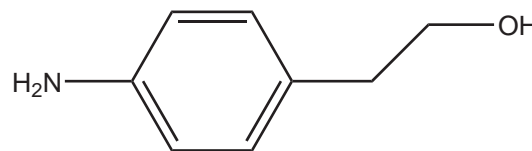


HYDROGEN BONDING IN 4-AMINOPHENYL ETHANOL: A COMBINED IR-UV DOUBLE RESONANCE AND MICROWAVE STUDY

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Both amine and hydroxyl functional groups are present in 4-aminophenyl ethanol (4-AE), and each functional group can form hydrogen bonds with carboxylic acids, such as formic acid and acetic acid. Predicting the structures of such complexes involving 4-AE is rather complex, given the many possible conformations and their similar (and method and basis-dependent) energies. In particular, the carboxyl group, -COOH, can act as both as a hydrogen bond donor or acceptor, or both at once.



In this study we report the formic acid – 4-AE hydrogen bonded complex. An infrared-ultraviolet double resonance spectrometer is used to examine the shifts in IR frequencies of 4-AE from the monomer to the complex. Fourier transform microwave spectroscopy is used to determine structures of the species. Results from both experiments are compared to DFT and *ab initio* results. Time permitting, results of the water complex with 4-AE will also be presented.