

MATRIX-ISOLATION FTIR SPECTROSCOPY OF THE 1-BUTYN-3-YL RADICAL

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The 1-butyn-3-yl radical (C_4H_5) is thought to play a role in the formation of hydrocarbons in the interstellar medium and planetary atmospheres, but it is not well characterized. In this study, the 1-butyn-3-yl radical was formed by the pyrolysis of gas-phase 3-bromo-1-butyne at temperatures of 800-1200 K. Nascent radicals were isolated in an argon matrix, followed by FTIR spectroscopy. Vibrational bands in the experimental spectra were matched to frequencies predicted by Gaussian 09. Pyrolysis of 3-methyl-1-butyne was also investigated as a possible pyrolytic precursor to the 1-butyn-3-yl radical under similar conditions. Evidence of 1-butyn-3-yl formation was observed, but other radicals may have formed as well.