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Quantum diffusion of atomic hydrogen isotopes in water DAVID BARTELS, JONATHAN WALKER, Univ of Notre Dame — Atomic hydrogen or deuterium radicals can readily be generated in water with a high energy electron beam, and studied using time-resolved electron paramagnetic resonance (EPR). The light isotope muonium, formed from an electron orbiting a positive muon (mass = 0.11 amu), can also be studied by muonium spin resonance (MuSR) at facilities where muon beams are generated. It is to be expected that the diffusion of these isotopes would depend on their mass, and particularly in the case of muonium there should be effects of quantum zero point energy. The ring polymer molecular dynamics (RPMD) simulation method has already been applied to predict a large reduction of diffusion coefficient for muonium relative to hydrogen atoms[1]. In the present work, we present both EPR and MuSR measurements of spin exchange rate between the atomic hydrogen isotope and $(Ni^{2+})_{aq}$ ions. The spin exchange is a diffusion-limited process, and so should directly indicate the relative diffusion rates of the atomic isotopes. Surprisingly, the muonium diffusion appears to be more classical than quantum in character. New RPMD simulations with a quantized water model will be presented to model the experimental result. .(1) Markland, T. E.; Habershon, S.; Manolopoulos, D. E. *J. Chem. Phys.* **2008**, *128*, 194506.

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