

Quantum Chemical Studies on Tautomerism and Acidity-Basicity Behaviours of Some 1,2,4-triazole Derivates

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The gas and liquid phase acidity-basicity behaviours of some 1,2,4-triazole derivates [1] were investigated using DFT (Density Functional Theory) calculation method. The preferred tautomeric forms were predicted using the DFT calculated acidity constants and physical parameters. The correlation attempt between the experimental and calculated acidity constants, pK_a values, revealed that the B3LYP/6-311G(d,p) calculated pK_a values are closer to the experimental values with a regression of almost unity ($R^2 = 0.99$).

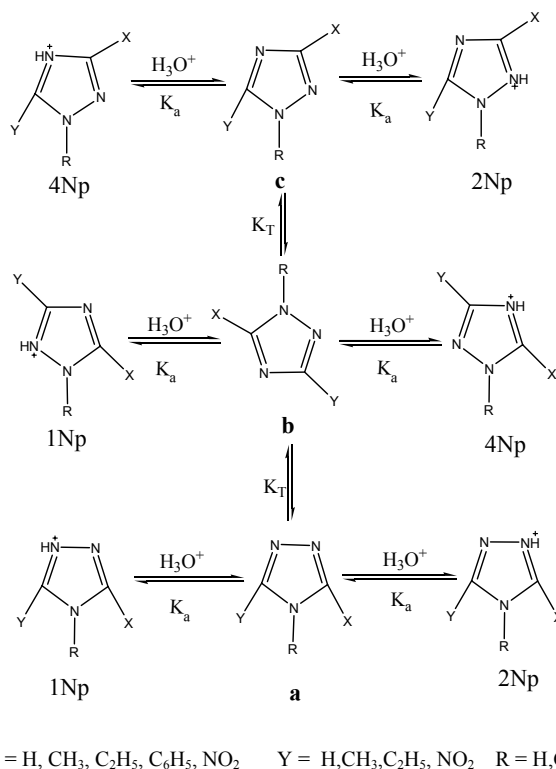


Fig. 1: Prototropic annular tautomerization and protonation patterns for c-substituted 1,2,4- triazole derivates.

[1] J. Catalan, J. Luis, M. Abboud, J. Elguero: *Basicity and Acidity of Azoles*, Copyright© by Academic Pres, Inc. 1987.

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