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Investigation into the Characteristics of Asymmetric substituted 4,5-Dialkoxy-2-Nitroanilines Using Spectroscopic and Theoretical Approaches

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This study aims to synthesize and explore the physicochemical properties of two distinct constitutional isomers of 4,5-dialkoxy-2-nitroanilines, wherein each isomer is asymmetrically substituted with an ethoxy group and an isobutoxy group.

By synthesizing the isomers and subjecting them to spectroscopic analysis, the study focuses on explaining the nature of electron and oscillatory transitions, providing insight into the complex relationship between molecular structure and spectroscopic properties.

There are no significant differences between the experimental and theoretically calculated infrared spectra. From the comparison of infrared spectra, we can conclude that hydrogen bonds are present in the crystal structure, as quantum mechanical calculations considered one molecule and molecular dynamics considered the elementary cell of the compounds studied. By calculating the energies of successive singlet states, analyzing the calculation results in detail, and visualizing the orbitals, it was possible to describe the HOMO orbitals from which the transitions come and the corresponding LUMO orbitals.

Field

Chemistry

Length

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