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, 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, $\Gamma_{\text{vib}}(\text{HCCCH}_2) = 5a_1 + 3b_1 + 4b_2$, 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: $a_1$ modes - 3308.5 +/- 0.5, 3028.3 +/- 0.6, 1935.4 +/- 0.4, 1440.4 +/- 0.5, 1061.6 +/- 0.8; $b_1$ modes - 686.6 +/- 0.4, 483.6 +/- 0.5; $b_2$ modes - 1016.7 +/- 0.4, 620 +/- 2. We recommend a complete set of gas-phase vibrational frequencies for the propargyl radical, HCCCH2 $X \ 2B_1$.

1 also at National Renewal Energy Laboratory