MASTER OF SCIENCES

"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Ageing of individual pollen grains under controlled environment

University 1: University of Lille 1
Main Laboratory: LASIR - Laboratoire de Spectrochimie Infrarouge et Raman (UMR CNRS 8516)
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Topic

The average adult respires 12,000 litres of air per day. Ambient air contains a variety of particulates that can induce several health effects. In particular, an increasing number of individuals suffer from pollinosis. Pollen allergens are found in respirable particles, including whole anemophilous pollen grains (10-30 µm mean diameter), pollen-derived starch cytoplasmic granules (2-4 µm) and submicrometric particles called orbicules. Alteration of pollen grain structure and rupture can be induced in the atmosphere by ageing of the pollen surface upon exposure to pollutants and hydration (Taylor et al, 2004; Visez et al., 2015).

In this Master project the candidate will study the (photo)reactivity of individual pollen grains to better understand the physical-chemical transformation of the pollen during their transport in the atmosphere. The student will use a combination of optic and spectroscopic techniques (Raman and FT-IR microscopies) coupled to adapted reactors (micro-reactors) to study the processes occurring in individual pollen grains exposed to pollutants and/or sunlight. The humidity effect on the processes will also be evaluated.

Keywords: Pollen, Ageing, Single particle analysis

References:

Taylor, P. E., Flagan, R. C., Miguel, A. G., Valenta, R. and Glovsky, M. M. (2004), Birch pollen rupture and the release of aerosols of respirable allergens. Clinical & Experimental Allergy, 34: 1591–1596.

Visez, N., Chassard, G., Azarkan, N., Naas, O., Sénéchal, H., Sutrac, J.-P., Poncet, P. and M. Choël (2015), Wind-Induced Mechanical Rupture of Birch Pollen: Potential Implications for Allergen Dispersal. Journal of Aerosol Science, 89: 77–84.

MASTER OF SCIENCES

"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Modeling and Spectroscopy of Flavonoid Complexes

University 1 : Univ. Lille
Main Laboratory : LASIR
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University 2 (if any):
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Topic

Flavonoids are organic compounds implied in the secondary metabolism of higher vegetables. They include several complexation sites that could bind with cations encountered in soils.

Due to the complexity of the systems, the elucidation of the structures of the complexes formed need a intricated approach of spectroscopy and molecular modeling.
More precisely, the methodology applied associates the measurements of spectra during titration. Then, hypotheses on the complexes actually formed are made, and their structures and spectra are computed by the means of DFT-based methods (stationary and time-dependant). By comparison between measured and theoretical results, it will then be possible to conclude on the nature of the formed species.
Once the structural elucidation achieved, it is possible to go further in the study on electron properties, especially the nature of bonding by the use of NBO and AIM-based methods.

Depending on the results obtained, it would be possible to compare the reactivity of several organic ligands towards a metal cation or of several cations towards a ligand.

The interested student will be involved in both aspects of the study: measurements of electronic spectra (absorption, possibly emission) and quantum chemistry computations. The precise part of the two aspects could be adjusted according the applicant's preferences.

Related references:

A. Moncomble, J.-P. Cornard, *RSC Adv.* **2014**, *4*, 29050-29061
A. Le Person, A. Moncomble, J.-P. Cornard, *J. Phys. Chem. A* **2014**, *118*, 2646-2655

keywords: complexes, DFT, electronic spectroscopy, flavonoids, molecular modeling, UV-vis