Estimating organic matter acid-base properties and electrical charge by spectrophotometry

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Natural Organic Matter (NOM) holds a crucial role in major environmental issues such as soil quality and contamination, because of its ubiquity and high reactivity. Both NOM (1) adsorption onto mineral surfaces and (2) reactivity towards various contaminants are mainly related to NOM acid-base functional groups such as, carboxylic and phenolic ones. Although acid-base potentiometric titration is the most reliable approach to quantify these groups, it is time-consuming and often impossible to apply to environmentally relevant NOM concentrations, because it requires several hundreds of milligrams per liter of dissolved organic carbon [1]. Spectrophotometric acid-base titration is a simple and powerful technique to evaluate NOM proton binding sites properties at environmentally relevant concentrations [2]. However, the quantitative determination of NOM electrical charge (Q), from the measured absorbance (A), remains a great challenge. In a previous work [2], a linear relationship between Q and the UV-vis differential absorbance (ΔA_λ) at a given wavelength (λ) was evidenced for a specific humic acid solution. Here, by using a simplified and efficient spectroscopic acid-base titration protocol [3], the present study proposes a novel method to extend this ΔA_λ vs Q relationship to various NOM samples. This approach deconvolutes the absorbance spectra into 3 components, proton-inert chromophores ($A_{0,\lambda}$), a signal related to the deprotonation process of carboxylic ($A_{1,\lambda}$) and phenolic groups ($A_{2,\lambda}$). This method enabled to select a sample-specific wavelength (λ_{mid}) where both $A_{1,\lambda}$ and $A_{2,\lambda}$ significantly contribute to the variation of the absorbance with pH. By linear regression analysis of $A_{\lambda mid,pH}$ vs Q for various NOM reference samples, sample-specific slope (S_{NOM}) and intercept (I_{NOM}) were found to be related to intrinsic sample spectroscopic properties ($A_{0,\lambda mid}$, $A_{1,\lambda mid}$ and $A_{2,\lambda mid}$), allowing the approximation of Q values of NOM at environmentally relevant concentrations. This approach will improve the understanding and enable more accurate predictions of NOM role in the metal ion fate in natural systems.

[1] Tesfa; Duval; Marsac; Dia; Pinheiro (2022), *Environ. Sci. Technol.* 56 (14), 10494–10503.

[2] Janot; Reiller; Korshin; Benedetti (2010), *Environ. Sci. Technol.* 44 (17), 6782–6788.

[3] Tesfa; Dia; Ollivier; Osorio-Leon; Marsac (2022), *MethodsX.* 56 (14), *9*, 101721.