Synthesis, characterization and photo physical-theoretical analysis of D-π-A compounds. 2. Chain length effect through even-odd effect on the photophysical properties

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Résumé en anglais	In the continuous search for new compounds for solar devices, the family of dipolar D-π-A molecules, which have a donor (D) and an acceptor (A) charge joined by a conjugate bridge, have been the focus of attention in the recent years due their different properties. As we have shown before, there is a connection between the geometry of molecules based on tertiary asymmetric amines and their quantum yield. In the current work, four new compounds based on the same backbone molecule ((E)-2-cyano-3-(5-((E)-2-(9,9-diethyl-7-(phenylamino)-9H-fluoren-2-yl)vinyl)thiophen-2-yl)acrylic acid), but with different substituent, were synthesized. It is shown that the chain-size of the substituent group modifies the quantum yield. The news substituents introduced are a propyl (M8-3), butyl (M8-4), pentyl (M8-5) or hexyl (M8-6) group. In general, it was possible to see that the new substituents were able to increase their performances. Furthermore, an odd-even substituent effect, between propyl/pentyl and butyl/hexyl, was found and the theoretical geometrical data was able to follow the trend. However, theoretically, this substituent effect was inverted in the case of M8-3 and M8-4, which may be due to the disappearance in the emission patterns of an excited state close to 450 nm (at λ2), as it was shown in the experimental data. The most suitable behaviour belongs to [(E)-2-cyano-3-(5-((E)-2-(9,9-diethyl-7-(phenyl(propyl)amino)-9H-fluoren-2-yl)vinyl)thiophen-2-yl)acrylic acid] (M8-3). M8-3 has the highest quantum yields on average in all studied solvents; even higher than the last reported compounds with methyl (M8-1) and ethyl (M8-2) groups. Theoretically, the most likely explanation is that the dihedral angle formed between the carbonyl acceptor and nitrogen electron donor (Aryl-CO), should be as small as the molecule M8-3. This isolated compound has an average quantum yield including all solvents of 58.1% (average value), showing that a long group is not necessary to improve the performance.
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