

International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: LPCA

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Eventually,

CaPPA Work Package: WP1 – From gas phase to aerosols

Kinetic studies of BVOCs ozonolysis using THz rotational spectroscopy

Biogenic volatile organic compounds (BVOCs) account for around 90% of global hydrocarbon emissions into the Earth's atmosphere. The gas-phase degradations of these reactive chemical species contribute to produce photooxidants in the atmosphere. These reactions are liable to aggravate the situations of pollution events by increasing the background level of ozone in the lower troposphere. A good knowledge of the mechanisms and the rate constants is necessary when describing the impact of these processes on air quality [1]. The ability of the LPCA terahertz (THz) spectrometer to monitor in real time the evolution of the gas phase concentrations of atmospheric polar compounds has been demonstrated with the kinetic measurements of H₂CO photolysis [2]. Moreover, the MULTICHARME project has allowed to build a CHERNIN type multi-pass cell operational from IR to THz frequencies inside the new LPCA atmospheric simulation chamber CHARME (Chamber for the Atmospheric Reactivity and the Metrology of the Environment) dedicated to the study of VOC reactivity [3].

For this research training, we propose to participate to the first THz kinetic studies of BVOCs ozonolysis. Two well-known reactions will be targeted: the ozonolysis of isoprene which is a source of OH radicals in the troposphere [1] and the ozonolysis of catechol which plays a key role in the secondary organic aerosol formation [4]. The rate constants will be determined at low pressure by THz rotational quantitative spectroscopy, first in a double path absorption gas cell, next in MULTICHARME. The data measured in the atmospheric chamber will be compared with those obtained at atmospheric pressure using PTR-ToF-MS and photometric analyzer for VOCs and ozone, respectively.

This experimental research training will allow the student to develop analytical skills both in physics and in chemistry with the unique opportunity to work with the state-of-the-art instrumentation. Some financial support will be provided and a continuation in PhD thesis is expected.

Key words: Kinetics, BVOCs, Terahertz, spectroscopy, atmospheric chamber, ozonolysis

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[2] A. Omar, S. Eliet, A. Cuisset, G. Dhont, C. Cœur-Tourneur, R. Bocquet, G. Mouret, F. Hindle, *Sensors*, 12087, 2015.

[3] <https://wp3.univ-littoral.fr/equipements/caracterisation-des-gaz-et-aerosols/>

[4] A. El Zein, C. Cœur, E. Obeid, A. Lauraguais, T. Fagniez, *J. Phys Chem. A.*, **119** (26), 6759-6765, 2015.