THE ROTATIONAL SPECTRA OF PERFLUOROPROPIONIC ACID AND ITS HYDRATES

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The pure rotational spectrum of perfluoropropionic acid, CF_3CF_2COOH, has been studied using a chirped pulse Fourier transform microwave spectrometer in the frequency range of $8-14$ GHz. A total of 81 transitions, including *a*-type, *b*-type, and *c*-type transitions have been observed and analyzed. The rotational constants and the five quartic centrifugal distortion constants have been determined for the first time. Quantum chemical calculations and the spectral analysis indicate that the observed conformer is the *gauche* form of perfluoropropionic acid with calculated dihedral angles $\angle$CCCO = 106° and 107° completed at the MP2/6-311G++(3df, 3pd) and MP2/aug-cc-pVDZ level, respectively. The rotational spectrum of the perfluoropropionic acid monohydrate has been assigned from the broadband spectrum. Most of the transitions exhibit doubling patterns belonging to the tunneling motion of the water molecule. Progress on the assignment of the perfluoropropionic acid dihydrate will also be presented.