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Model-based analysis for kinetic complexation study of Pizda and Cu(II)

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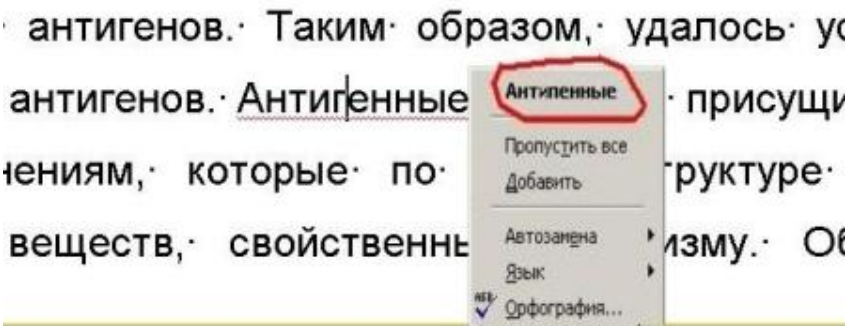
Abstract

In the present work, the multivariate kinetic complexation of a new synthesized ligand, 1-(2″-hydroxyl cyclohexyl)-3′-[aminopropyl]-4-[3′-aminopropyl]piperazine (Pizda) and Cu^{2+} in 50% ethanol–water solution is investigated using the UV–vis stopped-flow technique and state-of-the-art multi-wavelength numerical analysis. Model-based least squares fitting analysis or hard modeling is a specific part of chemometrics which is based on mathematical relationships for describing the measurements. Some recent developments include the incorporation of the effects of non-ideal experimental conditions into the fitting algorithm so it can substantially simplify experimental procedures. In this study no buffers are required because pH changes are taken into computations. Some 21 multi-wavelength kinetic measurements, taken at various initial concentrations of $[H^+]$ were analyzed globally, i.e. simultaneously applying an all inclusive reaction mechanism and a common set of species spectra. Using numerical analysis, the pH of the experimental solutions was allowed to vary as a consequence of the proceeding reactions. This enabled the complete kinetic analysis of the formation and dissociation of $Cu(Pizda)^{n+}$. Here protonation equilibria have been directly incorporated into the rate law, so thus variable pH values have been allowed during each measurement. Using the independently estimated stability constants (from spectrophotometric and potentiometric measurements) for the $Cu(Pizda)^{n+}$ complexes, a total of six rate constants and one protonation constant could be elucidated. The results of the analysis include the concentration distribution and spectra of all chemical species involved in the reaction. A low standard deviation and residual profiles obtained validate the results.

Keywords: Hard modeling; Stopped-flow measurements; Global analysis; Pizda



Самая маленькая разновеска для аналитических весов.

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