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Structural Characterization of Humic Materials Using ^{13}C NMR Techniques: A Comparison of Solution- and Solid-State Methods
CATHERINE CLEWETT, West Texas A&M University, TODD ALAM, Sandia National Laboratories, ERIC OSANTOWSKI, Environmental Protection Agency, MICHAEL PULLIN, New MexicoInstitute of Mining and Technology — The analysis of the carbon type distribution and chemical structure of natural organic matter (NOM) by ^{13}C NMR spectroscopy is an important technique for understanding its origins and reactivity. While prior work has used solution-state NMR techniques, solid-state NMR has the potential to provide this information using less instrument time and sample manipulation, while providing an array of advanced filtering techniques. Analyses of four isolated humic materials with ^{13}C solid-state magic angle spinning (MAS) NMR techniques are described, including three commercially available samples and one fulvic acid sample isolated from the Rio Grande in New Mexico. This study demonstrates the utility of solid-state ^{13}C NMR for aquatic NOM structural characterization, comparing these results to the existing solution-state determinations. The solid-state ^{13}C MAS NMR results are used to determine % carbon distribution, estimates of elemental composition (%C, %H, %(O+N)), aromatic fraction (f_a), nonprotonated aromatic fraction (f_{aN}), an estimate of aromatic cluster size, and ratio of sp^2 to sp^3 carbons. A Gaussian deconvolution method is introduced that allows for a detailed analysis of carbon type.

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