Abstract

In this study, a quantitative structure–property relationship (QSPR) approach was used for complexation formation of large set of structurally diverse organic ligands with Mn^{2+}, Fe^{2+}, Y^{3+}, La^{3+}, Pb^{2+}, UO_2^{2+}. Some models based on the linear (multiple linear regression) and nonlinear (support vector machine) relationship between logK and MOE descriptors were developed as global models, and a general equation as a simple way to calculate the complexation formation of organic ligands was provided. Moreover, local QSPR models were also developed for each subset of organic ligands and, as expected, the statistical results obtained from these models were better than the global one. The descriptors representing the potential energy and partial charge of organic ligands showed the highest correlation with logK.

Keyword: QSPR, complexation formation, global model, local model, MLR, SVM

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Faculty of Science
Department of Chemistry

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Local and global QSAR models and the overall shear stability constants of metal ions and organic ligands

Supervisors:
Dr. F.Shiri

Advisor:
Dr. M. Salahinejad
Dr. M. Sanchuli

By:
N. M. mooguei

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