MICROWAVE SPECTRA OF ¹⁸O-TROPOLONE AND D-TROPOLONE

WEI LIN, WALLACE C. PRINGLE, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, Middletown, CT 06459; THOMAS A. BLAKE, Pacific Northwest National Laboratory, Richland, WA 99352 (PNNL is operated for the US Department of Energy by the Battelle Memorial Institute under contract DE-AC05-76RLO 1830); JOHN C. KESKE, and DAVID F. PLUSQUELLIC, Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8441.

Tropolone is a seven-membered ring with an intramolecular hydrogen bond between the hydroxyl proton on C_1 and the carbonyl oxygen on C_2 . The proton tunnels between the two neighboring oxygen atoms. Microwave spectra of singly-substituted ¹⁸O-tropolone and of singly-deuterated tropolone were measured to determine the effect of these two substitutions on the proton tunneling dynamics. The 0^+ state of ¹⁸O-tropolone and both the 0^+ and 0^- states of D-tropolone were observed and assigned. Analysis of the spectra reveals complete quenching of the tunneling splitting of ¹⁸O-tropolone. The energy separation between the 0^+ and 0^- states in D-tropolone was determined and is found to be significantly smaller than that of normal tropolone.