



From Molecular Structure to Global Processes : NMR Spectroscopy in Analytical/Environmental Chemistry

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NMR Spectroscopy is arguably the most powerful tool to elucidate structure and probe molecular interactions. A range of NMR approaches will be introduced with emphasis on addressing and understanding structure and reactivity of soil organic matter at the molecular level. The presentation will be split into three main sections. The first section will look at evidence from advanced NMR based approaches that when considered synergistically describes the major structural components in soil organic matter. Multidimensional NMR spectroscopy (1-3D NMR), automated pattern matching, spectral simulations, diffusion NMR and hybrid-diffusion NMR will be introduced in context of molecular structure. Finally the structural components in soil will be contrasted to those found in aquatic dissolved organic matter.

Secondly molecular interactions of natural organic matter will be considered. Advanced structural studies have provided detailed spectral assignments which in turn permit the reactivity of various soil components to be elucidated. Aggregation and self-association of soil and dissolved organic matter will be discussed along with the structural components likely responsible for aggregation/colloid formation. Interactions of soil organic matter with anthropogenic chemicals will also be considered and NMR techniques based on "Saturation Transfer Difference" introduced. These techniques are extremely powerful and can be used to both; describe mechanistically how anthropogenic chemicals sorb to whole soils and identify the structural components (lignin, protein, cellulose, etc..) that are responsible for the binding/sorption in soil.

In the last section, the "big questions" and challenges facing the field will be considered along with some novel experimental NMR based approaches that should, in future, assist in providing answers to these questions.