

# Rapid Non-radiative Decay of Jet-cooled 2-hydroxyformanilide: IR-dip Spectroscopy and Computational Studies

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In this study, we present the conformational investigations and excited state dynamics of jet-cooled 2-hydroxyformanilide (2-HFA). The number of conformers and their structures of 2-HFA are assigned on the basis of resonance enhanced multiphoton ionization (REMPI), ultraviolet-ultraviolet hole burning (UV-UV HB), infrared-dip (IR-dip) spectroscopy. From comparison between REMPI and UV-UV HB spectra, three species coexist in the supersonic jet. Two species among them are 2-HFA-AC (Anti and Cis) and the other is 2-HFA-AT (Anti and Trans). The similar UV-UV HB spectra are due to the anharmonic coupling between the peptide group and some ring deformations in the excited state. We speculate that the observance of IR upstream in the IR-dip spectrum might come from the contribution of 2-HFA-ST (Syn and Trans). The structures of these conformers are determined by the IR-dip spectroscopy and Franck-Condon simulations. Also, the observed spectra are compared with the predictions of ab initio and density functional theory calculations.

