

SYNTHESIS AND EVALUATION OF NOVEL FLUORENE-BASED DYES FOR DSSC

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DSSCs (Dye-Sensitized Solar Cells) are devices capable of converting solar energy into electricity through semiconductor nanoparticles sensitized by dyes. In order to propose more sustainable and less expensive dye options, there is a growing interest in the development of efficient metal-free photosensitizers, produced through simpler syntheses [1]. The development of purely organic dyes aims at constructing a structure in which an electron-donating group is linked to a conjugated bridge, which is connected to an electron-accepting group capable of anchoring to the semiconductor (usually TiO₂) [2].

This work was based on the synthesis and characterization of novel dyes using fluorene as the main conjugated bridge in order to obtain suitable photosensitizers for DSSCs. Four fluorene derivatives were synthesized using different donor (D) and acceptor (A) groups in two molecular architectures: D-A-D for compound 2TPA-CA and A-D-A for compounds TPA-2CA, TPA-2CYA, and DPA-Th-2CYA. The synthesis of these products uses 2,7-dibromofluorene as the main starting material, which was submitted to the following reactions: Knoevenagel condensation using different aldehydes, and then Suzuki cross-

coupling using different boronic acids. Specifically for the compounds TPA-2CYA and DPA-Th-2CYA, a final step was carried out after the cross-coupling, consisting of another Knoevenagel condensation using cyanoacetic acid.

Photophysical studies of absorption and emission in solution were performed, as well as solid-state reflectance via DRUV-Vis. The compounds showed high molar absorptivity values in solution ($\epsilon \sim 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$). Furthermore, all compounds were applied in the sensitization of DSSCs in order to evaluate their photoconversion efficiencies (%) and compare them with the ruthenium complex N719, one of the best commercial dyes. Furthermore, the solar cells were also submitted to IPCE tests. Finally, the synthesized compounds showed η values ranging from 0.41% to 2.23%, while N719 achieved $\eta = 4.78\%$. Overall, compounds from the A-D-A architecture exhibited better efficiencies, specially DPA-Th-2CYA, reaching the highest efficiency of 2.23%. These results highlight the great potential of fluorene as a versatile “building block” for the development of new photosensitizers, especially in the A-D-A architecture, which is currently underexplored in the literature.

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