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Computational study of photosensitizing IR780 and its interaction with transition metals cations

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Abstract: Heptamethine dyes are chemical compounds within the indocyanine dye family, and have being explored in photodynamic therapy (PDT)[1], since they are reported to have photosensitizing characteristics. Besides, experimental results indicated that its interaction with magnetic nanoparticles influenced their thermal and spectroscopic properties. In this work we have studied the electronic and thermal properties of IR780 molecule (Figure 1), a lipophilic agent, using Density Functional Theory (DFT) simulations. DFT calculations were performed using B3LYP functional and D3BJ empirical dispersion correction, considering 6-31G(d,p) basis set and def2-TZVP auxiliary basis, as implemented in Orca software. Also, excited state optimization using time-dependent DFT (TD-DFT) methodology was performed in order to compare the infrared spectra in both cases.

In order to understand the role of the interaction with nanoparticles, molecule's bond with transition metals cations Mn^{+2}, Fe^{+2} and Co^{+2} were investigated, aiming to analyze the changes in dipole moment magnitude and direction, also changes in charge distribution.

Comparing IR780 in ground and excited states, dipole moment decreased substantially, and its direction also changes. In terms of charge distribution the largest differences were in atoms of the central ring. Considering the structures with cations, the larger charge distribution variations were observed in atoms nearer from the cations, as expected. Differences in single point energies of IR780 bonded to metal cations indicate formation of chemical bonds, and the difference increases proportionally with atomic radii.

Although it was not observed significant change in the molecule's geometry between ground and excited states, changes in the infrared spectrum were noticed. In order to clarify these results, further studies are in progress.

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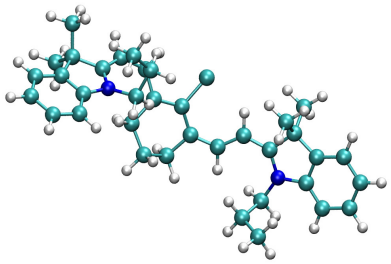

Figure 1: Optimized structure of IR780

Key-words: Density Functional Theory, IR spectrum, excited states, coordinated atoms.

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