

SEPTEMBER  
23-27<sup>TH</sup>  
2024



BRAZILIAN MEETING  
ON ORGANIC SYNTHESIS  
BENTO GONÇALVES, RS - BRAZIL

## Theoretical and Experimental approach to visible light-catalysed $6\pi$ -photoelectrocyclization

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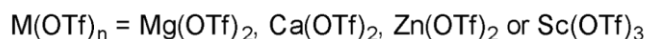
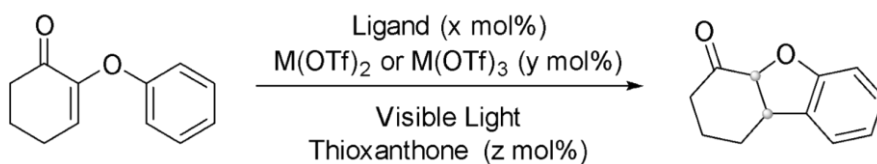
Keywords: Asymmetric Synthesis, Photocatalysis, DFT

### ABSTRACT

Photocatalyzed reactions are an excellent technique to generate chiral compounds. Combined with Lewis acids, these processes can be visible light driven. This work aims to investigate the effects operating on a recently published  $6\pi$  catalyzed electrocyclization [1] and explore catalysts that promote efficient visible light driven combining computational and experimental techniques.

Quiral ligands based on bisoxasoline, PyBox and N-Oxide structures coordinating with a metal entity were used to induce enantioselectivity in the studied reaction based on chiral complexation with the substrate. To achieve the triplet state, a photosensitizer is necessary. Efficient iridium photosensitizers are expensive and not commonly accessible. Instead, thioxanthone-based photosensitizers were utilized.

High level DFT calculations shows that neutral structures are more stable. Subsequent TDDFT calculations will examine its absorption and overlap with emission spectra photosensitizer. To prevent background reactions, the complex that results in the strongest bathochromic shift is desired.



### ACKNOWLEDGEMENTS

The authors acknowledge the STI-USP, CNPq, CAPES and the São Paulo Research Foundation (FAPESP).

### REFERENCES

[1] Edtmüller, V., Pöthig, A., Bach, T.: Tetrahedron, 73(33), 5038–5047 (2017)