LARGE AMPLITUDE MOTIONS IN 2,2,3,3,3-PENTAFLUOROPROPANOL AND ITS BINARY WATER COMPLEX

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2,2,3,3,3-pentafluoropropanol (PFP) is an important solvent for organic syntheses. It is also considered to be a greenhouse gas pollutant because it is radiatively active in the mid-infrared region. Understanding properties of PFP and its hydrogen bonding interactions with water in the gas phase may help to develop more realistic estimate of its effects because of the abundance of water in the atmosphere. In the current study, we apply both rotational spectroscopy and ab initio calculations to characterize large amplitude motions in PFP and its water complex and also hydrogen bonding interactions between PFP with water. Their rotational spectra were recorded using a cavity-based and a chirped pulse Fourier transform microwave spectrometers. Two most stable PFP conformers, Pg+g+ and Ptg+ were identified. The rotational transitions of the latter exhibit tunneling splittings. Two PFP-H2O conformers were identified and both of them show tunneling splittings. Deuterated species of the water complex were also investigated to assist the identification of the tunneling paths, in addition to the theoretical calculations. The large amplitude motions responsible for these splittings will be discussed.