A ROTATIONAL STUDY OF 2H-3H-PERFLUOROPENTANE AND ITS ISOTOPOLOGUES

CHINH H. DUONG, DANIEL A. OBENCHAIN, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT 06459-0180; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.

The chirped pulse Fourier transform microwave spectrum of 2H-3H—perfluoropentane has been observed and assigned. Given a racemic mixture sample of the four available structural isomers, only the (S,S) structure was observed in the broadband spectrum. Attempts at observing the ^{13}C isotopologues on a Balle—Flygare cavity type spectrometer and their assignments will be discussed, along with an examination of the theoretical predictions for the structure and rotational constants of the molecule against their experimental values. Structural results of the monomer will also be compared with those of the helical structure of C_2 perfluoropentane.

^a Joseph A. Fournier, Robert K. Bohn, John A. Montgomery Jr., Masao Onda. J. Phys. Chem. <u>114</u> (1118), 2010.