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Soil organic matter dynamics as characterized with 1H and 13C solid-state NMR techniques

Alex Jäger (1), Jette Schwarz (2), Marko Bertmer (3), and Gabriele E. Schaumann (4)

(1) Universität Leipzig, Germany, (ajaeger@physik.uni-leipzig.de), (2) Universität Koblenz Landau, Germany , (3) Universität Leipzig, Germany, (bertmer@physik.uni-leipzig.de), (4) Universität Koblenz Landau, Germany, (schaumann@uni-landau.de)

Soil organic matter (SOM) is a complex and heterogeneous matter. Characterization by solid-state NMR methods on 1H and 13C nuclei is therefore demanding. Our goal is to obtain information on the dynamic behaviour of soil samples and to study the influence of external parameters on both structure and dynamics. We regard water molecules to be the pivotal agent of soil dynamics by generating a network between organic matter via intermolecular hydrogen bonding, which leads to cross linking of organic matter and increases its rigidity.
Although 1H solid-state NMR on non-rotating samples are not so commonly used for soil characterization, they enable the differentiation of proton mobilities via their linewidths which are resulting from differences in the dipole-dipole coupling strengths. Therefore, even weak molecular interactions such as hydrogen bonding can be differentiated and changes due to heat treatments and the short and long term behaviour followed.
Though in principle a simple technique, static 1H measurements are complicated by several means, one of them is the high abundance in almost all matter including probe head material that has to be excluded for analysis. Finally, we selected 1H DEPTH [1] and Hahn-echo sequences to distinguish different mobilities in soil, mainly free moving water and water fixed in the soil matrix. After decomposition using Gaussian and Lorentzian lineshapes, the relative amounts of mobile and rigid water molecules can be obtained. By heating the samples above 100°C in sealed glass tubes, the proposed water network is destroyed and able to rebuild after cooling. This long term behaviour is studied on the course of months. Furthermore, the instant changes before and after heating are shown for a series of soil samples to characterize soils based on this water network model.
To combine the information obtained on the 1H mobility with focus on water dynamics, 13C 2D WISE (wideline separation) measurements were done. This method yields 1H mobilities of carbon containing molecules, in our case the soil organic matter. On the one hand, this can be correlated with the results from the static 1H measurements and on the other hand, mobility changes before, during and after a heating event can be studied.

Combining the various information from NMR together with data from DSC (differential scanning calorimetry), a better understanding and perhaps a contribution to a modern model of soil dynamics can be reached.