

ALTERNATING 1-PHENYL-2,2,2-TRIFLUOROETHANOL CONFORMATIONAL LANDSCAPE WITH THE ADDITION OF ONE WATER: TUNNELLING AND LARGE AMPLITUDE MOTIONS

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The 1:1 adduct of 1-phenyl-2,2,2-trifluoroethanol (PhTFE) with water was investigated using chirped pulse Fourier transform microwave spectroscopy and computational methods. PhTFE itself was previously reported to have two stable conformations, I (gauche) and II (trans), however, only the most stable conformer, PhTFE I, was experimentally observed.¹ Rotational spectra of the two most stable PhTFE-H₂O conformers along with several deuterium and oxygen-18 isotopologues were assigned and their structures analyzed. The most stable complex exhibits PhTFE in the gauche configuration with water inserted into the existing intramolecular OH-F hydrogen bond. This conformer is stabilized by two intermolecular hydrogen bonds in addition to the intramolecular interactions present in the PhTFE monomer. Those being a strong interaction between the alcohol hydrogen on PhTFE and the oxygen on water OH-OH₂ and a weaker interaction between a fluorine on PhTFE and a water hydrogen F-HOH. Water tunnelling splitting was identified in the rotational spectrum showing the characteristic ortho versus para intensity ratio, which was attributed to the interchange of bonded and non-bonded hydrogen atoms of the water subunit. The second observed complex exhibits PhTFE in the trans configuration, indicating that complexation with water sufficiently stabilized PhTFE II such that it can survive the supersonic expansion. Stabilization is achieved by water interacting with both the alcohol hydrogen and the phenyl ring of PhTFE. The nonbonded hydrogen of the water subunit was shown to exhibit a large amplitude motion in both conformers.

1. Carlson, C. D.; Seifert, N. A.; Heger, M.; Xie, F.; Thomas, J.; Xu, Y. J. *Mol. Spectrosc.*, 2018, 351, 62–67.