IR SPECTROSCOPY OF MATRIX-ISOLATED PROPARGYL RADICALS

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Organic radicals isolated in a rare gas (Ar or Ne) matrix at 10K can be prepared by UV photolysis of a suitable precursor. A precursor/rare gas mixture is deposited on a CsI window at 30K and cooled to 10K. The matrix is then irradiated with UV light for several hours to photodecompose the precursor. IR absorption spectra are recorded before, during, and after the photolysis using a Fourier transform spectrometer. We have prepared propargyl radical in the photodecomposition 1-butyn-3-nitrite ($HCCCH_2$ CH_2ONO) at 254 nm.

$$HCCCH_2CH_2ONO \longrightarrow HCCCH_2CH_2O + NO \quad HCCCH_2CH_2O \longrightarrow HCCCH_2 + CH_2O$$

We have identified the propargyl radical, along with formaldehyde and nitric oxide, in the photoproducts of the butynnitrite decomposition and assigned many of the IR fundamentals of propargyl in the Ar matrix.

ν_1 3316 cm^{-1}
ν_2 3102 cm^{-1}
ν_3 1955 cm^{-1}
ν_4 1446 cm^{-1}
ν_5 1028 cm^{-1}
ν_6 656 cm^{-1}
ν_{10} 986 cm^{-1}
ν_{11} 638 cm^{-1}

We are currently working to produce the propargyl radical and dueterated isotopes from a variety of other precursors, including propargyl bromide ($HCC\text{-}CH_2\text{-}Br$) and bromoallene ($CH_2{=}C{=}CHBr$).