



OFFRE D'ALLOCATION DE THESE / PhD GRANT

ÉCOLE DOCTORALE SCIENCES EXACTES ET LEURS
APPLICATIONS - ED 211 / NATURAL SCIENCES DOCTORAL SCHOOL
Avenue de l'université BP 1155 64 013 PAU Cedex – France

PhD SUBJECT

TITLE: Development and implementation of analytical methods for monitoring halogenated contaminants new energies type samples

New-generation biofuels or biogas, which are then refined to produce biomethane, SAF (Sustainable Aviation Fuel) or other non-fossil petroleum substitutes, are produced from waste. This waste, whether agricultural, household or industrial, is composed of organic matter that will be recycled, but also of numerous compounds added during the waste's life cycle, such as pesticides, flame retardants, additives, etc.

Certain compounds present in these raw materials are likely to end up as contaminants in the production cycle or even in the finished product, proving dangerous for the use of finished products or during refining during production. These compounds often include hetero-elements such as phosphorus, chlorine, fluorine...

The speciation of these trace elements in complex matrices such as bio-oils and biogases has therefore become an important issue for the further development of these new alternative energy sources. This thesis will therefore focus on the development of speciation of these elements (starting with fluorine) using coupling techniques (HPLC, GC, LA) with ICP MS and then FT ICR MS.

Keywords: Hetero-element, speciation, ICP MS, FT ICR MS

WORKING CONDITIONS

Laboratoire : UMR 5254 CNRS-UPPA, Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux (IPREM)

Site web : www.iprem.univ-pau.fr

PhD Director: Pierre Giusti / Brice Bouyssiére

PhD co-supervisor: Caroline Mangote

In Collaboration with:

Place: IPREM. Hélioparc, 2 Avenue du Président Angot 64053 Pau cedex 09

Start: October 2024

Duration: 3 years

Employeur (employer): Université de Pau et des Pays de l'Adour (UPPA)

Salaire mensuel brut (monthly salary before taxes): 2100 €

(Si enseignement : salaire mensuel brut pour 32h d'enseignement par année universitaire : 110 €)

HOST LABORATORY PROFILE

The PhD will principally work at IPREM, specifically, he/she will be member of the Analytical Chemistry, Physical and Theoretical (CAPT) Cluster. He will be part of the iC2MC Pau group that has a vast experience on analytical chemistry, trace metal speciation in complexes matrices. To reach the outlined objectives, the project will be supported by the unique instrumental facilities of the host laboratory. This platform possesses, among others, the state of the art instruments required for these project (ICP-MS, ICP HR MS, HPLC/GC/LA ICP MS, FT ICR MS (ESI and MALDI)).

This PhD will be also link with TotalEnergies iC2MC part and some stay at the TRTG Research center (Gonfreville) or at the Florida State University will be possible.

See details at <https://iprem.univ-pau.fr/fr/activites-scientifiques/poles-scientifiques/chimie-analytique-physique-et-theorique/capt-membres.html>

MISSION - ACTIVITES PRINCIPALES / MISSION – PRINCIPAL ACTIVITIES

I. Scientific Context

ICP MS is the instrument of choice for the characterization of metals in total analysis or speciation via coupling with chromatographic techniques. However, as far as hetero-elements are concerned, and more particularly halogens, their weak ionization in an ICP plasma does not allow acceptable detection limits to be reached. However, recent work has shown that it is possible to create polyatomic ions in ICP plasma from these poorly ionizable elements and a metal ion. Detection is then based on the mass of this polyatomic ion. This methodology is very promising, as it enables us to take advantage of the high sensitivity of ICP MS and its ability to analyze complex matrices, while continuing to use speciation techniques already developed for the analysis of petroleum products and applying them to these new samples.

II. Objectives

The aim of this research work is to improve the monitoring of halogenated contaminants, with priority given to fluorine, in matrices derived from new-generation biofuels. The aim is to set up a reliable protocol for analyzing fluorine by ICP MS, to bring it down to the detection limits sought after in the biofuel industry. Once the protocol for total analysis is in place, speciation techniques will be developed.

The thesis work will be carried out in partnership between the IPREM laboratory of the Université de Pau et des Pays de l'Adour based in Pau and the TRTG, Total's research center in Gonfreville. The PhD student will be based mainly at IPREM, an expert laboratory in the field of speciation by ICP MS.

III. Work plan

- Bibliographical study on contamination by possible halogenated compounds in différents types of bio-oil/biogas. Bibliographical study on the characterization of these elements in complex organic matrices.
- Development of a reliable method for total F analysis by ICP MS through polyatomic ion creation.
- Development of F speciation in complex matrices.
- Transfer to quadrupole ICP MS at TRTG
- Study on improving the characterization of other halogens via polyatomic ion creation in ICP plasma.

REQUIRED COMPETENCES

The candidate should have a Master (or BAC+5 homologated) on Analytical/Bioanalytical/Environmental Chemistry

Previous experience on hyphenated chromatographic techniques, mass spectrometry would be appreciated.

CRITERIA USED TO SELECT CANDIDATE

Selection process steps:

- Establishment of the selection committee.
- Evaluation of the applicants Cv's
- Interview with the selected candidates and ranking.

Criteria used in selection of the candidate:

- The candidate's motivation, scientific maturity and curiosity.
- Previous experience on hyphenated chromatographic techniques, mass spectrometry or stable isotopes would be appreciated

- Candidate's marks and rankings in M1 and M2.
- English proficiency

REQUIRED DOSSIER, DATE

Send an e-mail with your candidature containing (with "PhD Candidate in the object of the message"):

- CV
- Cover letter detailing candidate's motivations
- Candidate's MSc marks and ranking
- Minimum two contact details for 2 referees

Limiting date:

04/07/2024

CONTACTS

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