عنوان مقاله:

Synthesis, Solubility in Various Solvents, Spectroscopic Properties (FT–IR, 1H, 13C and 15N–NMR, UV–Vis), NBO, NLO, FMO Analysis of A MNDPPD Drug

محل انتشار:

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خلاصه مقاله:

In the present study, the complete structural and vibrational analysis of 3-methyle-4-(4-nitrophenyl)-4,8-dihydropyrazolo[4',3':5,6]pyrano[2,3-d]pyrimidine-5,7(1H,6H)-dione (MNDPPD) were evaluated using the theoretical and experimental methods. Then, the molecular structure of this drug optimized using the Gaussian 09 software with Hartree-Fock (HF) and density functional theory (DFT)methods with 6–311+G(d,2p) basis set. The 1H and 13C NMR spectra were computed using the gauge-invariant atomic orbital (GIAO) method, showing a good agreement with the experimental ones. The calculated vibrational frequencies and chemical shift values were compared using the FT-IR and NMR analysis. The last one UV–vis absorption spectra were analyzed at the presence of five solvent (H2O, DMSO, CH3CN, CH3NO2 and CH3CHCl2), saved at the range of 200–550 nm. The hyper-conjugative interaction energy and electron densities of donor and acceptor bonds were calculated using the natural bond orbital (NBO) analysis. In addition, frontier molecular orbitals analysis, non-linear optical (NLO)activity, electro negativity, ionization energy, global hardness, global softness, andthe energy gap between the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) were calculated. The results showed that the experimental and computational data are consistent with each other.

کلمات کلیدی:

Spectroscopic properties, NLO, NBO, FMO analysis, Global hardness, Global softness, Electronegativity, Electrophilicity index, Solvent effect