

International Master 2 Atmospheric Sciences: Research Training 2021-2022

Laboratory: LPCA

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Eventually, CaPPA Work Package: WP1 – From gas phase to aerosols: biogenic VOCs (volatils organic compounds) as precursors for particles

High temperature and high resolution millimeter-wave spectroscopy of semi-volatile organic compounds for their atmospheric interest

The Laboratory of Physico-Chemistry of the Atmosphere (LPCA) has an extensive experience in the conception and operation of THz spectrometers for gas phase applications. In particular, the frequency multiplication technique is used to measure the rotational spectra of gas phase samples between 70 GHz and 900 GHz with an accuracy of ten kHz [1]. These spectra are specific for each molecule and their analysis allows characterizing the dynamics and the structure of the molecules, while providing line lists for their future detection in atmospheric conditions.

In order to study semi-volatile organic compound whose vapor pressure is very low at room temperature ($< 10^{-3}$ mbar), the laboratory has recently acquired a heating coat associated with a temperature regulation system to heat the absorption cell and increase the vapor pressure of the gas sample. The first part of the internship project aims to implement the heating system on the spectrometer and to characterize the equilibrium temperature of the gas sample. Improvements of the setup could also be required to avoid condensation of the sample on the "cold" parts of the instrument. Through this improvement, new molecules that are not accessible by the current technique will be permitted.

The second part of the project will be dedicated to the measurement of rotational spectra of semi-volatile organic compounds for their atmospheric interest. Guided by previous studies performed in atmospheric simulation chambers of the LPCA, 3-methylcatechol, 4-methylcatechol, resorcinol and hydroquinone will be selected for spectroscopic measurements. The project will focus firstly on 3-methylcatechol (3-methyl-1,2-dihydroxybenzene) and 4-methylcatechol (3-methyl-1,2-dihydroxybenzene) which have been identified as secondary organic aerosol precursor during their ozonolysis [2]. Concerning the spectral analysis, the 3-methylcatechol will be studied in a global data analysis including the new millimeter-wave spectrum and already measured microwave spectra. We can expect at least one article in a peer-review international journal for this molecule.

The project is proposed by Anthony Roucou, assistant professor at the PCMI group of Laboratoire de Physico-Chimie de l'Atmosphère (LPCA) of the Université du Littoral Côte d'Opale in Dunkerque.

Key words: rotational spectroscopy, SOA precursors, heated absorption cell, spectral analysis, millimeter-waves.

[1] G. Mouret, M. Guinet, A. Cuisset, L. Croize, S. Eliet, R. Bocquet, F. Hindle (2012). Versatile sub-THz spectrometer for trace gas analysis. *IEEE Sensors Journal* 13(1): 133-138.

[2] C. Coeur-Tourneur, V. Foulon, M. Laréal. (2010) Determination of aerosol yields from 3-methylcatechol and 4-methylcatechol ozonolysis in a simulation chamber. *Atmospheric Environment* 44(6): 852-857.