

A study of different oxidation states of Zinc(II)-Phthalocyanines

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Abstract: The phthalocyanines and naphthalocyanines are important pigments on the industry, but more recently several studies reported their biological activity against tumors because of their photochemical properties. However their synthesis are expensive. [1, 2] Computational simulations can be used to estimate the molecules that may have good results in photodynamic therapy and reduce its costs. In order to analyses how the oxidation state can influence on the structural and optical properties of phthalocyanines and naphthalocyanines we have conducted computational studies with different oxidation states on monomers and dimers of Zinc(II)-phthalocyanine.[3] The computational method employed was based on Density Functional Theory (DFT). Geometry optimization and TD-DFT were carried out using the BLYP functional and 6-311G basis set and the dispersion correction included by the Grimme's approach (D3-BJ). The understanding of how the oxidated and reduced phthalocyanines have their optical properties changed can help us to understand the activity against tumors.

Key-words: Phthalocyanine, Density Functional Theory, Photodynamic Therapy, oxidized and reduced photosensitizers.

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References:

- [1] Bonnett R Chemical; Society Reviews 24, 19 (1995)
- [2] J, Simon; Molecular Semiconductors: Photoelectrical Properties and Solar Cells (1985)
- [3] Bettanin, F.; Fontinelles, T. A.; Maciel, C. D.; Dias, LG; Coutinho Neto, M. D.; Homem-de-Mello, P., Theoretical Chemistry Accounts 134, 152 (2015).