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Effect of cation loading of peat on low-field and high-field proton NMR characteristics

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Temperature and moisture dynamics induce swelling/shrinking processes and may irreversibly change surface characteristics of soil. We treated peat and soil samples by solutions of NaCl, CaCl2 or AlCl3 or with cation exchange resin, focusing on the hypothesis that multivalent cations induce cross-links in soil organic matter with impact on its matrix and surface characteristics. Water binding was characterized with low field 1H-NMR-Relaxometry (20 MHz) and 1H wideline NMR spectroscopy (400 MHz) and compared to contact angles.
From the 1H wideline measurement, we distinguished between mobile water and water involved in water molecule bridging interactions (WAMB). The mobile water was separated by 1H-NMR-Relaxometry into a more mobile and less mobile component. Relaxation rates indicate suggest relatively weak cross-linking in the Al sample, which is explained with the extremely low pH in this sample. We assume that Al retains its hydration shell and bridges uncharged hydrophilic groups via outer sphere complexes. The Ca sample reveals a more effective cross-linking than the Al sample, probably due to the higher abundance of carboxylate groups.
We found a relation between the percentage of mobile water and the wettability of the surface, i.e. the trend to a higher mobile film water volume with increasing wettability. The average sample information from the NMR analysis is correlated with the surface information provided by the contact angle measurements. The results might have significant implications since only a few percent of organic matter can affect the physical, chemical, and biological functioning of the entire 3-phase ecosystem.