The Influence of Hydrazo and Azo Bonds on the Conformation of New 4-Methyl-3,5-dinitro-2-(2-phenylhydrazinyl)pyridine and Its Azo Derivative—Structural Properties, Vibrational Spectra and Quantum Chemical DFT Calculations

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Rok wydania

2025

Czasopismo

International Journal of Molecular Sciences

Numer woluminu

26

Strony

12106/1-12106/24

DOI

10.3390/ijms262412106

Kolekcja

Naukowa

Język

Angielski

Streszczenie

A review of studies has shown that aromatic azo and hydrazo derivatives are used in a wide spectrum of fields, including food, pharmaceutical, and cosmetic products, as well as in technical and electronic technologies, which has contributed to the development of new such compounds. In this work, the structures of newly obtained 4-methyl-3,5-dinitro-2-(2-phenylhydrazinyl)pyridine (**4MDNPHP**) and its azo derivative, 4-methyl-3,5-dinitro-2-[(E)-phenyldiazenyl]pyridine (**4MDNPAP**), were established by spectroscopic (NMR, IR, Raman, and UV-Vis) and emission studies. Single-crystal X-ray diffraction analysis was used to determine the molecular structure of the studied compounds, and the results were compared with DFT calculations (B3LYP/6-311G(2d,2p)). The collected X-ray data revealed that the crystal of the hydrazo compound (**4MDNPHP**) belongs to the triclinic space group $P\underline{1}$ (Z = 2), whereas the crystal of the azo compound (**4MDNPAP**) follows the symmetry of the monoclinic space group $P2_1/n$ (Z = 4). Both presented derivatives crystallized with one molecule in the asymmetric unit. Specific properties of the hydrazo bridge $C_{\square}$-NH-NH-C_{θ} moiety and its azo counterpart $C_{\square}$-N=N-C_{θ} were considered in detail.

Słowa kluczowe

azo and hydrazo groups, pyridine derivatives, crystal structures, spectroscopic analyses, DFT calculations