Abstract

Thiazole-based derivatives with a wide range of biological activities, which can play an important role in the development of new drugs in the treatment of human diseases. Complexation properties of four 2-[(E)-(benzo[d]thiazol-2(3H)ylidene)(cyano)methyl]thiazoles derivatives with Ag⁺, Pb²⁺, La³⁺ in DMSO(20%)-water binary mixture have been studied by spectrophotometric methods. The absorption spectra were recorded at 25 °C, pH = 6.4 and 0.1 M ionic strength of KNO₃ by classical titration. From the results of exploratory analysis of data by soft-modelling approaches, the number of absorbing species was determined by a singular value decomposition of each data set. Multivariate nonlinear least squares as a hard-modelling approach on the experimental data matrix was applied to determine stability constants of each complex. Small values of standard deviation in the resulting parameters showed the proper selection of the model. The fitting of the predefined complexation model to the spectral - mole ratio data were estimated by SQUAD and ReactLab computer programs. The stability constants determined from SQUAD are in good agreement with the results obtained from the ReactLab.

Keywords: Thiazole-based derivatives, Hard-modelling, Soft-modelling, Singular value decomposition, SQUAD, ReactLab.
The Thesis Submitted for the Degree of Master of Science
(In the field of Analytical Chemistry)

Determination of stability constants of
complexes some metal ions with new Thiazole
derivatives by chemometrics methods

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October 2016