DETERMINATION OF THE PROTONATION CONSTANTS OF SOME 3-ALKYL(ARYL)-4-(SUBSTITUTED PHENYL)-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONES BY THE POTENTIOMETRIC METHOD IN AMFIPROTIC AND DIPOLAR APROTIC – WATER MIXTURES

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Acidity measurements of organic compounds have a long history dating back to the end of the 19th century, when the first pKa was measured. Since then a vast body of data on acidities in various solvents has been collected.¹-⁴ The measurements have mostly been limited to polar solvents, however, with water being by far the most exploited medium, followed by alcohols and dipolar aprotic solvents. Several studies, involving the formation and investigation of biological activities of some 4,5-dihydro-1H-1,2,4-triazol-5-one derivatives, have been reported.⁵

To gain more information about the effect of solvent on some 3-alkyl(aryl)-4-(substituted phenyl)-4,5-dihydro-1H-1,2,4-triazol-5-ones, the stoichiometric protonation constants of these triazole derivatives in amfiprotic – water (ethanol – water, methanol – water) mixtures and dipolar aprotic – water (dioxan – water) mixtures were determined at an ionic strength of 0.10 M NaCl and at 25.0±0.1 °C under nitrogen atmosphere. A potentiometric method was used and the calculation was carried out using the PKAS computer program. The corresponding pKa values of these triazoles were determined in these mixtures. Thus, the effects of solvent and molecular structure upon acidity were investigated.

![Chemical structure](image)

**References**

