Solvent and substituent effects on the electronic structures of triazoles: computational study

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Abstract

The tautomerisation reaction of 1,2,3-triazole and some of its derivatives has been studied and the transition states were located. The analysis of results indicates that 2H-triazole is more stable than the 1H-tautomer in all studied compounds in gas phase and in solution. The proton detachment energies and the geometries of the compounds studied were analysed using density functional theory (DFT) and Hartree-Fock (HF (methods in gas phase and solution. Deprotonation takes place in all cases studied by the detachment of N-H proton. The solvent effect on the stability the tautomeric and anion forms of studied compounds has been examined using B3LYP/6-31G* level of theory by applying the polarisable continuum model .

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