LABORATOIRE DE SPECTROCHIMIE
INFRAROUGE ET RAMAN
UMR 8516

Post-doctoral position at CReS (Total/MS) with LASIR

11 juillet 2018

Chemical science

Applications of EPR techniques in studying the stability of base oils and formulated lubricants

Understanding the factors that impact ageing is key to develop new products with high added values and long term stability. One of the priorities for the MS R&D is to develop products with low ageing properties and high durability. Today's engine lubricant must comply with manufacturers specifications that are more and more restrictive. The lubricant needs to be formulated to resist longer constrains linked to more and more compact and powerful engines. As a result, it is important for the formulation to comply with manufacturer specifications which rely on Fuel Economy and Durability.

Lubricant stability study can be divided into different steps : base oil stability, additive package stability and formulated lubricant stability. All of these events potentially involve single electron transfers that can be characterized by Electron Paramagnetic Resonance (EPR) spectroscopy with or without the use of spin straps to stabilize the radicals.

EPR technique is highly sensitive and can be easily applied, in the conventional continuous wave, CW, mode, to identify and quantify radicals in a petroleum product. Unlike most other analytical techniques, EPR spectroscopy enables the study of the early stages of the ageing process and allow to gain a deeper understanding on the precursors involved. Besides, pulsed EPR can also be used to get access to the chemical environment of the electron in order to better describe the structure of the active site. The other asset of pulsed EPR is that measurements are performed at low temperature which allow to study processes which are slowed down at 4K and cannot be studied at room temperature.

The objectives of this post-doctoral internship are as follow :

- Understand the ageing process of base oils depending on the group of origin : identify and quantify the different radicals present using spin traps and a computation approach such as DFT

- Screen base/additives couples in order to identify the best chemistries for anti-oxidants : assess the impact of an additive or an additive package on the formation of radicals in base oils

- Understand the stability of performance additives containing paramagnetic centers such as molybdenum : using pure additive or additive package, assess the structural and/or oxidation state changes of paramagnetic centers depending on the ageing process used

- Predict the stability of a base or a formulated lubricant depending on the ageing process involved : establish paramagnetic or radical markers that can be used to predict the stability of a formulated lubricant

This internship, in partnership with LASIR (Hervé Vezin's group), will be mostly localized in Lyon for the use of CW EPR EMX-nano. Stays in Lille will also be scheduled when pulsed EPR is required.

Keywords : EPR, lubricant, base oil, pulsed EPR, spin traps

Academic supervisor Dr. Hervé Vezin : laboratoire de Spectrochimie Infrarouge et Raman (LASIR) Lille

TOTAL supervisor Dr. Simon Pondaven : responsable du laboratoire de RMN et RPE, Département Analyse Physico-chimique, CReS, Lyon

Duration and start date 12 months

Employer CNRS

Academic requirements Ph.D. in EPR, knowledge of CW and pulsed EPR, use of Spin trap

Language requirements Fluency in French and/or English