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Performance Analysis of TD-DFT Calculations for a Series of Iron Complexes

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The optical properties of coordination complexes make them a class of compounds with important applications in the fields of materials and biology. With a view to low-cost applications, complexes of abundant metals in the Earth's crust, especially Fe, are frequently studied in the development of new materials. The accuracy and predictive capacity of computational chemistry approaches are extremely important for accelerating scientific discovery, providing deeper first-principles-based understanding of chemical phenomena, and enabling rapid *in silico* screening to reduce costs and waste in trial-and-error experimental approaches. This work aims to study the electronic excited states of a series of Fe complexes by TD-DFT using the CAM-B3LYP/def2-TZVP[3] method and comparing the results obtained with the experimental UV-Vis spectra available in the literature. The geometries of the complexes were optimized using the PBEh-3c[4] composite method, which was the most effective computational approach for electronic ground state geometries in a benchmark carried out for a series of 20 Fe complexes. TD-DFT calculations were carried out using the conductor-like polarizable continuum model (CPCM)[5] to evaluate the effects of the solvent according to the spectra available in the literature. The absolute percentage deviation ($\mathrm{APD} = (|\lambda_{\mathrm{max,calc}} - \lambda_{\mathrm{max,exp}}|/\lambda_{\mathrm{max,exp}}) \cdot 100$) values were calculated for all the complexes considering the calculated and experimental λ_{max} and are shown in **Figure 1**. TD-DFT calculations will also be carried out using other functionals to find the best method for describing the excited states of this type of complex.

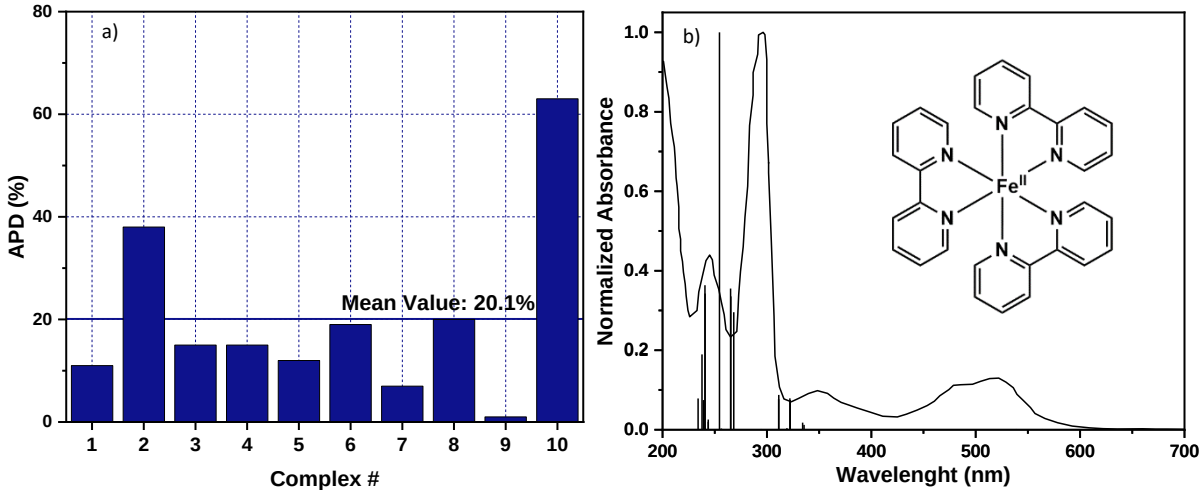

Figure 1: a) Comparison of the absolute percentage deviation (APD) values obtained for the series of molecules studied using the CAM-B3LYP/def2-TZVP method; b) Calculated and experimental electronic transitions for the $[Fe(bpy)_3]^{2+}$ (**4**) complex.

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