Interactions between a humic acid and a paramagnetic cation as assessed by CPMAS 13C NMR spectroscopy

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Humic substances (HSs) are natural organic materials playing a very important role in environment due to their ability in interacting with organic and inorganic compounds. From the one side, HSs can reduce the toxic effects of organic and inorganic contaminants, while, from the other side, they can enhance availability of nutrients, such as cations, to living organisms including plants. For this reason it is very crucial to understand the mechanisms of the interactions between humic substances and the environmentally relevant chemical components. In the present work, we have investigated the mechanisms of interaction between a HS and iron (III) by using cross polarization magic angle spinning (CPMAS) 13C NMR spectroscopy. For that, complexes between HS and different amounts of Fe(III) were prepared. All the HS-Fe(III) complexes were analysed by variable contact time (VCT) NMR experiments in order to obtain estimations of the values of the cross-polarization time (TCH) and the proton longitudinal relaxation time in the rotating frame (T1rho(H)). Results confirmed literature findings by which carboxyl groups are the most important humic fraction endowing with the ability to chelate Fe(III). However, our results also demonstrated that direct bondages between HS and Fe(III) involve the remaining polar systems such as carbohydrates and peptides. Conversely, alkyls and aromatics appeared not to be directly bound to the paramagnetic iron (III). We also evaluated the distances between Fe(III) and the different functional groups in the HS through the analysis of the proton spin diffusion into the HS-Fe(III) complexes.