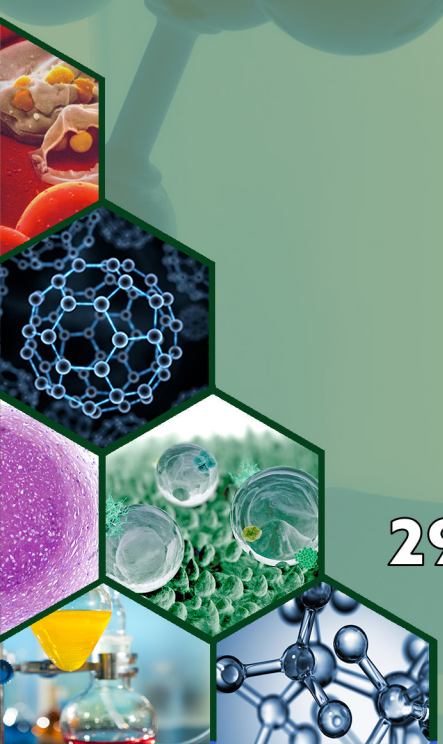
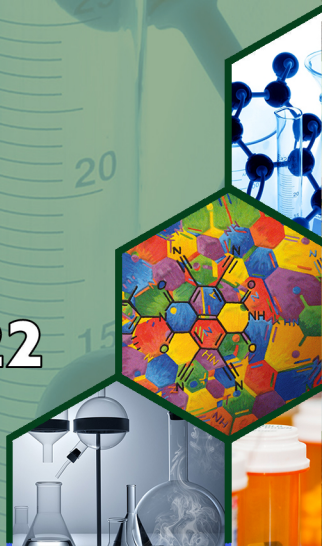
Serbian Chemical Society
Serbian Young Chemists' Club

Eight Conference
of the Young Chemists of Serbia

Book of Abstracts





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Editors
Jelena **MILOVANOVIĆ**
Marko **RODIĆ**
Vuk **FILIPOVIĆ**
Života **SELAKOVIĆ**
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

Page Layout and Design
Vuk **FILIPOVIĆ**
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

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Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

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Poster presentations

Analytical chemistry

AC PP 19

Comparative analysis of ionization constants determination using spectrophotometry and potentiometry: 3-aminobenzoic acid, 1,3,5-benzenetricarboxylic acid and tyrosine

Jelena Ž. Mrđinac[1], Olivera S. Marković[2], Miloš P. Pešić[1], Tatjana Ž. Verbić[1]

[1] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

[2] *University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia*

The ionization constant (usually expressed in logarithmic form, pK_a) is important physicochemical parameter which is used to characterize the acid-base chemistry of a compound. Since most drugs contain one or more ionizable functional groups, knowledge of pK_a values is necessary in drug research. The most common techniques used for pK_a determination are potentiometry and spectrophotometry. Potentiometry is a method of choice when ionization processes are overlapping, as in such case it is not possible to obtain the absorption spectrum of each species present in solution. The aim of this work was the comparative analysis of pK_a determination using potentiometry and spectrophotometry for model compounds with overlapping ionization processes: 3-aminobenzoic acid, 1,3,5-benzenetricarboxylic acid and tyrosine. The potentiometric titrations were performed with *p*SOL Model 3 instrument (*p*ION) equipped with *p*S software package for titration data analysis.[1] Avdeef–Bucher four–parameter equation was used for electrode standardization.[2] To overcome the above-mentioned limitation of spectrophotometry, the alternative approach was applied in this study. The new aminocaproate phosphate buffer (containing phosphoric and ε-aminocaproic acids) was used for the solutions preparation of the model compounds in pH range 1 – 12. This buffer has numerous advantages like UV-transparency, resistance to pH changes upon standing for several days, useful buffer capacity and constant ionic strength in the wide range of pH values. Absorption spectra were recorded according to specific procedure which was carefully designed to avoid systematic errors. Collected absorption spectra will be used for the development of the algorithm for the spectral deconvolution (using MATLAB). Such software can be very useful tool in the drug research, especially for the analysis of the compounds which pK_a values cannot be determined by potentiometry.

References

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2. A. Avdeef, J. J. Bucher, *Anal Chem*. **1978**, *50*, 2137.

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