mL of water and dried with Na_2SO_4. The organic layer was evaporated using a rotary evaporator to produce crude material in the form of colourless oil. Due to instability of the material observed, it is immediately proceeded to the next step as there is a chance of partial hydrolysis during aqueous workup.

2.3.1.1. Synthesis of 2,4-dichloro-6-methyl-1,3,5-triazine [MeTz]
The same procedure using 1.5 M Methyl-magnesium bromide (18 ml, 27.11 mmol, 1eq) was used to afford

colourless oil with 68 % yield.

2.3.1.2. Synthesis of 2,4-dichloro-6-ethyl-1,3,5-triazine [EtTz]

The same procedure using 1 M Ethyl-magnesium bromide (27 ml, 27.08 mmol, 1eq) was used to afford colourless oil with 75 % yield.

2.3.1.3 Synthesis of 2,4-dichloro-6-cyclohexyl-1,3,5-triazine [CyHTz]

The same procedure using 1 M Cyclohexyl magnesium bromide (27 ml, 27.11 mmol, 1eq) was used to afford colourless oil with 78 % yield.

2.3.2. General procedure for synthesis of 4,4'-((6-alkyl-1,3,5-triazine-2,4-diyl) bis(azanediyl)) diphenol

Due to instability, crude product from the first step (2,4-dichloro-6-alkyl-1,3,5-triazine, 38.42 mmol, 1 eq.) was suspended in 60 mL of acetone in a round-bottom flask. The suspension was cooled to 0°C with vigorous stirring. At 0°C, 80 ml of $NaHCO_3$ solution (6.45 g, 76.78 mmol, 2 eq.) was added dropwise. A suspended solution of p-aminophenol (8.37 g, 76.70 mmol, 2 eq.) in acetone (60 mL) was added portion-wise for 1 hr and stirred at 0°C. The contents were heated to 45°C for 3 hours before stirring at ambient temperature for an additional 15 hours. The reaction was monitored using TLC. Acetone was completely evaporated using a rotary evaporator when the reaction was completed. Ethyl acetate was used for extraction. The separated organic layer was dried over anhydrous sodium sulphate and then evaporated, yielding a crude product. The crude product was further purified by column chromatography in a 40% Ethyl acetate/Hexane system to produce a white solid that became blackish grey after a while, yielding 50%.

2.3.2.1. Synthesis of 4,4'-((6-Methyl-1,3,5-triazine-2,4-diyl) bis(azanediyl)) diphenol [Me-DAPTz]

The same process was performed with Me-Tz (6.30 g, 38.42 mmol, 1 eq.) to produce a blackish grey solid with a yield of 50%.

M.P.: 241.8 ^{0}C., IR (ATR, cm^{-1}): 3409 (-OH-Stretching), 3260 (-N-H Stretching), 1610.2, 1581.4, 1522.68, 1503.82 (C=N, C=C Ar.), 1201, 829.91 (=C-H Bending, Para substituted Phenyl ring), ^{1}H NMR (300 MHz, DMSO-D6) 2.23 (s, 3H, -CH3), 6.69-6.70 (d, 4H, Phenyl ring); 7.424-7.477 (d, 4H, Phenyl ring) and 9.11, 9.17, (Broad,4H,-NH and -OH), ^{13}C NMR (300 MHz, DMSO-d6$_3$): 25.30, 115.37, 123.00, 131.25, 153.25, 164.17, 174.66; ESI-MS (m/z) 310.48 [M+H]$^+$ and 308.25 [M-H]$^-$ Anal. Calcd for $C_{16}H_{15}N_5O_2$: C, 62.13; H, 4.89; N, 22.64; O, 10.34 Found: C, 62.08; H, 4.17; N, 21.99; O, 11.76.

2.3.2.2. Synthesis of 4,4'-((6-ethyl-1,3,5-triazine-2,4-diyl) bis(azanediyl)) diphenol [Et-DAPTz]

A blackish grey-colored solid with a 64% yield was obtained by following the same process with Et-Tz (5 g, 28.09 mmol, 1 eq.).

M.P.: 216.6 ^{0}C., IR (ATR, cm^{-1}): 3478 (-OH-Stretching), 3218 (-N-H Stretching), 3075 (=C-H Stretching), 2970.8 and 2933 (C-H Stretching -CH_2, -CH_3), 1617.98, 1504.76 and 1439.1 (C=N, C=C Ar. Stretching), 1238.44 (C-O stretching), 824.89 (=C-H Bending, Para substituted Phenyl ring), ^{1}H NMR (300 MHz, DMSO-D6): 1.21-1.24 (t, 3H, -CH_3 Ethyl group), 2.47 -2.48 (q, 2H, Ethyl group -CH_2), 6.67-6.69 (d, 4H, Phenyl ring), 7.45 (Broad peak, 4H, Phenyl ring) and 9.13, 9.35, (Broad,4H,-NH and -OH); ^{13}C NMR (300 MHz, DMSO-d6$_3$): 12.18, 31.82, 115.30, 122.91, 131.52, 153.41, 164.40, 178.89, ESI-MS (m/z) 324.35 [M+H]$^+$ and 322.26 [M-H]$^-$; Anal. Calcd for $C_{17}H_{17}N_5O_2$: C, 63.15; H, 5.30; N, 21.66; O, 9.90 Found: C, 63.29; H, 5.45; N, 22.02; O, 9.89.

2.3.2.3 synthesis of 4,4'-((6-cyclohexyl-1,3,5-triazine-2,4-diyl) bis(azanediyl)) diphenol [Cy-DAPTz]

A blackish-grey solid with a 58% yield was obtained by following the same process using CyH-Tz (6 g, 25.85 mmol, 1 eq.).

M.P.: 224.8 ^{0}C., IR (ATR, cm^{-1}): 3278 (-N-H Stretching), 3027.99 (=C-H Stretching), 2970.84 2931.29 and 2855.22 (C-H Stretching aliphatic -CH$_2$), 1607.96, 1574.66, 1535.2, 1504.83, 1436.09 (C=N, C=C Ar. Stretching), 1217.33 (C-O stretching), 827.83 (=C-H Bending, Para substituted Phenyl ring), ^{1}H NMR (300 MHz, DMSO-D6): 1.23-1.41 (m, 10H, Cyclohexyl -CH$_2$), 2.38-2.47 (m, 1H, Cyclohexyl -C-H), 6.69-6.71 (d, 4H, Phenyl ring), 7.40-7.47 (d, 4H, Phenyl ring) and 9.18, 9.34, 9.40 (Broad,4H,-NH and -OH), ^{13}C NMR (300 MHz, DMSO-d6$_3$): 26.09, 28.24, 31.04, 46.54, 115.34, 123.11, 131.64, 153.55, 164.01 and 180.97, ESI-MS (m/z) 378.40 [M+H]$^+$ and 376.34 [M-H]$^-$; Anal. Calcd for C$_{21}$H$_{23}$N$_5$O$_2$: C, 66.83; H, 6.14; N, 18.55; O, 8.48 Found: C, 66.50; H, 5.98; N, 18.23; O, 9.29.

Reaction Scheme
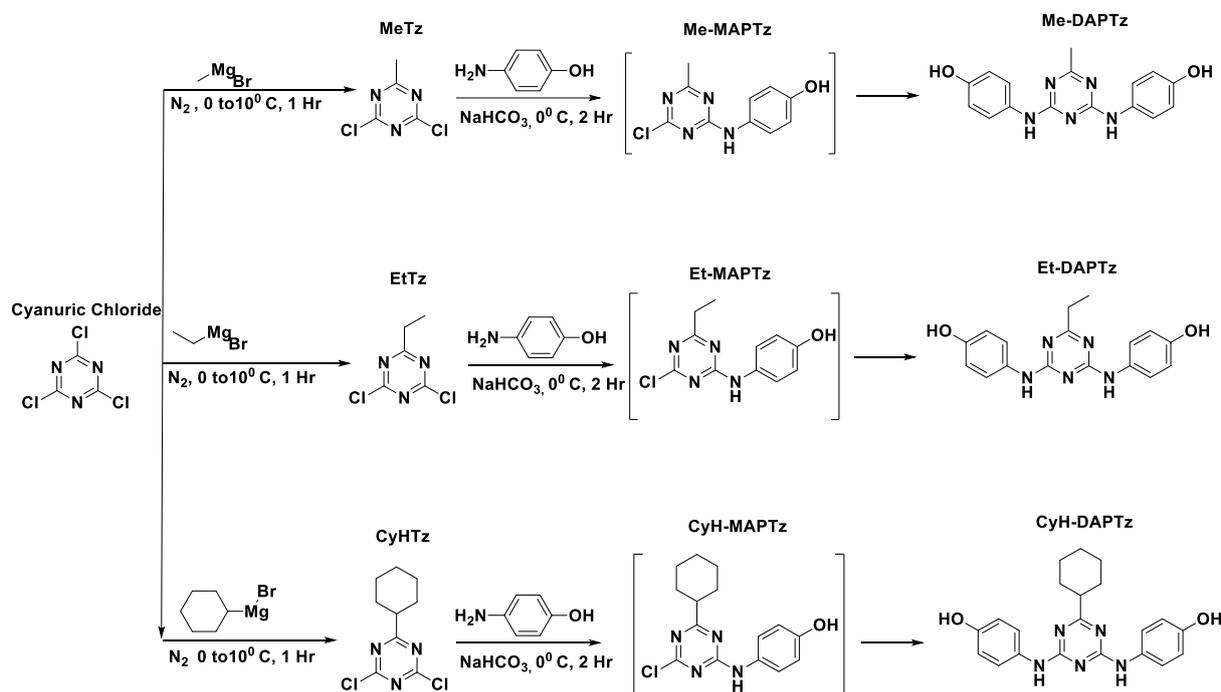
3. Result and Discussion

3.1 Photophysical properties

UV-visible photons carry energy levels that coincide with the electrical states of organic molecules.

It is possible to comprehend and investigate these electron transitions using UV-visible spectrometers. The Eopt represents the energy of the exciton absorption band's long wavelength edge.

Figures 1a and **1b**, respectively, show the compounds' UV/Vis absorption and emission spectra. Di-substituted triazine based compounds absorb and emit in the ultraviolet part of the spectrum (**Figure 1a** and **1b**). The primary absorption bands' shape and wavelength range alter just minimally in this series of compounds (Table 1). Characteristic peaks at 300-310 nm are observed. The first absorption peak in the shorter wavelength region at 262 nm is caused by the n-π* absorption bands of the triazine moiety in triazine derivatives. The second absorption peak at 310 nm was found to originate from the π-π* transition bands in the central core [16].

These electron transitions may be understood and studied with UV-visible spectrometers. Eoptical energy is the energy of the exciton absorption band's long wavelength edge.

The optical gap energy (Eg) is found using the longest absorption wavelength, λ. A formula may be used to compute the optical band gap, according to the equation.

$$Eg = 1242/\lambda \text{ nm}$$

Table 1 presents the optical energy band gap of substances as determined from the onset of their UV/Vis spectra.

The band gap ranges from 3.69 to 3.72 eV, with the sequence **CyH-DAPTz** > **Et-DAPTz** = **Me-DAPTz**. When one hydrogen in triazine was substituted with a cyclohexyl group, the molecule had a band gap of 3.72 eV (**CyH-DAPTz**). When the alkyl group is substituted with triazine, the band gap shifts to 3.69 eV. Thus, the band gap was greatly impacted by changing the functional group of the substituted triazine. Selecting the appropriate functional groups allows a material to have its band gap tuned [17].

Fluorescence spectra were collected at a variety of excitation wavelengths ranging from 270 to 320 nm. Exciting the material at $\lambda exc=270$ nm resulted in no emission, indicating triazine core absorption [18, 19]. Nonetheless, all compounds exhibited an emission centered at 340 nm when stimulated at 298 nm.
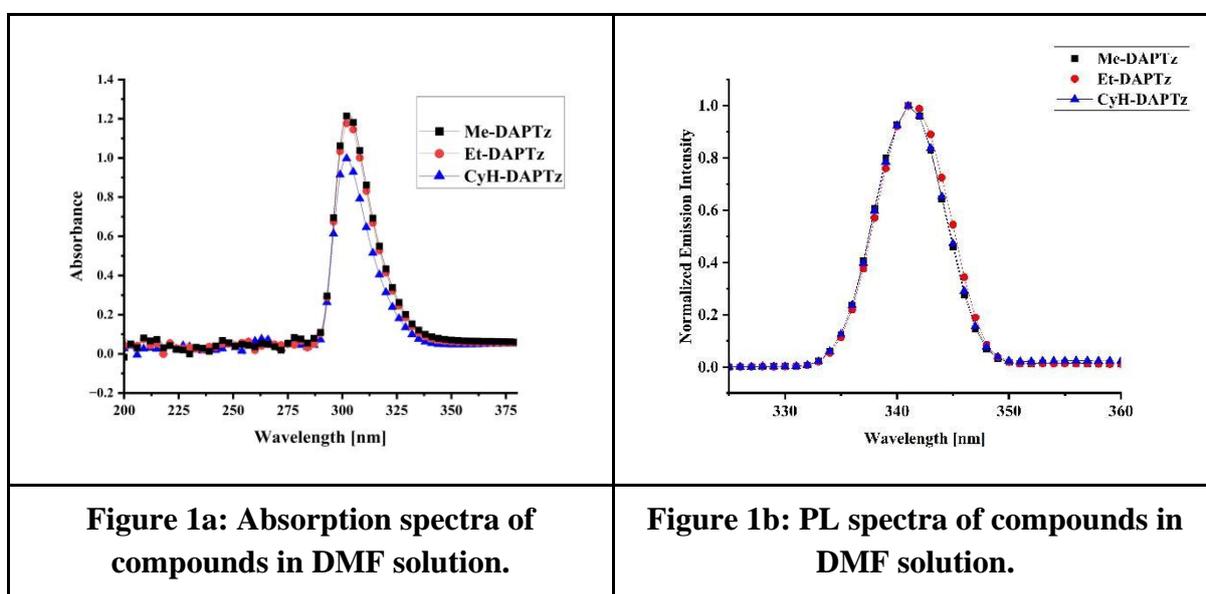

| Figure 1a: Absorption spectra of compounds in DMF solution. | Figure 1b: PL spectra of compounds in DMF solution. |

Table 1. Emission and absorption wavelength of disubstituted Triazine based compounds in DMF

Compound	λ^{*} (nm)	$\lambda^{\#}$ (nm)	S (nm)	Optical Band Gap
Me-DAPTz	300	341	41	3.69
Et-DAPTz	305	341	36	3.69
CyH-DAPTz	315	341	26	3.72

DMF= N,N-Dimethylformamide

λ^{*}= Absorption maxima; $\lambda^{\#}$= emission maxima; S= Stoke shift.

3.2 X-Ray Crystallographic studies

The stresses, preferred orientations, crystallographic structures, and grain size of crystalline materials may all be determined through X-ray diffractograms.

Figure 2's diffractograms revealed peaks with different intensities that were not well resolved. A somewhat higher intensity was seen in several of the diffractograms' peaks, and the measured crystallite size was less than 19 nm but larger than zero.
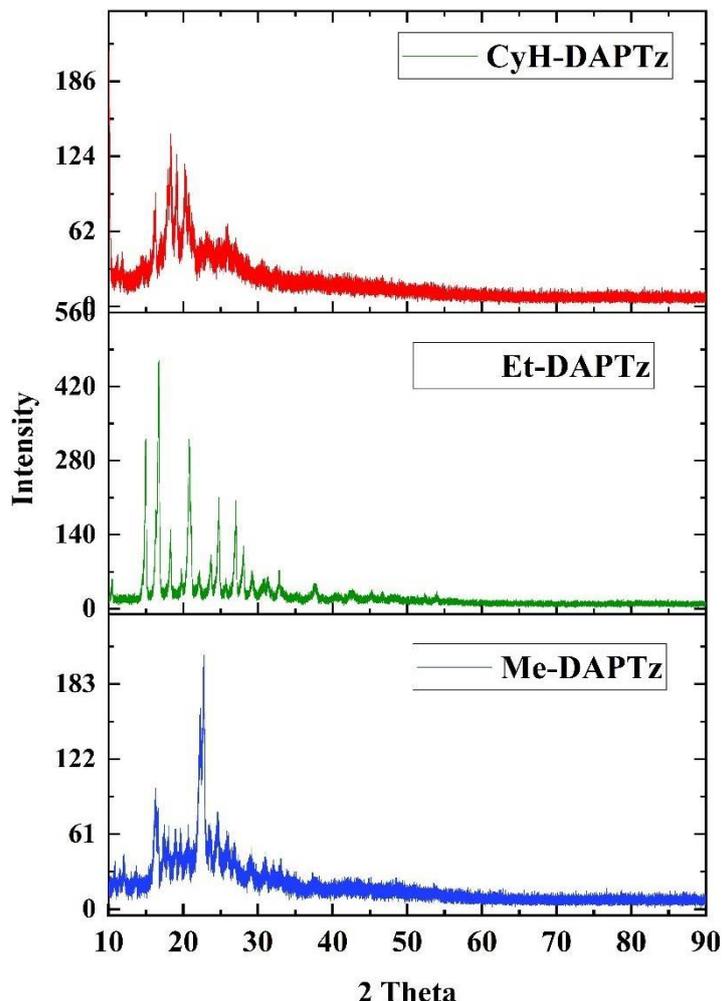

Figure 2. X-ray diffractogram of triazine based compound.

The triazine-based compounds' crystallite sizes did not exhibit a pattern that increased with the size of the connected alkyl moieties. The ethyl substitution **Et-DAPTz** had the largest size (19 nm), while the cyclohexyl group substitution **CyH-DAPTz** had the smallest size (3.94 nm).

The diffractogram for **Et-DAPTz** showed strong peaks, but there was also a discernible spreading region beneath the peak. Therefore, this discovery suggested that the nature of **Et-DAPTz** was more crystalline. The crystallite sizes of the remaining **Me-DAPTz** and **CyH-DAPTz** compounds ranged from 3.94 to 12.38 nm. Consequently, it has been discovered that these compounds are amorphous in nature. **Table 2** presents the information gathered from X-ray diffraction investigations.

Table 2. X-ray diffraction data of triazine based compound.

Peak Position [2Theta]	FWHM	Crystallite size [nm]	Mean Crystallite size [nm]
22.5353	0.8119	9.9760	

Me-DAPTz	16.3421	0.5611	14.3031	**12.39**
	22.5353	10.6162	0.7630	
	24.7848	44.4908	0.1828	
	14.9603	0.2723	29.4219	
	16.6651	0.4083	19.6621	
Et-DAPTz	18.2717	0.3604	22.3224	**19.29**
	20.81824	0.5134	15.7327	
	24.7343	0.3821	21.2833	
	26.9855	0.4051	20.1628	
	27.9896	0.4829	16.9520	
CyH-DAPTz	13.9453	4.2677	1.8753	**3.94**
	18.2145	0.6093	13.2028	
	18.2145	14.9386	0.5385	
	18.2145	52.8697	0.1522	

3.3 Thermal properties

The thermal stability of the compounds was investigated using thermogravimetry. **Figure 3** displays the TGA thermogram, while Table 3 lists the decomposition temperature. Excellent thermal stability is possessed by all substances.

The thermal stability order of the synthesized compound is **CyH-DAPTz**>**Et-DAPTz**>**Me-DAPTz**. The decomposition temperature can also be adjusted by substituting other groups in triazine's fundamental structure. Compounds are a good fit for optoelectronic devices because of their thermal properties. The synthesised compounds have good solubility in acetonitrile and chloroform, hence strengthening the processing characteristics and applications of materials based on triazine.
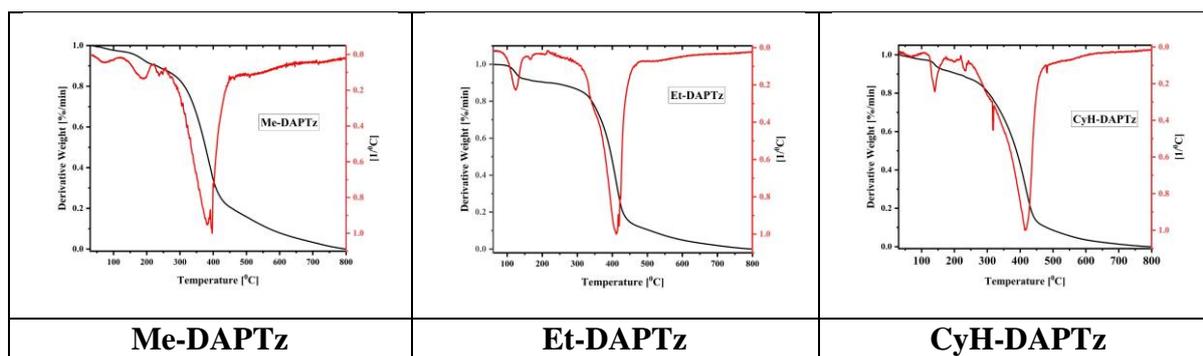

Figure 3. Thermogram of triazine based compound.

The absence of moisture content (free moisture or moisture bonding) was shown by the fact that none of the compounds significantly lost weight below 100^0C. Thermograms also indicated that di-substituted triazine based compound showed two steps of decomposition process. Almost 95-100% of compound decomposition occurs until 500^0C.

Me-DAPTz had a 6-7% decrease in weight during the first stage, which began at 30°C and ended in the 30-250°C range. The loss of the CH_3 moiety might be the cause of this. With a 94% reduction in weight,

the second breakdown phase began at 300°C and ended between 300 and 800°C. This may have resulted from the $C_{15}H_{12}N_5O_2$ moiety losing a significant portion of its residue.

For **Et-DAPTz,** the first step was carried out between 30°C and 200°C, resulting in a 9% reduction in weight. The deletion of the C_2H_5 moiety might be the cause of this. 91% of the weight was lost during the first phase of the second breakdown process, which began at 300°C and ended between 300 and 800°C. This may have resulted from the $C_{15}H_{12}N_5O_2$ moiety losing a significant portion of its residue.

For **CyH-DAPTz**, the first step started at 30°C and concluded within the 30-200°C range, coinciding with a 9% reduction in weight. The loss of the H_2O_2 moiety might be the cause of this. 91% of the weight was lost during the first phase of the second breakdown process, which began at 300°C and ended between 300 and 800°C. This might be ascribed to the $C_{21}H_{21}N_5$ moiety losing a significant portion of its residue.

Table 3 summarizes the observed and estimated weight loss, TG temperature, and DTA peak temperature data.

Table 3. Thermal data for di-substituted triazine based compound.

Compounds/ Mol. Formula/ Mol. Weight	Dissociation step	Temp. range in TG (^{0}C)	DTA peak Temp. (^{0}C)	Observed weight loss [in %]/Moiety lost
Me-DAPTz/ $C_{16}H_{15}N_5O_2$/ 309	I	30-200^{0}C	189	6-7/ **-CH$_3$**
	II	300-800°C	396	94/ **$C_{15}H_{12}N_5O_2$**
Et-DAPTCz/ $C_{17}H_{17}N_5O_2$/ 323	I	30-200^{0}C	124	9/ **-C$_2$H$_5$**
	II	300-800°C	411	91/ **$C_{15}H_{12}N_5O_2$**
CyH-DAPTz/ $C_{21}H_{23}N_5O_2$/ 377	I	30-200^{0}C	141	9/ **H_2O_2**
	II	300-800°C	418	91/ **$C_{21}H_{21}N_5$**

3.4 Surface morphology

Using the FEI Quanta 200 3D, SEM examined the surface morphological characteristics of di-substituted triazine based compound at an operating voltage of 3.00 kV. SEM microphotographs of the monomers based on Triazine are displayed in **Figure 4**. The pictures consisted of a big, asymmetrical crystal mixed with route debris. Additionally, the rock-shaped structure, amorphous globular structure, and platy rough structure are all visible in the microcrystal SEM photomicrographs. The separation of the microscopic and macroscopic phases was not seen in SEM micrographs. It was evident from the morphology that certain monomers were crystalline while others were amorphous.
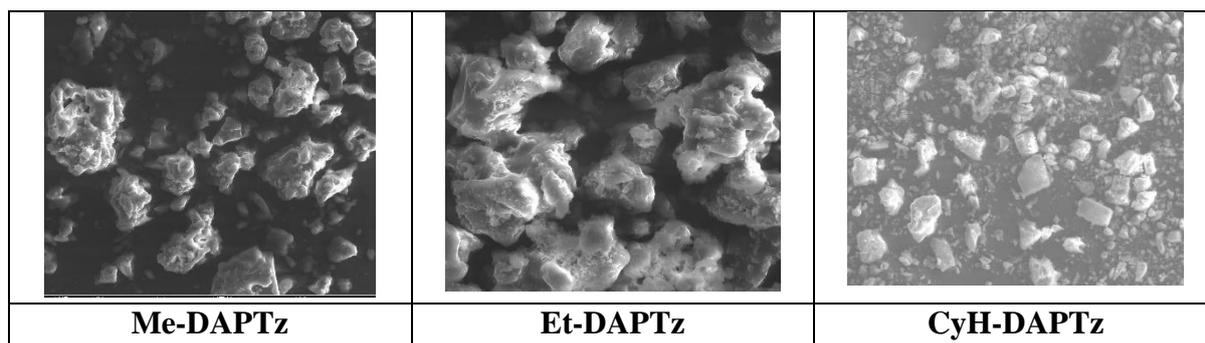
| Me-DAPTz | Et-DAPTz | CyH-DAPTz |

Figure 4. SEM images of di-substituted triazine based compounds.

Conclusion

UV-Vis and photoluminescence spectroscopy were used to do a thorough optoelectronic investigation of recently created triazine compounds based on the combination of 1,3,5-triazine as a central core with alkyl moieties.

The synthesized compound has high thermal stability up to $396\text{-}418^0$C and emits at 341 nm in DMF with a band gap of 3.69-3.72 eV determined from absorption spectra. The outcomes validated a theory in molecular design that adding additional electron-donating groups to molecules can control their ideal energy levels and band gaps, leading to better optoelectronic capabilities. The results also demonstrated that synthesized compounds could enhance the performance of optoelectronic devices. This molecular design idea might be advantageous in the development and exploration of novel 1,3,5-triazine derivatives with exceptional optoelectronic characteristics.

Acknowledgements

References:

1. Forrest, S. R.; Thompson, M. E. (2007), Introduction: organic electronics and optoelectronics, Chem. Rev., 107, 923.

2. M.A. Baldo, D.F. O'Brien, Y. You, A. Shoustikov, S. Sibley, M.E. Thompson, et al., (1998), Highly efficient phosphorescent emission from organic electroluminescent devices, Nature 395, 151.

3. L.X. Xiao, Z.J. Chen, B. Qu, J.X. Luo, S. Kong, Q.H. Gong, et al., (2011), Recent progresses on materials for electro phosphorescent organic light-emitting devices, Adv. Mater. 23(8):926-52.

4. P.L. Burn, S.-C. Lo, I.D.W. Samuel, (2007), The development of light-emitting dendrimers for displays, Adv. Mater. 19, 1675–1688.

5. L. Stagi, D. Chiriu, A. Ardu, C. Cannas, C.M. Carbonaro, P.C. Ricci, (2015), Luminescence enhancement by energy transfer in melamine-Y_2O_3:Tb^{3+} nanohybrids, J. Appl. Phys. 118,125502–125507.

6. Y.-J. Cheng, S.-H. Yang, C.-S. Hsu, (2009), Synthesis of conjugated polymers for organic solar cell applications, Chem. Rev. 109 (11), 5868–5923.

7. Shahbaz, M.; Urano, S.; LeBreton, P.R.; Rossman, M.A.; Hosmane, R.S.; Leonard, N.J. (1984), Tri-s-Triazine: Synthesis, Chemical Behavior, and Spectroscopic and Theoretical Probes of Valence Orbital Structure. J. Am. Chem. Soc., 106, 2805–2811.

8. Cannon, J.G. Comprehensive Heterocyclic Chemistry II Edited by A. R. Katritzky, C.W. Rees, and E. F. V. Scriven. Pergamon Press, Elsevier Science, Ltd., Tarrytown, NY. 1996. 12 Volumes: Vol. 1A, Xxvii + 505 Pp; Vol. 1B, 860 Pp; Vol. 2, Xiii + 1102 Pp; Vol. 3, Xiii +. J. Med. Chem. **1997**, 40, 4165–4166

9. T. Murase, M. Fujita, (2005) Highly blue luminescent triazine-amine conjugated oligomers, J. Organomet. Chem. 70, 9269–9278.

10. L. Stagi, D. Chiriu, C.M. Carbonaro, R. Corpino, P.C. Ricci, (2016) Structural and optical properties of carbon nitride polymorphs, Diam. Relat. Mater. 68, 84–92.

11. Z. Jiang, C. Zhu, W. Wan, K. Qiana, J. Xie, (2016) Constructing graphite-like carbon nitride modified hierarchical yolk–shell TiO2 spheres for water pollution treatment and hydrogen production, J. Mater. Chem. A 4 1806–1818.

12. X. Li, J. Yu, J. Low, Y. Fang, J. Xiao, X. Chen, (2015) Engineering heterogeneous semiconductors for solar water splitting, J. Mater. Chem. A 3, 2485–2490.

13. C. Butchosa, T.O. McDonald, A.I. Cooper, D.J. Adams, M.A. (2014), Zwijnenburg, Shining a light on s-triazine-based polymers, J. Phys. Chem. C 118 4314–4324.

14. B. Huang, W. Jiang, J. Tang, X. Ban, R. Zhu, H. Xu, W. Yang, Y. Sun, (2014) A novel, bipolar host based on triazine for efficient solution-processed single-layer green phosphorescent organic light-emitting diodes, Dyes Pigments 101, 9–14.

15. F. Pop, F. Riobé, S. Seifert, T. Cauchy, J. Ding, N. Dupont, A. Hauser, M. Koch, N. Avarvari, (2012), Tetrathiafulvalene-1,3,5-triazines as (multi)donor−acceptor systems with tunable charge transfer: structural, photophysical, and theoretical investigations, Inorg. Chem. 51 (15), 8545–8556.

16. Xu F, Wang Z, Gong Q (2007) Synthesis, characterization, and optical properties of two-photon-absorbing octupolar molecule with an s-triazine core. Opt Mater 29:723–727.

17. Rajeesh Pakkath, Eeda Koti Reddy†, Sheena Kuriakose, Saritha C, Ayyiliath M Sajith (2019) Synthesis, Characterization and Determination of HOMO-LUMO of the Substituted 1,3,5-Triazine Molecule for the Applications of Organic Electronics, J. of the Korean Chem. Soc., Vol. 63, No. 5 https://doi.org/10.5012/jkcs.2019.63.5.352

18. Deihmann VAF, Lisboa-Filho PN, Martins TD, Atwars TDZ, Akcelrud LJ (2007) Structural control of photoluminescence of four poly(urethane-urea-co-1, 3, 5-triazine)s: Synthesis and characterization. J. Lumin. 124:343–350

19. Halim M, Pillow JNG, Samuel IDW, Burn PL (1999) Conjugated dendrimers for light-emitting diodes: effect of generation. Adv Mater 11:371–374