

Área: FIS

Theoretical analysis of the influence of substituents on the charge distribution of anthraquinones

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Keywords: Anthraquinones, Aloe vera, DFT

Highlights

- DFT analysis performed for 9,10-anthraquinone and its derivatives aloe emodin, emodin, and rhein;
- Insights into the electronic properties of anthraquinones, essential for understanding their photochemical behavior

Abstract

Compounds derived from the *Aloe vera* plant, such as anthraquinones, are known due to their biological and photochemical properties¹. Anthraquinones are aromatic organic compounds formed by three conjugated benzene rings, whose basic structure derives from anthracene, with two carbonyl groups in positions 9 and 10. Emodin has been featured by infrared (IR) and ultraviolet (UV) to investigate the interaction with DNA *in vitro* indicating intercalation or external binding mechanisms². DFT simulations on the Aloe emodin showed electronic properties for Reactive Oxygen Species (ROS) associated with dichroism spectroscopy to study DNA interaction³. In this study, computational analyses were performed on the 9,10-anthraquinone (Fig. 1a), rhein (Fig. 1b), aloe emodin (Fig. 1c), and emodin (Fig. 1d) to investigate the charge distribution. Geometry relaxations were carried out using Density Functional Theory (DFT) with the B3LYP functional and the def2-TZVP and def2-TZVPP basis sets. Through the results, the charge distribution change occurred due to the presence of different substituent groups in each molecule. Therefore, this study contributes to characterizing the charge profiles of the anthraquinones, which is essential for their photochemical behavior.

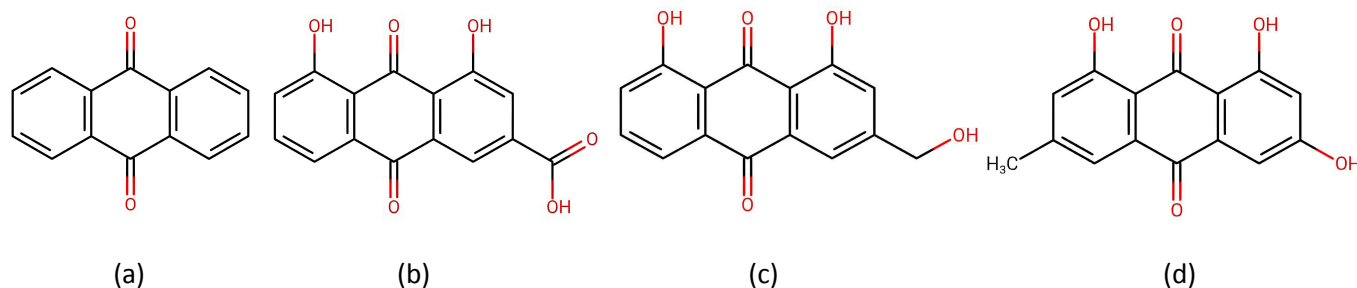


Figure 1. Molecular structures of (a) 9,10-anthraquinone, (b) rhein, (c) aloe emodin, and (d) emodin.

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Acknowledgments

The authors thank the CAPES, Araucária Foundation, CNPq, and UEPG.