

Área: TEO

TD-DFT Simulations on the UVA and UVB Absorptions of the Avobenzone, Octocrylene, Octisalate, Homosalate e Bemotrizinol Molecules

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Highlights

- UVA and UVB absorptions to investigate solar protection.
- Keto and enol structures have different ultraviolet absorptions.
- There is no red shift from water, methanol, and ethanol solvents

Resumo/Abstract

Photoprotection is intrinsically connected to human health, playing a crucial role in combating premature aging, skin cancer, and other dermatological pathologies. With the increase in greenhouse gas concentrations and the depletion of the ozone layer, high exposure to solar radiation becomes a more urgent issue. According to the World Health Organization, cancer is one of the leading causes of death worldwide, accounting for nearly one in six deaths in 2020. It occurs due to mutations in the genes responsible for the production and maintenance of cells and is therefore classified as a degenerative disease. Organic sunscreens protect against the UVA and UVB solar radiation. While UVB radiation exclusively affects the epidermis, UVA radiation can reach the deeper layer, the dermis. When UVB rays reach the cells of the epidermal layers, melanocytes stimulate the release of melanin in the affected areas, which act to absorb these rays and offer protection to the cells.

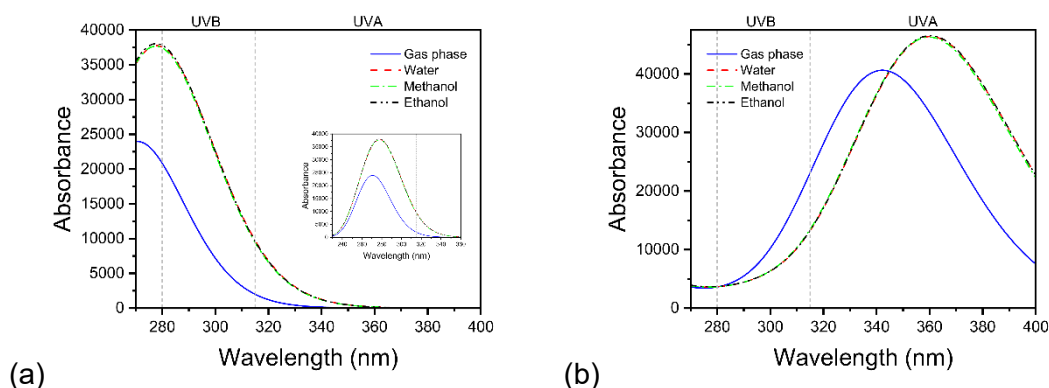


Figure 1. UVA and UVB absorptions spectra simulated by TD-DFT/B3LYP approach in singlet excitation. Keto Avobenzone (a); enol Avobenzone (b).

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