Deuteron Nuclear Magnetic Resonance Studies on Molecular Dynamics of F-moc Amino Acid

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Abstract

The purpose of devising and validating models for intramolecular motions for FMOC amino acids is to quantify side chain motion in proteins which plays an important role in understanding biological structure function relations of proteins. In this thesis, spin lattice relaxation times (T1) of FMOC amino acids were measured under both static and magic angle spinning (MAS) condition at variable temperatures. Lower activation energies of the relaxation times than the normal amino acids observed indicate a less sterically crowded environment for the rotation methyl group. A three-site jump model for the methyl group was developed to fit the T1z and T1Q anisotropy under static condition. Under MAS, Multiple deuterated sites can be resolved and studied independently. Finally, a temperature model for the spinning rotor was developed to account for the temperature gradient across the rotor. A comparison of using the single most probable temperature and the temperature distribution in the simulation of relaxation times concludes the difference between these two approaches is minimal.