
Photophysical properties of a dual emitter : a TD-DFT study

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Résumé

Optical properties of 5-(4-dimethylaminophenylethynyl)-1,10-phenanthroline (Phen-PENMe2)[1] in aprotic solvents were studied. Phen-PENMe2 displays a dual emission, which is stemming from the presence of two distinct emissive excited states : an intramolecular charge-transfer (ICT) state and a locally excited (LE) state. The dual emission of Phen-PENMe2 was studied using a combined experimental and theoretical approach. TD-DFT calculations were performed to give more insights to the optical behavior of the compound, linking the two excited states to two different conformations of the molecule. In view of the experimental and theoretical results, the Phen-PENMe2 compound can be seen as a potential local ratio-metric probe for medium polarity.

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