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IMPROVING STRUCTURAL CHARACTERIZATION OF SOIL ORGANIC MATTER BY 2-DIMENSTIONAL HETERONUCLEUS CORELATION SOLID-STATE 13C NMR (HETCOR) SPECTROSCOPY

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One emphasis of NMR spectroscopy is to determine, via chemical shift assignments, the gross chemical structure of a material, and to quantitatively correlate between the different signal intensities and the chemical composition. Up to now, in soil science mainly 1-dimensional solid-state NMR is used for chemical characterization of soil organic matter (SOM). However, additional structural information can be obtained with 2-dimenstional HETeronucleus CORelation 13C NMR (HETCOR) spectroscopy. Here, the C-signal intensity is modulated by the proton chemical shift via scalar coupling, which allows a more detailed correlation of proton chemical shifts to carbon chemical shifts. Combining this technique with relaxation time measurements gives further information about the mobility of the respective functional group and a rough measurement of the internuclear distance between H and C. Thus, applied in soil science, this technique offers a powerful means to relate spatial molecular properties to biochemical recalcitrance of SOM which opens new doors for a deeper understanding of the mechanisms, responsible for its retention and stabilization in soils. In the present work, we applied this approach to charred biomolecules and plant material. Combined with elemental analysis, we were able to show further evidence supporting that pyrogenic organic matter represents a heterogeneous mixture of partly altered molecules, rather than a highly condensed polyaromatic network. With those first experiments, important acquisition parameters were determined and we clearly demonstrated that this technique can also applied to more complex samples.