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Theoretical Study of the Photophysical Properties and Potential Use of Pseudo-Hemi-Indigo Derivatives as Molecular Logic Gates

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Abstract : Introduction: Molecular Logic Gates (MLGs) are considered molecular machines that can perform complex work, such as solving logic operations. Molecular switches, which are molecules that can experience chemical changes are examples of successful types of MLGs. Recently, a simple MLG that can perform basic and complex logic operations was experimentally developed by Quintana-Romero and Ariza-Castolo. They selected the hemi-indigo structure, as its interaction with visible light makes it an excellent candidate for the design of molecular switches. It undergoes Z and E isomerism where the axis of the molecular switch is a double bond. Methodology: In this study, the photophysical properties of pseudo-hemi-indigo derivatives are examined, i.e., derivatives of molecule 1 with anthracene, naphthalene, phenanthrene, pyrene, and pyrrole. In conjunction with some trials that were conducted, the level of theory mentioned subsequently was opted for. The structures under study were optimized in both cis and trans conformations at the PBE0/6-31G(d,p) level of theory. The absorption spectra of the structures were calculated at the PBE0/DEF2TZVP level of theory. In all cases, the absorption spectra of the studied systems were calculated including up to 50 singlet- and triplet-spin excited electronic states. Transition states (cis → cis, cis → trans, and trans → trans) were obtained for the molecules in cases where it was possible, as well as the corresponding absorption spectra. For this purpose, the PBE0/6-31G(d,p) level of theory was used for the optimization of the transition states and the PBE0/DEF2TZVP methodology was employed for the respective absorption spectra. Emission spectra were obtained for the first singlet state of each molecule in cis both and trans conformations in the PBE0/DEF2TZVP level of theory as well. All studies were performed in chloroform solvent that was added as a dielectric constant and the polarizable continuum model was also employed. Findings: Specifically, shifts of up to 30 nm are observed, while the transition state is shifted up to about 150 nm in the cis-cis isomerization. The electron density distribution is also examined, where charge transfer (CT) and electron transfer (ET) phenomena are observed regarding the three excitations of interest, i.e., H-1 → L, H → L and H → L+1. Using protonation as input, selected molecules act as MLG. Conclusion: The theoretical data so far indicate that both the cis-trans isomerization, and cis-cis and trans-trans conformer isomerization affect the UV-visible absorption and emission spectra. The computational data obtained are in agreement with available experimental data, which have predicted that the pyrrole derivative is a MLG at 445 nm and 400 nm using protonation as an input, while the anthracene derivative is a MLG that operates at 445 nm using protonation as an input. Finally, it was found that selected molecules are candidates as MLG using protonation and light as inputs. The results of this study will be submitted for publication.

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