

Synthesis and Characterization of 5,10,15,20-Tetrakis(4-ethylphenyl)porphyrin and (Zn²⁺, Mn²⁺, Sn²⁺, Ni²⁺, Al³⁺, V³⁺)-Derivatives: Photophysical and DFT study

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A novel family of porphyrins based on 5,10,15,20-Tetrakis(4-ethylphenyl)porphyrin (1) and six metallo-derivatives (Zn²⁺(2), Sn²⁺(3), Mn²⁺ (4), Ni²⁺ (5), Al³⁺ (6) and V³⁺ (7)) were synthesized via the Alder-cols method (synthesis yield between 59%-75%) and characterized through ¹H- and ¹³C- NMR, MALDI-TOF mass spectrometry and FT-IR assay. Photophysical study was carried out by UV-Vis and fluorescence spectrophotometry with the aim of assessing their potential as dye sensitizers for photodynamic therapy (PDT). In this regard, fluorescence quantum yield values are between 0.002-0.38, being the macrocycle 3, the porphyrin with the highest fluorescence quantum yield while the derivative 7 showed the lowest value. Quantum chemical calculations were carried out to study the molecular structure of the porphyrins and to get insight of the luminescent process for 1, which is the free metal system and 3 which includes Sn²⁺ as metal center. Results indicated that the emissive states involve the transitions with LLCT character for 1, while for 3 it is ML[?]LCT. This fact evidenced the metal effects on their photophysical properties. Finally, optical and spectroscopic properties and besides, DFT study suggest that 3 could be used as sensitizer in photodynamic therapy applications. © 2019 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

DFT

Fluorescence

metalloporphyrin

porphyrin

quantum yield