

NMR Study of HD Adsorbed in a Z-type Metal-Organic Framework

Yu Ji, Y. Tang, J.A. Hamida, and N.S. Sullivan

Department of Physics, University of Florida, USA

We report the results of measurements of the nuclear spin-lattice and spin-spin relaxation rates of hydrogen deuteride trapped in the mesoporous cages of a metal organic framework¹ (MOF) for temperatures $2.2 < T < 50$ K. There is considerable interest in the use of this class of material for hydrogen storage because of the high density of adsorption. NMR studies can provide important information about the molecular interactions and dynamics inside the cages of the MOF structure. Samples were studied with filling factors of 0.5 and 1.0 molecules per cage as determined by the adsorption isotherm at 77 K. The results show strong peaks in the relaxation times at several well defined temperatures that are very different from the adsorption energy levels. These peaks are discussed in terms of the quantization of the translational degrees of freedom of the molecules inside the cages and the associated discrete energy levels. Measurements of the nuclear spin-spin relaxation times provide an important measure of the diffusivity of hydrogen through the MOF structure which is a critical parameter for the use of MOFs for storage and transport.

¹Basolite[®] Z1200, Sigma Aldrich, 3050 Spruce St., St. Louis, MO 63103