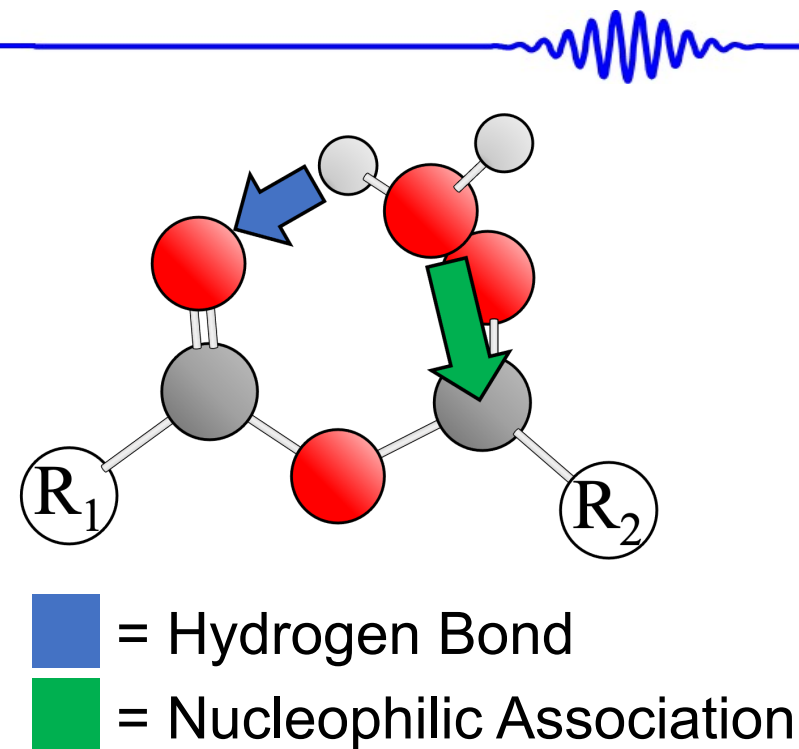


P4951: Microwave and Computational Studies of Hydrated Acid Anhydrides

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- Measured microwave spectra for the monohydrates of 3 different carboxylic anhydrides
- Measured all D₂O and DOH isotopologue spectra
- Observed water tunneling states (2 of 3 complexes)
- How do R groups dictate intermolecular interactions: Hydrogen Bonding vs. Nucleophilic Association
- Dominant Hydrogen Bond character in the t-butyl and mixed t-butyl—trifluoroacetic anhydrides
- Dominant Nucleophilic Association character in trifluoroacetic anhydride



R ₁	R ₂
t-butyl	t-butyl
t-butyl	-CF ₃
-CF ₃	-CF ₃