ABSTRACT

Complexes of water and biacetyl were isolated in argon and nitrogen matrices under vacuum. Infrared spectra of water, biacetyl, biacetyl*water complexes, and respective deuterated forms were then obtained. The matrices were irradiated using the filtered output of a mercury vapor lamp with short and long pass filters of varying wavelengths. Density Functional Theory (DFT) calculations of water, biacetyl, biacetyl*water complexes were optimized with an aug-cc-pVTZ basis set and uM06-2X method. Frequency calculations were then computed on optimized geometries, and excited state (time-dependent DFT) calculations were performed on stable molecules and complexes. Frequencies of possible isotopomers were also completed for comparison with experimental data. The theoretical infrared spectra were then compared to experimental infrared spectra in order to further understand the product species resulting from photochemical reactions of biacetyl and water. Ketene was observed in most irradiations at 2140 cm^{-1}. The 250-450 nm filter produced output with the most photoproducts, and the addition of water to matrices resulted in more ketene, carbon dioxide and photoproducts present in spectra.