



LABORATOIRE DE SPECTROCHIMIE
INFRAROUGE ET RAMAN
UMR 8516

Directeur : H. VEZIN

Fiche de poste pour stage de M2 en 2020

Titre du stage : Modeling and Spectroscopy of Flavonoid Complexes

Résumé du sujet :

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 joined 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.

The objective of the internship will be to fully understand a system that will be defined at the beginning of the period of practice depending on the team work.

Mots clés : DFT ; flavonoids ; complexes

Date prévisionnelle de démarrage du stage : février 2020

Durée : 6 mois

Lieu du stage : Campus Cité Scientifique, Université de Lille

Rémunération : 518 €/mois

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