Geophysical Research Abstracts
Vol. 19, EGU2017-4117-1, 2017
EGU General Assembly 2017

An original data treatment for infrared spectra of organic matter, application to extracted soil organic matter

Bruna Gomes Rossin (1,2), Roland Redon (1), Michel Raynaud (1), Nadia Regina Nascimento (2), and Stéphane Mounier (1)

(1) Laboratoire PROTEE - Université de Toulon - CS 6058483041 TOULON CEDEX 9, France, (2) Universidade Estadual Paulista (UNESP). Campus de Rio Claro. Instituto de Geociências e Ciências Exatas (IGCE), Av. 24 A, 1515, CEP 13506-900, Rio Claro - SP, Brasil

Abstract :
Infrared spectra of extracted organic matter are easy and rapid to do, but generally hard to interpreted over the presence or not of certain organic functions. Indeed, the organic matter is a complex mixture of molecules often having absorption overlapping and it is also difficult to have a well calibrated or normalised spectra due to the difficulty to have a well known solid content or homogeneity for a sample (Monakhova et al. 2015, Tadini et al. 2015, Bardy et al. 2008).
In this work, the IRTF (InfraRed Fourier Transform) spectra were treated by an original algorithm developed to obtain the principal components of the IRTF spectra and their contributions for each sample. This bilinear decomposition used a PCA initialisation and the principal components were estimated from vectors calculated by PCA and linearly combined to provide non-negative signals minimizing a criterion based on cross-correlation. Hence, using this decomposition, it is possible to define IRTF signal of organic matter fractions like humic acid or fulvic acid depending on their origin like surface of depth of soil profiles.
The method was used on a set of sample from Upper Negro River Basin (Amazon, Brazil) (Bueno,2009), where three soils sequences from surface to two meter depth containing 10 slices each. The sequences were sampled on a podzol well drain, a hydromorphic podzol and a cryptopodzol. From the IRTF data five representative component spectra were defined for all the extracted organic matter , and using other chemical composition information, a mechanism of organic matter fate is proposed to explain the observed results.

Bardy, M., E. Fritsch, S. Derenne, T. Allard, N. R. do Nascimento, and G. T. Bueno. 2008. “Micromorphology and Spectroscopic Characteristics of Organic Matter in Waterlogged Podzols of the Upper Amazon Basin.” Geoderma 145 (3-4): 222–30.

Bueno, G.T. Appauvrissement et podzolisation des latérites du baissin du Rio Negro et gênese dês Podzols dans le haut bassin amazonien. [PHD] .Universidade Estadual Paulista “Júlio de Mesquita Filho”;2009.

Monakhova, Yulia B., Alexey M. Tsikin, Svetlana P. Mushtakova, and Mauro Mecozzi. 2015. “Independent Component Analysis and Multivariate Curve Resolution to Improve Spectral Interpretation of Complex Spectroscopic Data Sets: Application to Infrared Spectra of Marine Organic Matter Aggregates.” Microchemical Journal, Devoted to the Application of Microtechniques in All Branches of Science 118 (January): 211–22.

Tadini, Amanda Maria, Gustavo Nicolodelli, Stephane Mounier, Célia Regina Montes, and Débora Marcondes Bastos Pereira Milori. 2015. “The Importance of Humin in Soil Characterisation: A Study on Amazonian Soils Using Different Fluorescence Techniques.” The Science of the Total Environment 537 (December): 152–58.