



NMR spectrometry to study aging processes in soil organic matter

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One of the most valuable ecological potentials of soil organic matter (SOM) is based on its highly dynamic nature, which enables flexible reactions to a variety of environmental conditions. SOM controls a large part of the processes occurring at biogeochemical interfaces in soil and may contribute to sequestration of organic chemicals. This contribution focuses weak intermolecular interactions in soil organic matter studied by NMR spectroscopy. Our central hypothesis is that SOM undergoes physicochemical matrix aging, driven by dynamics in intermolecular cross-linking via bridges of water molecules. In this contribution, aging processes occurring in soil organic matter in heating-cooling cycles are monitored with proton NMR relaxation, proton and deuterium wideline NMR with and without Hahn-Echoes and wideline separation techniques. Furthermore, spin-diffusion experiments, multidimensional ¹³C-¹H experiments including the 2D WISE technique and 2D correlation experiments have been employed to deduce connectivities in SOM structure especially in connection with bridging of functional groups, e. g. carboxyl groups and bound water and the hypothesized water bridges.

The results indicate changes in NMR behavior induced by manipulations of thermal history, and they suggest an increase in side-chain mobility upon heating that remains after cooling. Side-chain mobility slowly decreases again within at least one to two weeks. Our current results strongly suggest even longer aging periods. This observation supports the hypothesis that water molecules bridge molecular segments of SOM. The bridges may be easily disrupted, while re-formation is slow due to diffusion limitation in the SOM matrix.