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Crystal structure, Hirshfeld surface and interaction energy analysis, and quantum chemical investigation of a heteroaryl–phenyl chalcone derivative

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Streszczenie

The molecular structure and supramolecular features of a heteroaryl-phenyl chalcone derivative (HPCN) were investigated through a combined experimental and computational approach. The crystal structure was determined by single-crystal X-ray diffraction, revealing the molecular conformation and packing arrangement stabilized by intermolecular interactions. Experimental spectroscopic studies, including FT-IR, NMR, and powder X-ray diffraction, were employed to confirm the molecular integrity and phase purity of the compound. Density functional theory calculations performed using the B3LYP functional were used to support vibrational and electronic spectral interpretations. The FT-IR spectrum was analysed with the aid of computed vibrational frequencies, while electronic absorption properties were examined using TD-DFT, ZINDO, CIS and EOM-CCSD methods. Frontier molecular orbital analysis, molecular electrostatic potential mapping, and natural bond orbital analysis provided insight into the electronic structure and intramolecular charge-transfer characteristics of the chalcone framework. Hirshfeld surface analysis and two-dimensional fingerprint plots were employed to quantify intermolecular contacts, and interaction energy calculations based on the experimental crystal data revealed that dispersion forces play a dominant role in crystal stabilization. The calculated first hyperpolarizability reflects the intrinsic molecular charge-transfer characteristics, however, due to the centrosymmetric crystal structure, no bulk second-order nonlinear optical response is expected. The combined results offer a comprehensive understanding of the structural, spectroscopic, electronic, and intermolecular characteristics of the Heteroaryl-phenyl chalcone derivative.

Słowa kluczowe

Single-crystal X-ray diffraction, Heteroaryl-phenyl chalconem, DFT, TD-DFT, Hirshfeld surface, Interaction energy

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