Evaluation of genetic potential and of source rocks by ^{13}C nuclear magnetic resonance (NMR) spectroscopy

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Kerogen, or the insoluble fraction of organic matter in sediments, is a vast, structurally-complex, and economically-important organic carbon reservoir. Due to kerogen's inherent insolubility and structural complexity, the analytical techniques capable of providing molecular structure information in the solid-state are relatively limited. The present study seeks to explore relationships between chemical attributes of kerogen isolates and conventional methods for determining source rock potential, organic matter evolutionary pathway, and thermal maturity using solid-state carbon-13 Nuclear Magnetic Resonance (^{13}C NMR) spectroscopy. We have used 3 distinct ^{13}C NMR techniques: direct polarization, cross polarization, and dipolar dephasing to delineate structural properties and elemental ratios of kerogens of marine, lacustrine, and terrestrial origin (types I-III). Specifically, ^{1}H-^{13}C cross-polarization NMR spectra, and the amount of nonprotontated C and mobile CH_3/CH_2 obtained by C-H dipolar dephasing are applied as predictive tools in describing the genetic potential of shales and humic coals. These data are also explored as a method for kerogen classification when used in conjunction with a molecular mixing model. It is our assertion that NMR analyses of this type provide advantages in source rock characterization compared to standard pyrolysis methods due, in part, to the non-destructive nature of the NMR analysis as well as the bevy of structural information it provides.