International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.11 No.05, pp 476-487, 2018

Spectroscopic and Thermodynamic Properties of Novel 1-(4-Methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzylideneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

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Abstract : In this study, 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one was optimized by using B3LYP/6-31G(d) HF/6-31G(d) basis sets. ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of GIAO using the program package Gaussian G09W. Experimental and theoretical values were inserted into the graphic according to equitation of δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Also, calculated IR data of compound were calculated in gas phase by using of 631G(d) basis sets of B3LYP and HF methods and are multiplied with appropriate adjustment factors. Theoretical infrared spectrums are formed from the data obtained according to B3LYP and HF methods. In the identification of calculated IR data were used the veda4f program. Furthermore, molecule's theoretical angles, dipole moments, mulliken charges, HOMO-LUMO energies, total energy of the molecule, ionization potential, electron affinity, electronegativity and thermodynamic properties for both methods were calculated.

Key words : 4,5-Dihidro-1H-1,2,4-triazol-5-one, GIAO, B3LYP, HF, 6-31G(d).

International Journal of ChemTech Research, 2018,11(05): 476-487.

DOI= http://dx.doi.org/10.20902/IJCTR.2018.110552

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