# Impact of Solvent Choice and Molecular Blend on Y6 Molecular Arrangement

**Megan Davis**
Organic Chemistry Department
Humbolt University
Brook-Taylor-Straße 2, 12489 Berlin

Present address:
Department of Mechanical Engineering
University of Colorado at Boulder
1111 Engineering Dr, Boulder, CO 80309
meda1086@colorado.edu

## Abstract

Y6 is a leading non-fullerene acceptor in organic photovoltaic (OPV) devices due to its molecular flexibility, tunable energy levels, and optimal optical band gap for efficient solar energy conversion. However, the arrangement of Y6 at the nanoscale remains a key factor limiting device performance, as morphology strongly influences charge separation and transport. In this work, we use scanning tunneling microscopy (STM) to investigate how solvent environment and molecular additives influence the Y6 unit cell structure at the solid–liquid interface. Y6 solutions were drop-cast onto highly oriented pyrolytic graphite (HOPG), and the resulting STM images revealed notable changes in lamellar spacing, unit cell angle, and molecular packing under different conditions. These findings provide direct structural insight into how backbone and side-chain organizations respond to processing environment, offering guidance for morphological control in high-performance OPV systems.

## Introduction

Organic photovoltaics (OPVs) are an increasingly attractive renewable energy technology due to their low cost, mechanical flexibility, and potential for sustainable manufacturing. While crystalline silicon solar cells currently dominate the market with power conversion efficiencies (PCEs) approaching 26%, OPVs have recently achieved efficiencies of around 19%, highlighting their rapid progress[1]. A key factor in this improvement is the development of high-performance non-fullerene acceptors, with Y6 emerging as a benchmark material thanks to its strong absorption, tunable energy levels, and efficient electron-accepting properties.

In OPVs, the active layer typically consists of a bulk heterojunction (BHJ) blend of a donor polymer and an acceptor like Y6. The efficiency of charge generation and transport in these blends depends critically on nanoscale morphology. Strong π–π stacking and well-defined lamellar spacing within Y6 domains can enhance charge mobility and boost device performance. In this study, we use scanning tunneling microscopy (STM) to directly visualize the molecular packing of Y6 and measure its unit cell dimensions under varying solvent conditions and molecular blends. By linking these structural observations to known morphology-performance relationships, we aim to provide insights into how processing conditions influence the nanoscale arrangement of Y6 and, ultimately, OPV performance.

## Results & Discussion

For samples containing additives, 100 μL of coronene in 100 μL of 1-phenyloctane (PO) was mixed 1:1 with the Y6-phenyloctane solution. For Y6-only samples, the molecule was dissolved directly in either octanoic acid or PO. Immediately before measurement, all solutions were further diluted 1:1, yielding a final Y6 concentration of approximately 25%. Solutions were deposited dropwise onto freshly cleaved HOPG surfaces for STM imaging at the solid–liquid interface.

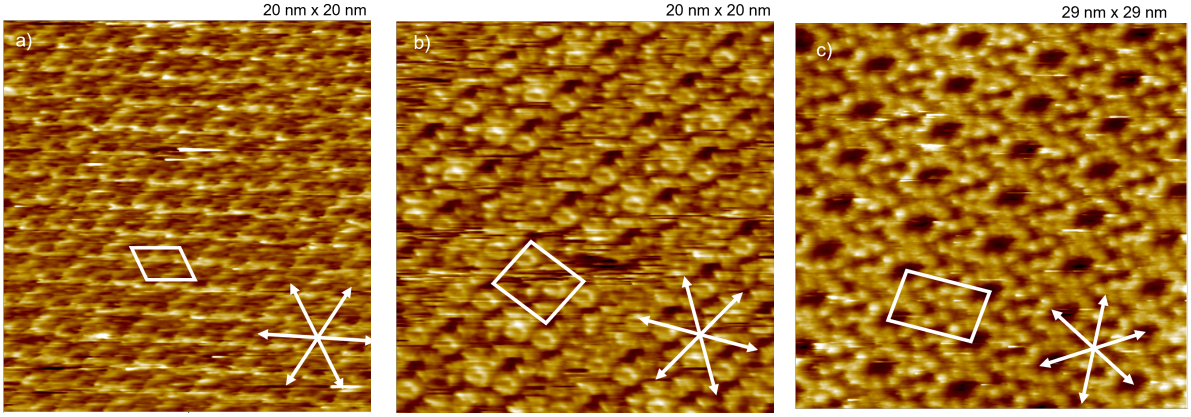


**Figure 1**. STM images (20 nm × 20 nm for a and b, 29 nm × 29 nm for c) showing the influence of solvent and blending on Y6 packing at the solid–liquid interface with HOPG. Lattice parameters a and b correspond to the measured lamellar spacings along the two principal crystallographic directions, and θ is the unit cell angle.
(a) Y6 in octanoic acid (OA), a = 1.4 nm, b = 2.3 nm, θ = 76.
(b) Y6 in 1-phenyloctane (PO), a = 3.6 nm, b = 6.0 nm, θ = 91°.
(c) Y6 in PO with coronene, a = 2.9 nm, b = 3.9 nm, θ = 65°.

STM imaging revealed clear differences in Y6 packing depending on the solvent and the presence of a molecular additive. Films deposited from octanoic acid (OA) showed relatively tight molecular packing, with lamellar spacings of a = 1.4 nm and b = 2.3 nm, and a unit cell angle of 76°. This compact arrangement likely reflects the limited extension of the alkyl side chains, as OA is a weaker solvent for them. Poor solvation restricts side-chain mobility, allowing the conjugated backbones to come closer together, which strengthens π–π stacking and leads to smaller lamellar spacings, particularly along the $a$ lattice direction.

In contrast, Y6 deposited from 1-phenyloctane (PO) exhibited much larger lamellar spacings (a = 3.6 nm, b = 6.0 nm, θ = 91°). PO is a better solvent for Y6, solubilizing both the backbone and side chains more effectively. This allows the side chains to stretch out, creating a more open lamellar structure. The nearly orthogonal unit cell angle suggests a packing arrangement that accommodates the extended side chains while still allowing strong π–π interactions along the backbones.

When Y6 was blended with coronene in PO, the lamellar spacings were intermediate (a = 2.9 nm, b = 3.9 nm, θ = 65°), and the unit cell became noticeably distorted. This points to strong π–π interactions between Y6 backbones and coronene, which pull molecules closer together along certain directions. At the same time, the presence of coronene disrupts the overall packing symmetry, leading to a skewed unit cell. The result is a delicate balance between backbone–backbone interactions, backbone–additive interactions, and steric effects from the side chains.

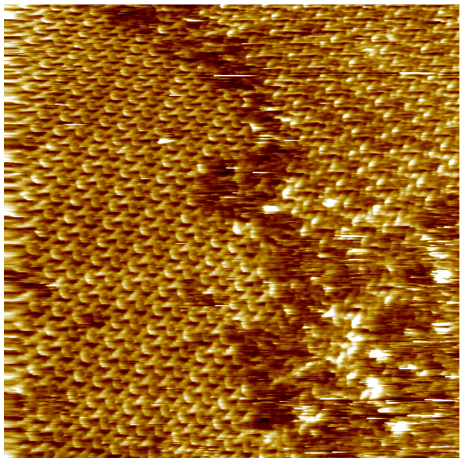

**Figure 2**. STM image (60 nm × 60 nm) of Y6 blended with coronene in 1-phenyloctane (PO) at the solid–liquid interface with HOPG. Multiple domains with distinct orientations are observed, highlighting how coronene influences Y6 molecular packing.

Overall, these observations demonstrate that the choice of solvent and molecular additives can subtly, yet significantly, influence Y6 packing. Tight packing in poor solvents may favor strong electronic coupling along the backbone, while expanded or distorted arrangements in good solvents or blends could influence charge transport by changing how molecules interact at the nanoscale. Understanding these effects provides a clearer picture of how processing conditions shape Y6 structure and, ultimately, OPV performance.

## Conclusions

Our STM results show that Y6 packing is highly sensitive to both the choice of solvent and the presence of molecular additives. In a poor solvent like octanoic acid, Y6 molecules pack tightly with limited side-chain extension, whereas in a good solvent such as 1-phenyloctane, the side chains stretch out, creating a more open structure. Adding coronene further alters the packing, leading to intermediate spacings, distorted unit cells, and the formation of multiple domains due to strong π–π interactions with the Y6 backbones. These findings highlight how subtle changes in processing conditions can significantly influence nanoscale order, which in turn affects charge transport. Understanding these effects gives valuable insight into how to tune Y6 morphology for better-performing organic photovoltaic devices.

## Acknowledgements

I would like to thank my supervisor, Filippo Giovanni Fabozzi, and staff scientist, Nikolai Severin, for training me in using the STM machine along with the data analysis involved in interpreting the images. I also appreciate my advisor, Stefan Hecht, who graciously hosted me in his lab group along with the IRES program, for allowing me to work abroad in Berlin.

**References**

[1] National Renewable Energy Laboratory. Best Research-Cell Efficiency Chart | Photovoltaic Research | NREL. NREL.gov, 2024. https://www.nrel.gov/pv/cell-efficiency.html.

[2] Ossila. Y6 Acceptor in Solar Cells: Structure, Benefits and Compatible Donors. Available online: https://www.ossila.com/pages/what-are-y6-acceptors.

[3] Zhang, G.; Li, X.; Chen, Y.; Wang, J.; Liu, H.; Zhao, W.; Ma, W.; Ade, H.; Hou, J. What We Have Learned from PM6:Y6. Adv. Mater. 2023, 35 (24), 2302005. https://doi.org/10.1002/adma.202302005

# Development of a UPyDAE Photo Switch

Photo-switchable molecules such as UPyDAE are valuable tools for controlling molecular properties with light, offering potential applications in smart materials and molecular devices. This study reports progress toward the synthesis of UPyDAE, focusing on the development and application of key synthetic techniques, including Schlenk line manipulations, thin-layer chromatography (TLC), column chromatography, nuclear magnetic resonance (NMR) spectroscopy, ultra-performance liquid chromatography (UPLC), and mass spectrometry (MS). While the full synthesis of the target photo switch was not completed, several intermediates were successfully prepared, monitored, and characterized, providing insight into reaction behavior and purity. The results highlight both the potential pathways for achieving the synthesis and the practical skills gained in modern organic synthesis.

## Introduction

Photo-switchable molecules are a versatile class of compounds capable of reversible structural changes in response to light. This property allows dynamic control over molecular polarity, shape, and optical behavior, which has been exploited in applications ranging from actuation and drug delivery to energy storage, tunable material surfaces, and advanced manufacturing techniques such as xolography. Despite their potential, implementing efficient photo switching in solid-state or crystalline systems remains challenging. Steric constraints and limited molecular mobility often impede the full conformational changes required for robust switching. In addition, the strong intermolecular interactions present in densely packed solids, such as π–π stacking, hydrogen bonding, or van der Waals forces, can restrict motion, reduce switching efficiency, or even lock molecules in one configuration. Achieving reversible switching in these environments thus requires careful molecular design to balance light responsiveness with structural flexibility, as well as precise control over assembly and aggregation.

This work focuses on synthesizing Ureidopyrimidinone–Diarylethene (UPyDAE), a photo-switchable molecule that combines two key features. The diarylethene core acts as a light-sensitive "switch," changing its shape when exposed to UV or visible light. Attached to this is a UPy unit, which can form self-complementary hydrogen bonds that encourage molecules to assemble into organized structures. These interactions may influence how UPyDAE behaves in solid or aggregated states. By exploring its synthesis and characterization, this study highlights both the challenges of making complex photo-switchable molecules and the strategies used to optimize their assembly and function.

## Results & Discussion

Reactions were carried out under an inert nitrogen atmosphere using Schlenk techniques

to prevent moisture- or oxygen-sensitive reactions. TLC was used to monitor reaction progress at each step. Column chromatography was employed to purify intermediates when necessary.

For analytical characterization, UPLC was used to separate reaction components, mass spectrometry confirmed molecular weights and NMR spectroscopy provided structural verification of the intermediates. Due to incomplete synthesis, no full UV-Vis characterization of UPyDAE was possible; however, the previously stated methods offered critical insight into the purity and identity of the compounds prepared.

The synthetic strategy toward UPyDAE is outlined in Figure 1. Key intermediates were successfully prepared, with observed yields summarized in Table 1.

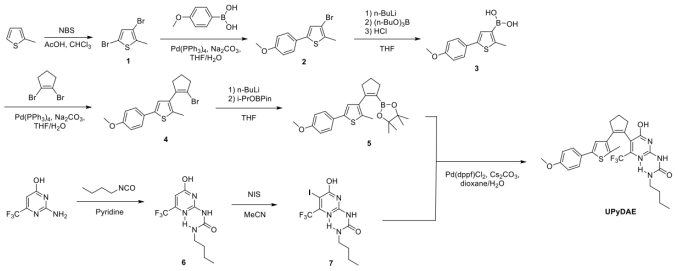


**Figure 1.** The synthetic route of UPyDAE[1]

**Table 1**. Reaction yields of UPyDAE intermediates (Steps 1 through 4)

| Step | Intermediate | Yield (%) |
|---|---|---|
| 1 | 4-dibromo thiophene | 13.52 |
| 2 | 3-bromo-5-(4-methoxyphenyl)-2-methylthiophene | 16.02 |
| 3 | (5-4-methoxyphenyl)-2-methylthiophen-3-yl) boronic acid | 39.19 |
| 4 | 3-(2-Bromo-1-cyclopenten-1-yl)-2-methyl-5-(4-methoxyphenylthiophene | 32.66 |

After purification, TLC analysis revealed clear separation of intermediates from starting materials and side products, demonstrating that reactions proceeded as expected. The identity and purity of intermediates were further confirmed by 1H NMR spectroscopy, UPLC, and mass spectrometry.

*Analytical Characterization*

UPLC-MS analysis confirmed the presence of targeted intermediates and allowed estimation of purity. Peaks observed in UPLC chromatograms corresponded to the expected molecular weights in mass spectrometry, validating the success of the partial syntheses. Even without the completion of the full UPyDAE molecule, this data provided confidence in the reaction design and approach.

As seen in Table 1, the initial steps, involving halogenation and early functionalization, gave relatively low yields (13–16%), likely reflecting the inherent challenges of these transformations, including side reactions and incomplete conversion. In contrast, later steps, particularly the formation of the boronic acid intermediate and its subsequent coupling, proceeded more efficiently, with yields increasing to 33–39%.
These findings emphasize that synthetic organic chemistry often involves iterative troubleshooting and intermediate characterization before the final target is realized. The skills developed-particularly handling air-sensitive compounds, purification, and analytical evaluation are directly transferable to completing the UPyDAE synthesis in future work.

**Conclusions**

This work represents progress toward the synthesis of the UPyDAE photo switch, demonstrating practical experience with Schlenk techniques, TLC, NMR, column chromatography, UPLC, and mass spectrometry analysis. While the complete photo switch was not obtained, intermediate compounds were successfully synthesized and characterized, providing important insights into reaction pathways and conditions. It is hoped that future efforts, independent of this work, will achieve full synthesis of the molecule and allow UV-Vis characterization to gain further insight into its photophysical properties.

## Acknowledgements

I would like to thank my research mentor, Jordan Thelemann, for his assistance in training me on several techniques involved in the synthesis of the UPyDAE molecule and several other molecules. Additionally, for his supervision in monitoring and purifying the reaction and interpreting the subsequent data. I would also like to thank Kailey Sun Marco for her additional assistance in training me in synthesis techniques. I also appreciate my advisor, Stefan Hecht, who graciously hosted me in his lab group along with the IRES program, for allowing me to work abroad in Berlin.

## References

[1] Tang, B.; Pauls, M.; Bannwarth, C.; Hecht, S. Photoswitchable Quadruple Hydrogen-Bonding Motif. J. Am. Chem. Soc. 2024, 146(1), 45–50. https://doi.org/10.1021/jacs.3c10401