

NMR and DFT Study of the Enol Imine \leftrightarrow Enaminone Tautomeric Equilibrium in Schiff Bases in Some Organic Solvents

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The tautomeric enol imine \leftrightarrow enaminone equilibrium of the N-(2-hydroxynaphthylidene)-methylamine, N-(2-hydroxynaphthylidene)-aniline and N-(1-hydroxynaphthylidene)-methylamine have been investigated in carbon tetrachloride, chloroform, acetonitrile, dimethylsulphoxide and methanol by ^1H and ^{13}C NMR spectra and density functional theory (B3LYP/6-31G(d,p) methods using the conductor-like screening continuum solvation model (COSMO). Correlations between the experimental ^1H and ^{13}C NMR chemical shifts of the investigated molecule in solutions and GIAO/B3LYP/6-31G(d,p) calculated magnetic isotropic shielding tensors (σ_{cal}) using the screening solvation model (COSMO), $\delta_{\text{exp}} = a + b \sigma_{\text{cal}}$, are reported.

