

A Spin-Lattice Relaxation Time Study of Organic Thin Films on Silica Particles.
Edward. W. Hagaman; Michelle. K. Kidder; A. C. Buchanan, III, Chemical Sciences
Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6201

An organic substance covering the surface of a nonporous silica particle may be described as a thin liquid film. The organic residue may be attached through a robust chemical bond or a much weaker and less well-defined hydrogen bond. Chemical attachment of the organic residue virtually guarantees monolayer coverage. Phenyl rings bonded to the surface of fumed silica by an Si-O-Ph linkage provides two rotational degrees of freedom for the organic moiety – rotation around the silicon-oxygen and the oxygen-carbon bonds. At room temperature rotation rates are fast enough to completely average dipolar and CSA line widths (Sigman, M. E.; Read, S.; Barbas, J. T.; Ivanov, I.; Hagaman, E. W.; Buchanan, A. C., III; Dabestani, R.; Kidder, M. K.; Britt, P. F. *J. Phys. Chem. A*, **2003**, *107*, 3450-3456.). In this case, the high resolution ^{13}C NMR spectrum can be recorded using conventional solution state NMR techniques. Physical adsorption (hydrogen bonding) of the organic at equivalent concentrations does not guarantee monolayer coverage. Nonetheless, we show here by solid state and solution relaxation time measurements that both the chemisorbed and physisorbed organics exhibit similar motional regimes that differ from that of the corresponding bulk liquid. The spin-lattice relaxation time data are used to describe the motion of the organic residues that occurs in these systems. This research was sponsored by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences, U. S. Department of Energy under contract DE-AC05-96OR22464 with Oak Ridge National Laboratory, managed by UT-Battelle for the Department of Energy.

NMR Symposium

Poster Session

Edward W. Hagaman, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6201, phone 865-576-2751, fax 865-574-6721, hagamanew@ornl.gov

"The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes."