

Influence of solvents on the ^1H -NMR chemical shifts of 4-(4-acetyl-5-methyl-1H-1,2,3-triazol-1-yl)-N-(6-chloropyridazin-3-yl)benzenesulfonamide

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A heterocyclic compound 4-(4-acetyl-5-methyl-1H-1,2,3-triazol-1-yl)-N-(6-chloropyridazin-3-yl)benzene sulfonamide (M2) was prepared by 1, 3-dipolar cycloaddition of 4-Azido-N-(6-chloro-3-pyridazinyl)benzene sulfonamide to acetylacetone. Mass spectrometry (MS), Fourier-transform infrared (FTIR) spectroscopy, and ^1H NMR spectroscopy were used for structure characterization of the compound. The effects of several solvents (DMSO- d_6 , CD_3OD and CDCl_3) on the experimental ^1H -NMR chemical shifts of the title molecule are explored. Significant change in chemical shifts values $|\Delta\delta| > 0.2$ ppm was observed when converted from low polar solvent (CDCl_3) to high polar solvent (DMSO- d_6). The ^1H -NMR of the title molecule was computed using GIAO/B3PW91/6-311++G(d,p), and GIAO/B3PW91/6-311++G(d,p) levels with IEFPCM in DMSO, CH_3OH and CHCl_3 . Study of the correlation between experimental ^1H -NMR chemical shifts and theoretical values suggests that GIAO/B3PW91/6-311++G(d,p) results gave lower RMSE values compared with results which were obtained from GIAO/B3PW91/6-311++G(d,p). The relationship between experimental ^1H -NMR chemical shifts and solvatochromic parameters, as well as dielectric constant of DMSO, CH_3OH , and CHCl_3 solvents, values were observed. Many experimental ^1H -NMR chemical shifts of title molecule have strong negative correlation ($R = -0.90$ to -1) with solvatochromic parameters, and dielectric constant of solvents under study.

Key words: DFT, NMR, solvatochromic, triazole**INTRODUCTION**

Nuclear magnetic resonance (NMR) is an effective tool in structural analysis of organic compounds. The proton NMR experiment is the most widely used NMR technique. Many factors influence on ^1H chemical shifts in NMR including temperature [1, 2], concentration [1, 3], anisotropies, steric effects [4], substituents [5], and solvent effects [3, 6]. Solvent selection has an influence on the chemical shift, and coupling pattern [6]. The effects of solvents in proton resonances are caused by four interactions: van der Waals interactions, solvent anisotropy, hydrogen bonding, and polar effects [7].

Many investigations on the ^1H and ^{13}C NMR chemical shifts of a variety of molecules in various solvents have been reported. Hashimoto and Sakata have given the proton chemical shifts for six compounds in