HAL
open science

Simplified spectrophotometric acid-base titrations to assess organic matter reactivity

Marawit Tesfa, Remi Marsac, Aline Dia, Fabrice Mahé

To cite this version:

Marawit Tesfa, Remi Marsac, Aline Dia, Fabrice Mahé. Simplified spectrophotometric acid-base titrations to assess organic matter reactivity. Goldschmidt Conference 2021, Jul 2021, online, United States. 2021, 10.7185/gold2021.5105 . insu-03320501

HAL Id: insu-03320501

https://insu.hal.science/insu-03320501v1

Submitted on 16 Aug 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Simplified spectrophotometric acid-base titrations to assess organic matter reactivity

Marawit TESFA[1*], Rémi MARSAC[1], Aline DIA[1], Fabrice MAHE[2]

1 CNRS - UMR 6118 Géosciences Rennes, 35042 Rennes cedex, France
2 IRMAR, UFR Mathématiques Équipe d'analyse numérique, Université de Rennes 1, 35042 Rennes Cedex France
(*marawit.tesfa@univ-rennes1.fr)

In environmental issues, including soil quality and contamination studies, Natural Organic Matter (NOM) holds a crucial role because of its size, ubiquity and high reactivity. NOM's adsorption onto mineral surfaces and reactivity towards various contaminants and trace elements are mainly related to their acid-base groups such as, carboxylic and phenolic ones. To study these groups, different characterization and quantification methods have been developed. Acid-base potentiometric titration is the most reliable one but, is time-consuming and often impossible to apply to environmentally relevant NOM concentrations. Recent studies showed the great potential of spectrophotometric titrations in NOM analysis [1,2]. UV-vis spectra of a NOM solution are recorded for different values of pH. The relative absorbance ($\Delta A(\lambda,pH)$) with respect to a reference pH (e.g. pH 3) was shown to evolve according to:

$$\Delta A(\lambda,pH) = A_1(\lambda)\times f_1(pH) + A_2(\lambda)\times f_2(pH) \qquad \text{eq.1}$$

Where $A_1(\lambda)$ and $A_2(\lambda)$ are specific absorbance of carboxylic and phenolic groups, respectively, $f_1([H^+])$ and $f_2([H^+])$ are functions of pH. However, the proposed methods face some limitations. Firstly, data acquisition is time-consuming (~ 4h) and can hardly be automated. Secondly, the analysis of $\Delta A(\lambda,pH)$ instead of the absorbance $A(\lambda,pH)$, leads to larger analytical errors and a loss of spectroscopic information. Thirdly, eq.1 is generally applied for a single wavelength, overlooking information in the rest of the spectra. Finally, absorbance data do not allow direct quantification of carboxylic and phenolic groups concentration, which requires potentiometric titration.

In this study, a method based on the use of pH buffer in acid-base titration speeded up to 4 times the sample preparation, and gave similar results to the published method. Equation 1 was modified to elaborate a MATLAB script allowing the use of $A(\lambda,pH)$ and the estimation of functional groups' proportion, behavior and specific UV-vis spectrum. By analyzing NOM reactivity for seven IHSS standard samples, empirical equations are proposed for a direct estimation of carboxylic and phenolic groups concentrations.

The present development will help measuring NOM reactivity, hence providing constraints for the modeling of contaminants' fate in the environment.

(1) Janot et al.. *Environ. Sci. Technol.* **2010**, *44* (17), 6782–6788.
(2) Liu et al., *Chemosphere* **2020**, *261*, 128189.