41. VERY HIGH RESOLUTION COSY NMR SPECTRA OF HUMIC SUBSTANCES: IMPLICATIONS FOR THE ELUCIDATION OF HUMIC SUBSTRUCTURES

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While one dimensional NMR spectroscopy in the solid and liquid state has contributed enormously to an understanding of structural detail of humic substances, two dimensional NMR spectroscopy is the most important tool to enhance the reliability of NMR resonance assignments.

Proton homonuclear shift correlated 2D NMR spectra offer high sensitivity and long range connectivity information and enable to assemble individual proton resonances and CH cross peaks (available from one bond heteronuclear correlation spectroscopy) into humic substructures. The rather long transfer times in COSY and TOCSY NMR spectra imply loss of magnetization caused by transverse relaxation, so homonuclear 2D NMR spectra of humic materials are in general acquired from rather concentrated samples. High quality homonuclear 2D NMR spectra would significantly improve the currently rather limited knowledge of accurate structural detail of humic materials.

We will present selected very high-resolution COSY NMR spectra of various soil derived humic materials to demonstrate the feasibility of high-resolution 2D NMR spectroscopy and computer aided assignment procedures to elucidate extended humic substructures. This methodology will contribute to a better understanding of humic genesis and transformations in various environmental compartments.