INFRARED SPECTRUM OF MATRIX-ISOLATED METHYLHYDROXYCARBENE

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The ultraviolet irradiation of matrix-isolated biacetyl results in the formation of a complex of methylhydroxycarbene (CH_3COH) and ketene (CH_2CO). The infrared spectrum of the carbene exhibits broad features at 3270 cm^{-1} (OH stretch) and 1240 cm^{-1} (CO stretch); the vibrational frequencies for CH_2CO are shifted from those observed for the uncomplexed molecule. The complex was also observed when the parent was fully or partially deuterated, with appropriate isotopic shifting. The observed spectra are consistent with predictions from DFT and MP2 calculations for *trans*-CH_3COH hydrogen bonded to the adjacent CH_2CO. The wavelength, matrix and isotope dependence for the formation of this complex was studied: parent deuteration decreases the apparent efficiency of production at 405 nm by a factor of 11 (O_2 matrix) to 300 (Kr matrix).