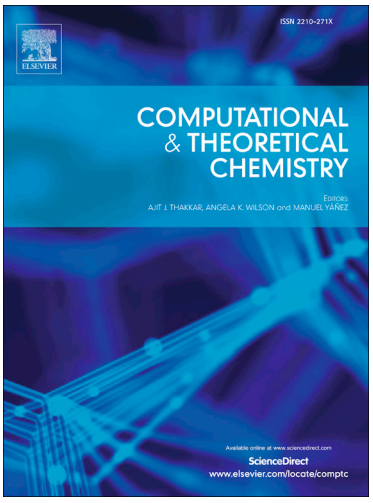

Molecular Structure and Absorption Spectral Properties of Corrole Isomers: DFT and TDDFT-IEFPCM investigations

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Molecular Structure and Absorption Spectral Properties of Corrole Isomers: DFT and TDDFT-IEFPCM investigations

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Abstract: Corrole has become one of the most important branches of porphyrin chemistry for the better optical properties than traditional porphyrin. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) have been utilized to simulate the molecular structures and electron absorption spectra of corrole and isomers. The molecular structure and charge distribution results revealed that the inner hydrogen atoms of the homologous isomers exhibit similar charge distribution. The corrole isomers show better absorption than corrole in Q band due to the carbon-nitrogen-swap structure, especially in isomers NCC1/NCC2. The diverse Q bands illuminate that the light absorption performance of corrole isomers vary in different polarity solvents based on the integral equation formalism polarizable continuum model (IEF-PCM) results. Obviously variations of NCC5 and NCC6 spectra in the three solvents indicated that both isomers are sensitive to the polarity of solvents and could be applied to regulate the light absorption ability of them by adjusting the polarity of the solvent. These theoretical researches would be conducive to the molecular design of novel multi-band photon absorption corrole isomers.

Keywords: Corrole isomers; DFT; TD-DFT; Absorption spectrum

1 Introduction

Corrole is a new series of multifunctional porphyrin compounds. The one less methylene bridge in structure lead to its smaller internal cavity and lower symmetry than general porphyrin [1]. Like trivalent anions, corrole can form stable metal complexes with high oxidation state transition metals [2]. Erben [3] found that when interconverting among internal NH protons happened frequently enough, the configuration of both the two configurational isomers of corrole became symmetrical similar to that of the C_{2v}. Corrole, with unique chemical and photochemical properties, has been widely used in catalysis [4], electrochemistry [5], sensors [6], non-linear

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