Accepted Manuscript

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PII:	S1386-1425(17)30596-6
DOI:	doi: 10.1016/j.saa.2017.07.034
Reference:	SAA 15321
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	26 January 2017
Revised date:	12 July 2017
Accepted date:	20 July 2017

Please cite this article as: Aslı Eşme, Seda Güneşdoğdu Sağdınç , Molecular structures, spectroscopic (FT–IR, NMR, UV) studies, NBO analysis and NLO properties for tautomeric forms of 1,3-dimethyl-5-(phenylazo)-6-aminouracil by density functional method, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2017), doi: 10.1016/j.saa.2017.07.034

Molecular structures, spectroscopic (FT–IR, NMR, UV) studies, NBO analysis and NLO properties for tautomeric forms of 1,3-dimethyl-5-(phenylazo)-6-aminouracil by density functional method

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ABSTRACT

The equilibrium geometry, nuclear magnetic resonance (NMR) and UV–Vis analysis, and vibrational frequencies for the azo and hydrazone isomers of 1,3-dimethyl-5-(phenylazo)-6-aminouracil have been performed using density functional theory (DFT/B3LYP) method with 6–311G(d,p) basis set. A detailed interpretation of the vibrational spectra has been made on the basis of the calculated potential energy distribution (PED) obtained from the Vibrational Energy Distribution Analysis (VEDA4) program. The ^{1}H NMR chemical shifts with respect to TMS were calculated by the gauge independent atomic orbital (GIAO) method and compared with the experimental data. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. Using the TD–DFT method, electronic absorption spectra in $CHCl_3$ solvent of the title compound have been predicted, and good agreement is determined with the experimental one. The NLO properties such as mean polarizability ($<\alpha>$), the anisotropy of the polarizability ($<\Delta\alpha>$) and the mean first–order hyperpolarizability ($<\beta>$) were computed by using finite field method. The computed values of μ, α and β for the azo and hydrazone forms of the title molecule are 5.4717 and 3.8905 D, 2.7773×10^{-23} and 2.7598×10^{-23} esu, and 3.4499×10^{-30} and 6.8504×10^{-30} esu, respectively. The high β values and non-zero values of μ indicate that the title compound might be a good candidate for NLO material.

Keywords: 1,3-dimethyl-5-(phenylazo)-6-aminouracil; NLO and NBO analysis; Infrared spectroscopy; ^{1}H NMR and UV–Vis analysis

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