INFARED SPECTROSCOPY AND PHOTOCHEMISTRY OF BIACETYL-WATER COMPLEXES ISOLATED IN INERT GAS MATRICES

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We report the results of a study of biacetyl and biacetyl-d_6 with water and water-d_2 trapped in inert gas matrices. In solution, irradiation has been shown to produce an enol (2-hydroxy-1-butene-3-one), although no indication of this compound is observed in the gas phase or for matrix-isolated biacetyl. DFT calculations predict the existence of three stable enol conformers, as well as several enol-water and biacetyl-water complexes. The calculations also predict that biacetyl-water complexes should have lower barriers to enolization than the uncomplexed biacetyl. The pre-irradiation infrared spectra contain features attributed to biacetyl-water complexes. Irradiation at 405 nm yields a different set of photoproducts than was found with uncomplexed biacetyl. These experimental results will be discussed in light of the DFT predictions.