

## MICROWAVE SPECTROSCOPY OF BIS-(TRIFLUOROMETHYL) PEROXIDE, $\text{CF}_3\text{OOCF}_3$

LU KANG, *Department of Biology, Chemistry, and Physics, Southern Polytechnic State University, Marietta, GA 30060*; STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06457*.

The microwave spectrum of bis-(trifluoromethyl) peroxide,  $\text{CF}_3\text{OOCF}_3$ , was measured between 5 and 20 GHz frequency region. The spectrum of its  $^{13}\text{C}$  isotopologue was also recorded in natural abundance. All observed transitions were ambiguously assigned. The rotational and centrifugal distortion constants for the dominant  $\text{CF}_3\text{OOCF}_3$  species are:  $A = 2806.6567(2)$  MHz,  $B = 795.3253(2)$  MHz,  $C = 790.3212(2)$  MHz,  $\Delta_J = 68.0(3)$  Hz,  $\Delta_{JK} = 179(1)$  Hz, and  $\delta_J = -0.44(9)$  Hz. The ab initio and the density functional theory level of calculations were performed to optimize the molecular geometry and to predict the spectroscopic constants. The theoretical predictions are in moderate agreement with the experimental measurements.