ChemTech

International Journal of ChemTech Research
CODEN(USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.11 No.03, pp 140-148,2018

Theoretical Study of Tetrazole and Oxazepine Compounds by Hartree-Fock Method

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Abstract: In this work, oxazepine and tetrazole compounds were synthesizedfrom the Schiff base (bis(Cinnamylidene)-biphenyl-4,4'-diamine) and this Schiff base synthesized from benzidine and p-nitro benzaldehyde. The IR and UV spectroscopy were measured, These compounds were studied theoretically using computational programs by (Hartree-Fock) method. The results showed that there is a great convergence between practical and theoretical values, but if there is a small difference, the reason is that the chemical computations calculate the values in very standard conditions.The thermodynamic properties (ΔH, ΔG and ΔS) of these compounds were calculated theoretically using the same method (Hartree-Fock), It was found that the reactions of the composition of these compounds are (endothermic and non spontaneous) reactions.

Keywords : Tetrazole, Oxazepine, Computational study, Hartree-Fock method and Thermodynamic Study.

International Journal of ChemTech Research, 2018,11(03): 140-148.

DOI :http://dx.doi.org/10.20902/IJCTR.2018.110315

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