Solid-state ^{17}O NMR Study of Small Biological Compounds

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We present a systematic experimental and theoretical investigation of the oxygen chemical shielding and electric-field-gradient tensors in polycrystalline amino acids and a peptide. Analysis of the ^{17}O magic-angle-spinning (MAS), multiple-quantum MAS, and stationary nuclear magnetic resonance (NMR) spectra yield the magnitudes and the relative orientations between the two NMR tensors. The obtained ^{17}O NMR parameters are sensitive to the hydrogen bond environments. We also demonstrate that solid-state ^{17}O NMR is potentially useful for studying the secondary structures of peptides and proteins.

Key words: Solid-state ^{17}O NMR, Electric-field-gradient Tensor, Chemical Shielding Tensor, Amino Acid, Peptide