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Electronic structure, ionic equilibria and complex formation of some derivatives of 1-phenyl-3-methylpyrazolone-5

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Abstract

The processes of complex formation of a series of derivatives of phenylazopyrazolone-5 are studied in ethanolic-aqueous solutions. The constants of deprotonation of organic molecules and of complex formation are determined by spectrophotometric titration. The tautomeric equilibria of organic molecules was performed using B3LYP/6-31+G(d). The modeling of electronic absorption spectra of azo-, hydrazo- and anionic forms is presented.