ABSTRACT

The objective of this dissertation was to develop prediction models for some important physico-chemical properties and an analytical method for determination of organic compounds in atmospheric particles in order to better understand formation of secondary organic aerosols. Doctoral dissertation is divided into two parts. In the first part, I focused on theoretical study of mechanisms of secondary organic aerosols formation. I developed models based on quantitative structure-property relationship (QSPR) by using a novel modeling software MACI (angl. Molecular Activity Characterization Indices) which I developed together with my colleagues. QSPR models were developed for prediction of vapor pressure, octanol-air partition coefficient – K_{oa} and semiempirical hygroscopicity parameter – κ. Furthermore, two separate models were developed for prediction of partial reaction rates of hydroxyl radicals with nonconjugated alkenes. Novel zero order variable connectivity index was used for the development of the first model; the second model was built by taking into an account quantum-chemical calculations and experimental data. Both models were compared with an established prediction model. Results show that allylic site is much more reactive than it is currently assumed in global models. In the last part of the dissertation I developed an analytical method for determination of organic acids (dicarboxylic acids and hydroxybenzoic acids) in atmospheric particles PM_{10} in $PM_{2.5}$. I used coupled technique of liquid chromatography and tandem mass spectrometry. Analytical method was used for determination of organic acids on two sites (urban – Maribor center and remote – Iskrba) and in two parts of the year (summer and winter). With inclusion of measurements done by Slovenian Environment Agency, I was able to determine possible sources of organic acids for Maribor site in summer and winter.

Keywords: secondary organic aerosols; hydroxyl radicals; partial reaction rates; variable connectivity indices; tandem mass spectrometry; dicarboxylic acids.