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Quantum chemical studies on tautomerism and basicity behavior of some 1,2,4-triazole derivatives

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Abstract: The acidity constants, relative stabilities, and tautomeric equilibrium constants of some 1,2,4-triazole derivatives were determined using the density functional theory (DFT) with the B3LYP method and 6-311G(d,p) basis set. The integral equation formalism version of the polarizable continuum model (IEFPCM) was used in the calculations of the aqueous phase. The calculated tautomeric equilibrium and relative stabilities values revealed that the 4H-1,2,4 triazole form for all studied molecules was favored over the 1H-1,2,4 triazole form. Protonation processes indicated the predominance of the 1H-1,2,4 triazole form over the 2H-1,2,4 triazole form. The correlation attempt between the experimental and the calculated acidity constants, pK_a values, revealed that they are quite close to the experimental values and they correlate well with a regression of around unity (R^2 = 1).

Key Words: 1,2,4-Triazole, proton affinity, tautomerism, acidity constant, nucleophilicity

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