Structures and spectroscopic properties of indigo in complex with \( \beta \)-cyclodextrin and its derivatives

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Abstract: Indigo (IG) is a deep blue dye utilizing for dyeing industry. It is interesting to find a new technique to increase amount of IG in water for a direct dyeing of fabric. In our experimental study, \( \beta \)-cyclodextrin (\( \beta \)-CD) and 2,6-hydroxypropyl-\( \beta \)-cyclodextrin (2,6-HP-\( \beta \)-CD) can help indigo (IG), a vat dye, more dissolve in water. The descriptions of structures and how IG interacts with \( \beta \)-CD and 2,6-HP-\( \beta \)-CD are of interests since it will be useful to add hydrotropic substance to improve a water solubility of IG. In this work, a 1:1 ratio of IG and each \( \beta \)-CD and 2,6-HP-\( \beta \)-CD were studied. The IG/\( \beta \)-CD and IG/2,6-HP-\( \beta \)-CD inclusion complexes were predicted using the Autodock Vina program followed by optimization. The CPCM model was applied to include solvent effect in the calculations. The fully optimized structures obtained from the B3LYP/6-31G(d) calculations were further applied to simulate the UV-Visible spectra of the inclusion complexes. The time-dependent density functional theory (TD-DFT) calculations with the B3LYP functional was selected. The predicted UV-visible spectra of each inclusion complex showed that the maximum absorption wavelength is in a range of 708 and 710 nm. The intramolecular and intermolecular charge transfer were observed.

Keywords: Indigo; 6-HP-\( \beta \)-CD; AutoDock Vina; MD simulation