EVIDENCE FOR A COMPLEX BETWEEN THF AND ACETIC ACID FROM BROADBAND ROTATIONAL SPECTROSCOPY

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Evidence for a complex between tetrahydrofuran (THF) and acetic acid from broadband rotational spectroscopy will be presented. Transitions believed to belong to the complex were first identified in a gas mixture containing small amounts of THF, triethyl borane, and acetic acid balanced in argon. Ab initio calculations suggest a complex between THF and acetic acid is more likely to form compared to the analogous acetic acid complex with triethyl borane, the initial target. The observed rotational constants are also more similar to those predicted for a complex formed between THF and acetic acid, than for those of a complex formed between triethyl borane and acetic acid. Subsequently, multiple isotopologues of acetic acid have been measured, confirming its presence in the structure. No information has yet been obtained through isotopic substitution within the THF sub-unit. Ab initio calculations predict the most likely structure is one where the acetic acid subunit coordinates over the ring creating a ”bridge” between the THF oxygen, the carboxylic O-H, and the carbonyl oxygen to a hydrogen atom on the back of the ring.