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TD-DFT study of octinoxate UV-Visible spectra

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Abstract

Ultraviolet radiation from sunlight is the main cause of non-melanoma skin cancer.[1] In order to mitigate the effects of ultraviolet radiation on the skin, many chromophores have been used in the photoprotectors.[2] The goal of this work is to study the ultraviolet spectrum of octinoxate molecule, using the Time Dependent Density Functional Theory at the PBE0/6-31+G(d,p) level of theory, and analyzes the solvent effects (n-Hexano, Chloroform and dimethyl sulfoxide. They were computed through the integral equation formalism of the polarizable continuum model. Our outcomes show that the main energy absorption is due to the HOMO–LUMO transition. The results mainly suggest π→π* contribution for this transition. Thus, despite the solvation model is implicit it reproduces the qualitative effects of solvatochromic shifts.

Keywords: octinoxate, PBE0, IEF-PCM

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