

Exploring Triplet State Formation and Excited State Dynamics of a Group of Corrole with Saccharide Ligands

D F DE OLIVEIRA¹, B A IGLESIAS², AND L DE BONI¹

¹*Physics and Materials Science, São Carlos Institute of Physics, São Carlos, Brazil*

²*Department of Chemistry, Federal University of Santa Maria, Santa Maria, Brazil*

Contact Email: diegofdeoliveira@usp.br

Intersystem crossing (ISC) is a spin-forbidden process of transition from singlet to triplet states present in specific molecules like photosensitizers, useful in various biological applications such as photodynamic therapy and antimicrobial inactivation. However, quantifying ISC in molecules is challenging due to its non-radiative nature. Corroles, being biocompatible molecules, undergo ISC and can be further optimized with lateral ligands [1]. This study aims to characterize a group of corroles bearing two pentafluorophenyl ligands and a distinct saccharide ligand, focusing on determining their ISC quantum yield and excited-state decay rates. Fluorescence quantum yield is determined by comparison with a standard, while fluorescence lifetime is obtained by observing fluorescence exponential decay post-excitation. ISC quantum yield is gauged using a technique involving double excitation-induced fluorescence, where two laser pulses are applied a few nanoseconds apart. The long-lived triplet population generated after the first excitation do not have time to return to the ground state, reducing fluorescence induced by the second pulse, allowing the triplet population determination [2]. Finally, radiative, intersystem crossing, and internal conversion decay rates are calculated, providing a comprehensive understanding of molecules' excited-state dynamics on the nanosecond timescale. Results indicate low fluorescence quantum yields yet significant ISC quantum yields across all molecules. Notably, the lactose ligand corrole exhibits the highest ISC quantum yield (67%) and also the higher fluorescence quantum yield (9%), suggesting the potential molecular stabilization benefits of longer saccharide chains. Saccharide ligands generally enhanced ISC efficiency and reduced decay via heat transfer, hinting at expanded possibilities for corrole functionalization.

References

- [1] A Kumar, D Kim, S Kumar, A Mahammed, D G Churchill and Z Gross, *Chem. Soc. Rev.* **52**, 573 (2023)
- [2] R de Q Garcia and L De Boni, in: *Ultrafast Optics 2023 - UFOXIII, Technical Digest Series*, Optica Publishing Group, 2023, paper P2.8