PÔSTER - RESUMO - DIVULGAÇÃO

UNEXPECTED PHOTOINDUCED ENHANCEMENT OF FLUORESCENCE QUANTUM YIELD IN AN ISOXAZOLINE–CARBAZOLE-BASED COMPOUND

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Carbazole-based organic compounds [1] have garnered considerable attention for applications in optoelectronic devices owing to their chemical versatility and favorable photophysical properties. Carbazole derivatives exhibit high thermal stability and molar absorption coefficients on the order of 10^4 L/mol.cm [2–4], absorption and fluorescence in the UV–Vis region and act as hole-transporting materials in OPVs [5].

In this study, we investigate the photophysical properties of carbazole/isoxazoline derivatives in acetonitrile solution (10^-5 mol/L) with four distinct substituents: a phenyl (1a), chlorophenyl (1b), bromophenyl (1c) and an aldehyde group (1g). The photophysical properties of the carbazole unit are clearly identified in the spectroscopic measurements performed for all compounds, including absorption bands at 233, 289, and 330 nm, as well as

fluorescence emission at 342 nm, which are attributed to the carbazole moiety [6]. Additionally, a molar absorption coefficient on the order of 10^4 L/mol.cm at 290 nm, a Stokes shift of 970 (1/cm), and an excited-state lifetime of 7 ns were observed. For the aldehyde-substituted compound (1g), additional bands overlapping with the carbazole bands were identified in both the absorption and fluorescence spectra. Notably, these compounds exhibited an unexpected enhancement of fluorescence quantum yield after UV irradiation, with the quantum yield increasing by factors of 2.1, 5.4, 3.4, and 4.6 for 1a, 1b, 1c and 1g, respectively.

The isoxazoline moiety in the chlorophenyl (2b) and bromophenyl (2c) compounds was oxidized and converted into isoxazole. This structural modification changes the chemical nature of the heterocyclic moiety, rendering it more rigid and aromatic. Although the absorption and fluorescence spectra retained profiles very similar to those of the isoxazoline-based compounds, the remarkable photoinduced enhancement of fluorescence quantum yield previously observed for the isoxazoline derivatives was completely absent in the isoxazole derivatives after UV irradiation. This result indicates that the conformational mobility of the isoxazoline moiety is crucial for the occurrence of this effect. The result was further validated through computational simulation. The ability to manipulate the photophysical properties of a compound, particularly to modulate its fluorescence quantum yield, enables the development of diverse applications in optoelectronic devices.

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Palavras-chave: photophysical; oxidized; isoxazoline; carbazole.