Resümee

Käesolevas töös uuriti 2-atsüülbensoehapetes ning monoasendatud 2-atsetüülbensehapetes toimuvat ring-ahel tautomeeriat. Mainitud ühendite abil uuriti ring-ahel tasakaalu termodünaamikat ja kineetikat kasutades temperatuurisõltuvuse mudelina van't Hoffi ja Eyringi kõveraid. Samuti modelleeriti kvantkeemiat kasutades 2-atsetüülbensoehappe ja selle monoasendatud amino- ja nitroderivaatide termodünaamikat. Solvendiefekti implitsiitseks arvutuskeemiliseks hindamiseks kloroformis ja metanoolis kasutati SMD mudelit.

Abstract

In the current study, we researched ring-chain tautomerism in 2-acylbenzoic acids as well as in various monosubstituted 2-acetylbenzoic acids. Thermodynamic and kinetic parameters for the ring-chain tautomerism in the aforementioned group of compounds were explored using the van't Hoff and Eyring equations. This study also contains a computational part, where thermodynamic parameters of equilibrium in the studied 2-acetylbenzoic acids were calculated, and the solvent effect was estimated implicitly with the SMD solvent model in chlorform and methanol.