



Laser-based studies of OH radical reactions in aqueous solution

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Oxidation processes initiated by radical reactions are the major loss processes for organic compounds in the troposphere. Among the atmospheric radicals, OH represents the most reactive and reactions involving OH radicals are often the most important sinks for volatile organic compounds (VOCs) both in the gas and aqueous tropospheric phases.

In this work the reactions of OH radical with the following oxygenate organic compounds, (1) ethylene glycol, (2) propylene glycol, (3) 1,3-propanediol, (4) 1,2-butanediol and (5) 1,4-butanediol have been studied as function of the temperature, between 288 K and 328 K.

The temperature dependent rate constants of the OH radical reactions with the above mentioned oxygenated organic compounds in aqueous solution have been investigated using a laser flash photolysis long path absorption (LP-LPA) set-up and applying the competition kinetics method.

Several studies suggest that the prevailing reaction mechanism between OH radical and a saturated organic aliphatic compound is the abstraction of the most loosely bonded hydrogen atom. In previous kinetic studies of OH radical reactions in aqueous solution from our laboratory correlations between the bond dissociation energy (BDE) of the weakest C-H bond, activation parameters and kinetic data have been developed using the Evans and Polanyi equation. The obtained data have been used to expand available reactivity correlations which can be used for the prediction of unknown rate constants of reactions of OH radical in the aqueous phase.

The obtained kinetic data represent input parameters for aqueous phase tropospheric models such as CAPRAM.