

MICROWAVE AND COMPUTATIONAL STUDIES OF HYDRATED ACID ANHYDRIDES: CAPTURING A LOCAL POTENTIAL ENERGY MINIMUM AND EXPLORING THE EFFECT OF C(CH₃)₃ AND CF₃ SUBSTITUENTS

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Microwave studies of hydrated acid anhydrides (RCOOCOR-H₂O) provide an interesting venue for characterizing local minima on the potential energy landscape of reactive systems. This talk reports the microwave spectra of the monohydrates of pivalic anhydride (R = R' = C(CH₃)₃), trifluoroacetic anhydride (R = R' = CF₃), and the mixed pivalic-trifluoroacetic anhydride (R = C(CH₃)₃, R' = CF₃). While the ultimate fate of these species in bulk aqueous solution is hydrolysis to form the parent acids, this work captures the precursor complexes and investigates the effect of R and R' on the geometry of the monohydrate. Microwave spectra of the parent species and their D₂O and DOH isotopologues are reported, as is an in-depth computational analysis at different levels of theory. Calculated structures show varying degrees of hydrogen bonding and electrophilic-nucleophilic interaction, depending on the particular combination of R and R' groups. Additionally, closely spaced pairs of tunneling states arising from internal water motion were observed in the monohydrate spectra except in the case where R = R' = CF₃.