ABSTRACT (EN)

The solvation model based on LSER was applied to study the retention behaviour of analytes in liquid and gas chromatography. In a first chapter, a retention description of 21 solutes was investigated by using the solvation model in a wide range of mobile phase composition methanol-water and acetonitrile-water. Generally, the retention of aromatic compounds was better described by the solvation model, compared to aliphatic compounds.

Effect of the particular analytes used to formulate the LSER model on ability of retention description was studied. Different results of a retention estimation was achieved by using the regression set of compounds including aromatic solutes only or by contrast aliphatic solutes only. The solvation model developed on the basis of oxygen derivatives provided distinct results in comparison to model formulated with nitrogen derivatives only.

The second chapter of this work, focused on gas chromatography, dealt with a description of retention of 152 isomers C5-C8 alkenes by the LSER model. The solvation descriptor *L* was obtained by using two estimation methods Havelec-Ševčík (HS) and Platts-Butina (PB), the descriptor *E* was calculated according to its definition.

Two models for retention description of alkenes were constructed, the HS model and the PB model, derived from the methods for estimation of descriptors. Higher error of the estimated retention calculated by the HS model was found for cis isomers of alkenes. After a modification of the HS model by omitting the contribution for cis interaction was achieved a significant improvement in the retention description.

Both the models were used to estimate the retention of 59 alkenes C5-C7. The HS model with descriptors $L_{,\mathrm{HS\ no\ cis}}$ and $E_{,\mathrm{calc}}$ provided the more accurate retention description compared to the PB model. Next, a retention description of 93 octenes was carried out and the best results were achieved by the PB model using the descriptors $L_{,\mathrm{PB}}$ and $E_{,\mathrm{calc}}$. Finally, retention of all 152 alkenes C5-C7 was studied, where noticeable heteroscedasticity of residuals occurred at the two-descriptor models. In case of the one-descriptor models HS and PB, heteroscedasticity was not entirely proved. The best retention description of 152 alkenes with only single descriptor *L* provided the HS model.