PÔSTER - RESUMO - DISPOSITIVOS OPTOELETRÔNICOS

INVESTIGATION OF FLUORESCENCE QUENCHING OF BENZAZOLE DERIVATIVES BY FULLERENE AND NON-FULLERENE ELECTRON ACCEPTORS FOR APPLICATION IN ORGANIC SOLAR CELLS

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Photoinduced electron transfer (PET) in organic donor–acceptor (D–A) systems plays a central role in photocurrent generation in organic solar cells (OSCs). In this work, we investigated the photophysical interactions between three benzazole-based fluorophores (BST, BSe, and NC-68) and electron acceptors of the fullerene type (C60 and PyC60) and non-fullerene type (Y18), with emphasis on fluorescence quenching driven by PET mechanisms. The addition of electron acceptors led to pronounced fluorescence quenching of the benzazole derivatives, accompanied by significant modifications in their excited-state properties. Furthermore, analysis of the absorption and emission spectra of both fluorophores and acceptors indicated that fluorescence quenching is not governed by resonance energy transfer. Thus, the results point to photoinduced

electron transfer as the primary quenching mechanism. The efficiency of this process was evaluated through Stern–Volmer analysis using data obtained from five experimental concentration points. Stern–Volmer constants (Ksv), excited-state lifetimes (t0), and bimolecular quenching rate constants (Kq) were determined. The results show that, for the three fluorophores studied, quenching efficiency follows the order Y18 » PyC60 > C60. For the BST fluorophore, Ksv values were on the order of 4.3 × 10^3 L/mol for C60, 8.0 × 10^3 L/mol for PyC60, and 5.1 × 104 L/mol for Y18. The BSe fluorophore exhibited Ksv values of approximately 3.4 × 10^3 L/mol for C60, 5.3 × 10^3 L/mol for PyC60, and 5.8 × 104 L/mol for Y18. A similar behavior was observed for NC-68, which showed highly efficient quenching in the presence of the non-fullerene acceptor Y18, indicating strong electronic coupling between donor and acceptor. The bimolecular quenching rate constants associated with Y18 reach values on the order of 10^{12} L/mol·s for all three fluorophores, suggesting extremely efficient processes close to the diffusion-controlled regime. The higher efficiency observed for PyC60 compared to C60 is attributed to its greater electron affinity. Theoretical predictions, based on electronic structure calculations and energy level alignment between the frontier orbitals of the fluorophores and the acceptors, corroborate the experimental results and indicate that photoinduced electron transfer is energetically favored, particularly in the case of the non-fullerene acceptor Y18. The agreement between experimental data and theoretical predictions highlights the decisive role of molecular structure and acceptor nature in modulating the photophysical properties of benzazole-based fluorophores, contributing to the rational design of new functional materials.

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Palavras-chave: photoinduced electron transfer; fluorescence quenching; benzazole derivatives; fullerene acceptors; non-fullerene acceptors;.