

Experiments and calculation on new N,N-bis-tetrahydroacridines

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New bis tetrahydroacridines were synthesized by Pfitzinger condensation of 5,5'-(ethane-1,2-diyl) diindoline-2,3-dione with several cyclanones [1]. They were characterized by NMR, MS, FT-IR. Their optical and electrochemical properties were investigated by use of UV-Vis and voltammetric (cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry) measurements [2]. The computational study was carried out with the software Spartan14 from Wavefunction, Inc. Irvine CA, USA for the lowest energy conformers of each structure, in vacuum conditions, at ground state using DFT models. B3LYP levels of theory [3] with basis set 6-311G (d, p) [4] was chosen for properties computations.

Their study recommended this class of π -conjugated heteroaromatic compounds for potential applications in different branches of medicinal chemistry, dye industry and metal chemosensing.

References

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