THE LOW FREQUENCY BROADBAND FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF HEXAFLUOROPROPYLENE OXIDE, CF_3CFOCF_2

LU KANG[a], *Department of Natural Sciences, Union College, Barbourville, KY 40906*; STEVEN T. SHIPMAN, JUSTIN L. NEILL, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*; ALBERTO LESARRI, *Departmento de Quimica Fisica, Universidad de Valladolid, Facultad de Ciencias, Valladolid, 47005 SPAIN*; and BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*.

The pure rotational spectra of hexafluoropropylene oxide (HFPO), CF_3CFOCF_2, as well as its ^{13}C (1.07%) and ^{18}O (0.205%) isotopomers were recorded in natural abundance from 2.0 to 26 GHz. Low frequency transitions (2 - 8 GHz) were measured by a recently designed chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer at the University of Virginia. The observed spectra lines of ^{13}C isotopomers (in natural abundance) demonstrate the capability and sensitivity of the CP-FTMW spectrometer operating in 2 - 8 GHz region. The spectra in 8.0 - 26 GHz region were recorded by a Fabry-Pérot cavity Fourier transform microwave (FP-FTMW) spectrometer. All the five isotopologues of HFPO were found, and their spectroscopic constants were fit from assigned spectral lines using JB95 and Pickett's SPFIT suite of programs. For the dominate HFPO isotopomer: A_0 = 2217.04887(11) MHz, B_0 = 1101.48958(5) MHz, C_0 = 936.60131(5) MHz, Δ_J = 55.0(2) Hz, Δ_{JK} = 107.5(9) Hz, Δ_K = -20(2) Hz, δ_J = 8.49(6) Hz, and δ_K = -266(2) Hz. The experimentally determined molecular structure and rotational constants are in a good agreement with our density functional theory calculation using B3LYP/6-31g(d) method.

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