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Propargyl Radical: ab initio Anharmonic Modes and the Polarized Infrared Absorption Spectra of Matrix-Isolated HCCCH2 BARNEY ELLISON, University of Colorado, XU ZHANG, University of Colorado, EVAN JOCHNOWITZ, University of Colorado, MARK NIMLOS[1], University of Colorado, JOHN STANTON, University of Texas, MYCHEL VARNER, University of Texas
— Propargyl Radical: ab initio Anharmonic Modes and the Polarized Infrared Absorption Spectra of Matrix-Isolated HCCCH2 The propargyl radical has twelve fundamental vibrational modes, Gamma(vib)(HCCCH2) = 5a1 + 3b1 + 4b2, and nine have been detected in a cryogenic matrix. Ab initio coupled-cluster anharmonic force field calculations were used to help guide the assignments. The experimental HCCCH2 matrix frequencies (cm-1) and polarizations are: a1 modes - 3308.5 +/- 0.5, 3028.3 +/- 0.6, 1935.4 +/- 0.4, 1440.4 +/- 0.5, 1061.6 +/- 0.8; b1 modes - 686.6 +/- 0.4, 483.6 +/- 0.5; b2 modes - 1016.7 +/- 0.4, 620 +/- 2. We recommend a complete set of gas-phase vibrational frequencies for the propargyl radical, HCCCH2 X 2B1.

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