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Determination of the pKa value of some 1,2,4-triazol derivatives in forty seven different solvents using semi-empirical quantum methods (PM7, PM6, PM6-DH2, RM1, PM3, AM1, and MNDO) by MOPAC computer program

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Abstract. In this study, we calculated the enthalpy (ΔH, kcal/mol), entropy (ΔS, cal/K·mol) and free energy (ΔG, kcal/mol) thermodynamic values of each molecule for forty-seven different solvent media according to semi-empirical quantum methods (PM7, PM6, PM6-DH2, RM1, PM3, AM1, and MNDO) using the MOPAC computer program. The theoretical pKa values were calculated by placing these values in the thermodynamic cycle. It was determined that the triazole derivative molecules examined in this study showed a very high acidity in trifluoroacetic acid and a very low acidity in cyclohexane. The fifth molecule of the triazole derivative molecules examined in this study showed a very high acidity (pKa :1.2457) in trifluoroacetic acid according to the RM1 semi-empirical quantum method. On the other hand, it was determined that the fourth molecule showed a very low acidity (pKa : 69.5668) in cyclohexane according to the RM1 semi-empirical quantum method.

***Keywords*:** pKa; 1,2,4-triazole; semi-empirical quantum method; MOPAC computer program.

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