Oxygen-17 Nuclear Magnetic Resonance of Organic Solids

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We report solid-state ¹⁷O NMR determinations of the oxygen chemical shift (CS) and electric field gradient (EFG) tensors for a series of ¹⁷O-enriched organic compounds containing various functional groups. In several cases, analysis of the ¹⁷O magic-angle-spinning (MAS) and static NMR spectra yields both the magnitude and relative orientations of the ¹⁷O CS and EFG tensors. We also demonstrate the feasibility of solid-state ¹⁷O NMR as a potentially useful technique for studying molecular structure and hydrogen bonding.

Key words: Oxygen-17; Solid State NMR; Organic Compounds; Chemical Shift Tensor; Quadrupole Coupling Constant.