REVIEW ARTICLE

JOURNAL OF PHARMACOLOGY AND BIOMEDICINE

Published by RB Science Home Page: www.jpbiomed.com

Triazatruxene Derivatives: A Review of Their Advancements and Applications in Optoelectronics & Biological Technologies

Shivanshu Tripathi[1], Varsha Nigam Gour[1]*

[1]Department of Chemistry, Sanjeev Agrawal Global Education (SAGE) University, Bhopal, Madhya Pradesh, India

Article History

Received on: 05/02/2025

Revised on: 18/04/2025

Accepted on: 22/04/2025

Published on: 13/05/2025

Keywords

Triazatruxene

Organic light emitting diodes

Perovskite solar cells

Thermally activated delayed fluorescence

Internal quantum efficiency

ABSTRACT

This review article provides a comprehensive analysis of triazatruxene (TAT) and its derivatives, highlighting their properties, synthesis history, and photophysical characteristics. Recently, triazatruxene-based molecules have shown excellent efficiency for thermally activated delayed fluorescence (TADF) organic light emitting diodes (OLEDs) and hole transporting materials (HTMs) for perovskite solar cells. Triazatruxene (TAT) and its derivatives, first synthesized in 1965, have garnered significant interest due to their remarkable properties like solubility, thermal stability, and electronic features, making them suitable for advanced technologies. TAT-based discotic liquid crystals (DLCs) enhance charge transport in organic electronics like OLEDs and organic photovoltaic (OPVs) through their ordered columnar structures. TAT derivatives also show promise as hole transport materials in perovskite solar cells and as thermally activated delayed fluorescence materials for efficient OLEDs. Additionally, they exhibit potential as G-quadruplex ligands with anticancer properties, encouraging further exploration.

.

*Corresponding Author

Dr. Varsha Nigam Gour

Email: varsha.g@sageuniversity.edu.in

JOURNAL OF PHARMACOLOGY AND BIOMEDICINE

ISSN No. 2456-8244

Publication Hosted by jpbiomed.com

Scan QR to visit website

Introduction

In 1965, Baars et al. successfully synthesized triazatruxene (TAT) for the first time by reacting indole with formaldehyde using a Lewis acid catalyst. This innovative achievement laid the groundwork for further investigation into TAT derivatives and their possible uses, especially in organic electronics and optoelectronics. Building on this initial synthesis, recent studies have explored the different properties of TAT-based materials, revealing their prominent solubility, thermal stability, and electronic features, which make them highly appropriate for a range of advanced technological applications. [1-3]

Triazatruxene (TAT) based discotic liquid crystals (DLCs) hold great potential for semiconductor applications because of their disc-shaped structure, which elevates the formation of well-ordered columnar phases that improve charge transport productiveness. Noted for their ability to self-assemble and their thermal stability, TAT-based DLCs create uniform columnar structures that are essential for reliable charge mobility in devices such as organic light-emitting diodes (OLEDs) and organic photovoltaic cells (OPVs). This consistent structural arrangement enhances the implementation of semiconductor devices by providing stable pathways for charge transport. [4-5]

Researchers have utilized a unique methodology known as single crystal X-ray diffraction to investigate the crystal structures of TAT derivatives. This study provides insights into the interactions between these molecules and their formation of columnar structures.

Triazatruxene derivatives have been studied for their potential use as Hole Transport Materials (HTMs) in Perovskite Solar Cells (PSCs) because of their beneficent electronic properties and stability. In particular, HTMs based on triazatruxene have substantiated encouraging outcomes in improving both the efficiency and stability of PSCs[6].

Thermally activated delayed fluorescence (TADF) materials play an important role to making OLEDs highly efficient because as they enable the achievement of 100% internal quantum efficiency (IQE)[8].

These materials are good at transforming non-light-emitting triplet states into light-emitting singlet states, thereby enhancing the overall external quantum efficiency of OLEDs. Recent research has focused on optimizing these materials through punctilious design, leading to produce various colors and improve device performance. [7] The triazatruxene derivatives demonstrate strong potential as selective G-quadruplex ligands, justifying further study of their biological activity. Their supremacy water solubility and DNA binding properties indicate enhancing pharmacological effects, especially in the inhibition of tumor cell growth; place them as promising candidates for future studies. [9]

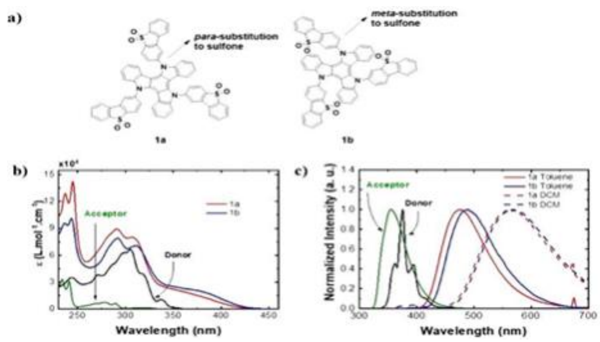


Figure 1. (a) Chemical structure of para-substituted emitter (1a) and meta-substituted emitter (1b), (b) extinction coefficient absorption spectra of the acceptor (A) and donor (D)

In **Figure 2,** complex of AZATRUX (stick model with yellow transparent surface) with the human monomeric G-quadruplex DNA (red surface), obtained by simulated annealing, (a) top view, (b) lateral view. [9]

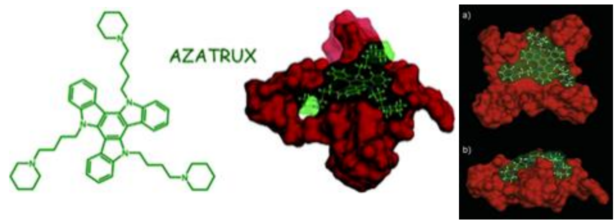


Figure 2. Azatrux complex with DNA

SYNTHESIS OF TRIAZATRUXENE DERIVATIVES [2,3,4]

The synthesis of triazatruxene (TAT) derivatives typically begins with the reaction of indole and formaldehyde using Lewis acid catalysts, as pioneered by Baars et al. This foundational method has since been expanded to include a variety of functionalization strategies to tailor the electronic, thermal, and solubility properties of TAT for specific applications.

1. Functional Group Modifications: Introduction of alkyl, aryl, or heteroaryl substituents at the nitrogen or core positions to enhance solubility and electronic behavior.

2. Cross-Coupling Reactions: Use of Suzuki, Stille, or Sonogashira reactions to introduce complex substituents for improved charge transport or optical properties.

3. Cyclization Reactions: For generating discotic liquid crystals, ensuring better columnar stacking.

4. Post-Synthetic Modifications: Tailoring TAT for optoelectronic and biomedical applications through further chemical modifications.

PROPERTIES OF TRIAZATRUXENE DERIVATIVES [5,6]

Thermal Stability and Electronic Properties : Triazatruxene derivatives exhibit remarkable thermal stability due to their rigid planar structure and conjugated core. These properties ensure durability under operational conditions in optoelectronic devices. Their extended π-conjugation also provides excellent electronic properties, including high charge mobility, making them suitable for applications such as organic photovoltaics (OPVs) and OLEDs [10, 8, 3].

2. **Self-Assembly Behavior and Structural Organization:**

The discotic structure of triazatruxene facilitates self-assembly into columnar liquid crystal phases. These well-ordered phases improve charge transport by forming stable pathways, critical for enhancing the performance of semiconducting devices. [13]

APPLICATIONS IN OPTOELECTRONIC DEVICES

1. Organic Light-Emitting Diodes (OLEDs) [10, 11, 12]

Role of TAT Derivatives in Enhancing Quantum Efficiency and Charge Transport: Triazatruxene (TAT) derivatives contribute to OLEDs by improving charge transport due to their self-assembly into stable columnar phases. Their extended conjugated core enhances quantum efficiency, reaching internal quantum efficiencies (IQEs) close to 100% in some devices.

2. Organic Photovoltaic Cells (OPVs) [10, 11, 12]

Contributions to improved charge mobility and device stability of the disc-shaped structure of TAT derivatives facilitates efficient π-π stacking, enhancing charge mobility and stability. Their ability to form well-ordered phases aids in optimizing OPV performance.

3. Perovskite Solar Cells (PSCs) [10, 12]

Use as Hole Transport Materials (HTMs) and Their Impact on Efficiency: TAT derivatives serve as effective HTMs, offering excellent thermal stability, energy level alignment, and improved device efficiency. They play a key role in enhancing PSC stability and power conversion efficiency.

4. Thermally Activated Delayed Fluorescence (TADF) Materials[4, 5]

Enhancing External Quantum Efficiency (EQE): TAT-based TADF materials efficiently harvest triplet excitons, converting them to singlets for light emission. This property significantly enhances EQE, contributing to the development of highly efficient OLEDs.

BIOLOGICAL APPLICATIONS OF TRIAZATRUXENE (TAT) DERIVATIVES

1. **Role as G-quadruplex Ligands and Anticancer Potential [9]**

TAT derivatives exhibit remarkable potential as G-quadruplex ligands, targeting the G-quadruplex structures in DNA. These unique non-canonical DNA structures, present in the promoter regions of oncogenes and telomeres, are vital in regulating cancer cell proliferation. By stabilizing these G-quadruplexes, TAT derivatives can inhibit telomerase activity, leading to anticancer effects. The planar and aromatic structure of TAT enables strong π-π stacking interactions with G-quadruplexes, enhancing selectivity and binding affinity. Studies have demonstrated their potential in reducing tumor growth and inducing apoptosis.

2. DNA Binding Properties and Pharmacological Prospects [9]

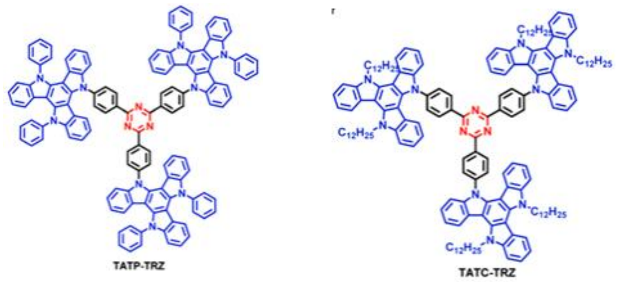
TAT derivatives possess strong DNA binding capabilities due to their amphiphilic nature and well-defined π-conjugated systems. These properties enable them to interact with the major and minor grooves of DNA, influencing transcriptional and replication processes. Their water solubility and high binding efficiency position them as promising agents for drug delivery and DNA-targeted therapy. In pharmacological studies, TAT derivatives have shown potential in the treatment of cancers, viral infections, and neurological disorders.

Literature Review

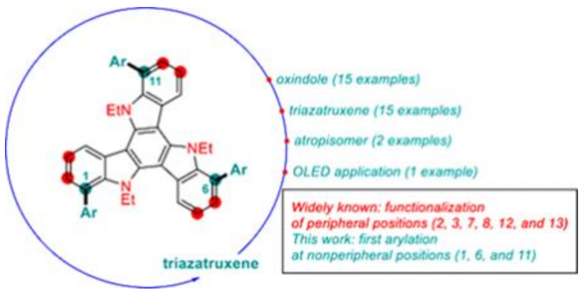
In 2021, Zhou *et* al presented the development of two star-shaped TADF emitters**, TATC-TRZ** and **TATP-TRZ**, with distinct side chains. Both emitters exhibited comparable photo physical properties and TADF characteristics. Notably, the flexible alkyl chain in TATC-TRZ significantly enhances film formation and stability, leading to superior device performance. Consequently,

TATC-TRZ-based OLEDs achieved markedly higher efficiencies (EQE_{max} of 7.5% and CE_{max} of 19.9 cd/A) than TATP-TRZ-based OLEDs (EQEmax of 2.8% and CE_{max} of 7.4 cd/A), highlighting the efficacy of flexible alkyl tails in improving solution-processed devices.[10]

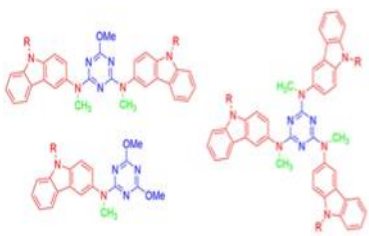
In 2021, Aslan *et* al., have successfully synthesized arylated-triazatruxene motifs at the **C1, C6**, and **C11** positions through a functionalization/cyclotrimerization process, influenced Significantly by the nature of substituents at non-peripheral positions of oxindoles. This method is operationally simple, broad in substrate scope, and scalable, hence providing a practical route to functionalized triazatruxene derivatives. We also demonstrated the synthesis of a new type-two atropisomer for oxindole and triazatruxene. Notably, the triazatruxene scaffold 9a showed potential in OLED technology when used as an emitting layer in a white OLED device. Future efforts will focus on extending the synthetic functionalization of triazatruxene and enhancing their OLED performance, considering the commercialization.[11]

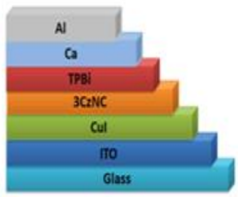


Recently, researchers have synthesized three novel bridged triazatruxene derivatives named **1FTAT-2Ph, 2FTAT-1Ph, 3FTAT**, as solution-processed host materials for TADF OLEDs, featuring diphenyl methylene bridging groups that enhance molecular rigidity, thermal stability, and high T1 energy levels (~**2.8 eV**). The 2F-TAT-1Ph based device achieved the best performance with a maximum EQE of **20.9** and a maximum PE of **72.7 lm/W**, showing balanced charge transport and high QY in the EML (Emitter layer). The elevated HOMO levels of bridged triazatruxene derivatives matched well with the Fermi level of the ITO/PEDOT anode, improving hole injection and transport. This resulted in a power efficiency of 72.7 lm/W, much higher than the 36.1 lm/W of the classical CBP host-based device, showcasing a new strategy for high-performance solution-processed TADF OLEDs. [12, 13, 14]



In 2017 Pawel Zassowski and co-workers propose a series of compounds with carbazole arms and a 1,3,5-triazine core connected by an amino group were synthesized and analyzed. The relationship between their electrochemical properties, quantum efficiency, charge transport properties, and structure was studied. The ability of the synthesized compound to form exciplexes as a donor was explored with two known acceptors, 4,7-diphenyl-1,10-phenanthroline (Bphen) and 2,2′,2"-(1,3,5-benzenetriyl)-tris(1-phenyl-1-H-benzimidazole) (TPBi). The results showed that the star-shaped structure of the compound 3CzNC achieved the best exciplex OLED performance, with an EQE of up to 6.84%.





In China, Nan Wu, Long Ma, Shan Zhao, Debao Xiao and their team propose a dual-band electrochromic device (Db-ECD) can control visible and near-infrared (NIR) light separately. These devices are useful for smart windows and camouflage. While organic materials have been studied, finding good dual-band electrochromic compounds is still difficult. [8, 11] **In this study**, triazine-based viologen analogs, TPPT and TPBT, showed excellent dual-band electrochromic properties. TPPT had contrast levels of 66.63% at 887 nm and 50.71% at 600 nm, while TPBT showed 59.79% at 900 nm and 66.90% at 600 nm. Devices made using a gel electrolyte with TPPT or TPBT operated at a low voltage (~0.6V) and had high efficiency (up to 230.94 cm^2C^{-1}). TPPT also had a strong absorbance change (2.58 at 1037 nm). This study helps develop new organic materials for advanced electrochromic devices.

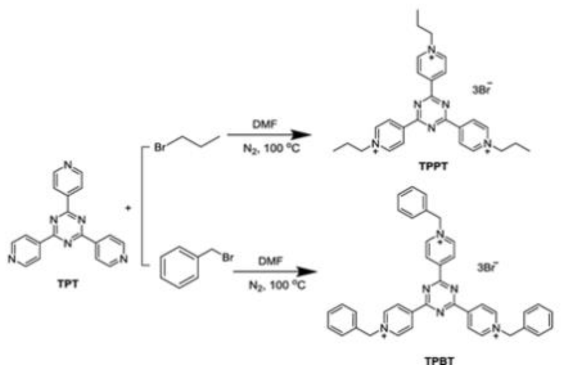


Figure explains transmission changes of a) TPPT-based ECD. b) TPBT-based ECD. under three different applied voltages. Schematic diagrams of modulation for solar radiation during various modes. These devices were able to switch between three distinct modes of operation by varying the plied electrochemical voltage: transparent (0.0 V), NIR light blocking (−0.8V) and broadband-blocking of the NIR and visible light (−1.0V). [8]

CHALLENGES AND FUTURE DIRECTIONS FOR TRIAZATRUXENE DERIVATIVES

1. Current Limitations in Synthesis and Application [10, 11]

While triazatruxene (TAT) derivatives exhibit promising properties, their synthesis can be complex and challenging due to the need for precise control over functionalization. Additionally, the scalability of these compounds remains an issue for large-scale industrial applications. The application of TAT derivatives in optoelectronics is still limited by factors such as poor solubility in certain solvents and stability under operational conditions.

2. Potential Areas for Future Research in Optoelectronics [10, 11]

Future research could focus on enhancing the synthesis of TAT derivatives with improved solubility, stability, and efficiency. Investigating new derivatives with enhanced photophysical properties may improve their performance in organic light-emitting diodes (OLEDs) and organic photovoltaic cells (OPVs). Additionally, further exploration of TAT derivatives in flexible electronics, perovskite solar cells, and their interactions with various acceptor molecules will provide insights into their full potential in optoelectronic applications.

Conclusion

Triazatruxene derivatives have great potential in optoelectronics, improving devices like OLEDs and solar cells with better efficiency, stability, and charge transport. Their biocompatibility also opens doors for biological applications. As research progresses and synthesis methods improve, these materials could lead to more efficient, flexible, and sustainable electronic devices. With growing energy demands, advancements in TADF OLEDs and perovskite solar cells may help develop energy-saving technologies and promote their commercial use for societal benefits.

References

1. Vogel, I. (1974). Practical organic chemistry.

2. Li, X. C., Wang, C. Y., Lai, W. Y., & Huang, W. (2016). Triazatruxene-based materials for organic electronics and optoelectronics. Journal of Materials Chemistry C, 4(45), 10574-10587.

3. Goubard, F., & Dumur, F. (2015). Truxene: a promising scaffold for future materials. RSC advances, 5(5), 3521-3551.

4.Tao, L., Xie, Y., Zhao, K. X., Hu, P., Wang, B. Q., Zhao, K., & Bai, X. Y. (2024). Triphenylene Trimeric Discotic Liquid Crystals: Synthesis, Columnar Mesophase and Photophysical Properties. New Journal of Chemistry.

5. Bisoyi, H. K., & Li, Q. (2014). Directing self-organized columnar nanostructures of discotic liquid crystals for device applications. In Nanoscience with Liquid Crystals: From Self-Organized Nanostructures to Applications (pp. 209-256). Cham: Springer International Publishing.

6. Pal, K., Raza, M. K., Legac, J., Rahman, M. A., Manzoor, S., Rosenthal, P. J., & Hoda, N. (2021). Design, synthesis, crystal structure and anti-plasmodial evaluation of tetrahydrobenzo [4, 5] thieno [2, 3-d] pyrimidine derivatives. RSC Medicinal Chemistry, 12(6), 970-981.

7. L. dos Santos, P., de Sa Pereira, D., Eng, J., Ward, J. S., Bryce, M. R., Penfold, T. J., & Monkman, A. P. (2023). Fine-Tuning the Photophysics of Donor-Acceptor (D-A3) Thermally Activated Delayed Fluorescence Emitters Using Isomerisation. ChemPhotoChem, 7(2), e202200248.

8. Wu, T., Zhang, D., Ou, Y., Ma, H., Sun, A., Zhao, R., ... & Hua, Y. (2021). Efficient perovskite solar cells enabled by large dimensional structured hole transporting materials. Journal of Materials Chemistry A, 9(3), 1663-1668.

9. Ginnari-Satriani, L., Casagrande, V., Bianco, A., Ortaggi, G., & Franceschin, M. (2009). A hydrophilic three side-chained triazatruxene as a new strong and selective G-quadruplex ligand. Organic & Biomolecular Chemistry, 7(12), 2513 -2516.

10. Pathak, S. K., Liu, H., Zhou, C., Xie, G., & Yang, C. (2021). Triazatruxene based star-shaped thermally activated delayed fluorescence emitters: modulating the performance of solution-processed non-doped OLEDs via side-group engineering. Journal of Materials Chemistry C, 9(23), 7363-7373.

11. Aslan, M., Taskesenligil, Y., Pıravadılı, S., & Saracoglu, N. (2021). Functionalization at non-peripheral positions of triazatruxene: modular construction of 1, 6, 11-triarylated-triazatruxenes for potentially organic electronics and optoelectronics. The Journal of Organic Chemistry, 87(8), 5037-5050.

12. Liu, Y., Wu, Y., Wang, T., Wang, Q., Han, X., Wu, X., & Wang, L. (2023). Bridged triazatruxene-based host materials for solution-processed thermally activated delayed fluorescence organic light emitting diodes with high power efficiency. Organic Electronics, 113, 106720.

13. Ahn, D. H., Kim, S. W., Lee, H., Ko, I. J., Karthik, D., Lee, J. Y., & Kwon, J. H. (2019). Highly efficient blue thermally activated delayed fluorescence emitters based on symmetrical and rigid oxygen-bridged boron acceptors. Nature Photonics, 13(8), 540-546.

14. Peng, X., Qiu, W., Li, W., Li, M., Xie, W., Li, W., & Su, S. J. (2022). Synergetic Horizontal Dipole Orientation Induction for Highly Efficient and Spectral Stable Thermally Activated Delayed Fluorescence White Organic Light-Emitting Diodes. Advanced Functional Materials, 32(28), 2203022.

Cite this article as

Tripathi S, Gour VN. Triazatruxene derivatives: A review of their advancements and applications in optoelectronics & biological technologies. J Pharmacol Biomed. 2025; 9(2): 823-829