Density Functional Theory calculations were performed on biacetyl*water complexes and expected photoproducts using the computational software, *Gaussian*. The method used in this study was uM06 with the aug-cc-pVTZ basis set. Geometry optimizations, frequencies and excited states were the specific calculations performed. Biacetyl, water, and biacetyl*water complexes, as well as deuterated forms, were isolated in argon and nitrogen matrices under vacuum. Infrared spectra of the matrices were obtained pre- and post-irradiation using a mercury vapor lamp and filters of various wavelengths. The resulting IR spectra were analyzed to determine the photoproducts formed after each irradiation. These results were then compared to the theoretical IR frequencies obtained from the computational analysis in order to assign possible photoproduct identities. The two major observed photoproducts were ketene, at 2140 cm⁻¹, and a peak 1160 cm⁻¹ previously believed to be a cyclic carbonyl. Based on new computational data obtained, the 1160 cm⁻¹ peak may possibly be assigned to an epoxide, 2-methyl-3-methylidene-2-oxiranol.