International Master 2 Atmospheric Sciences: Research Training 2021-2022

Laboratory: PC2A

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Eventually,

CaPPA Work Package: WP-1

Insights in a better understanding of the atmospheric reactivity of RO_2

Peroxy radicals are key radicals in tropospheric chemistry. They react, as recently shown, with the hydroxyl radical in the gas phase at an unexpectedly high rate. For instance, for ethyl peroxy, formation of activated ethylhydrotrioxide, followed by dissociation into methoxy and hydroperoxy radicals, is found to be the main reaction pathway, whereas ethylhydrotrioxide stabilization and methanol formation (from activated and stabilized ethylhydrotrioxide) are viable minor channels. Criegee intermediate formation is found to be negligible.

Since water vapor is the most abundant trace gas in the troposphere and it has been proved that atmospheric relative humidity has a strong influence in many atmospheric reactions, the effect of water vapor on this reaction has to be evaluated.

Molecular simulations will be performed by the intern to determine the thermochemical properties and kinetic parameters for the water-assisted reaction of OH with some RO_2 for which no literature data exist. Calculations will be compared to experimental data from the FAGE reactivity setup existing at the laboratory in order to discuss simulations.

This project will also aim to contribute to a larger research program devoted to the study of atmospheric processes (Labex CaPPA, CPER Ecrin). This work will be conducted in collaboration with the Comenius University in Bratislava.

The work will take place at PC2A laboratory, Lille University.

Key words: Atmospheric chemistry, OH, RO2, CH_3O_2, $C_2H_5O_2$, relative humidity, molecular simulations