ROTATIONAL SPECTRA OF T-SHAPED CYANOACETYLENE – CARBON DIOXIDE COMPLEX, HCCCN — CO_2

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The rotational spectra of T-shaped cyanoacetylene carbon dioxide complex, HCCCN — CO_2, were measured using two Balle-Flygare type Fourier transform microwave (FTMW) spectrometers between 1.4 GHz and 22 GHz. The low J transitions were recorded using the low frequency FTMW spectrometer at the University of Arizona with a state-of-the-art resolution of "full width at half maximum" (FWHM) 1 kHz. The spectra above 4 GHz were recorded at Wesleyan University. Spectral hyperfine structures due to the ^{14}N nuclear quadrupole coupling interactions can be fully resolved in low frequency bands. Since all K_a = 1 branches were not observed, this implies that HCCCN — CO_2 possesses a rigorous T-shaped structure. Assuming that A_0 is the same as that of HCN — CO_2, 11824 MHz, the spectroscopic constants of HCCCN — CO_2 are: B_0 = 794.59686(63) MHz, C_0 = 715.74488(60) MHz, Δ_J = 0.50067(18) kHz, Δ_{JK} = 120.892(12) kHz, δ_J = 0.04253(31) kHz, δ_K = 65.32(12) kHz, H_J = -0.00117(33) Hz, H_{JK} = 0.034876(21) kHz, H_{KJ} = -0.68254(73) kHz, $\chi_{aa}(^{14}\mathrm{N})$ = -4.12873(78) MHz, $\chi_{bb}(^{14}\mathrm{N})$ = 2.110(25) MHz, and $\chi_{cc}(^{14}\mathrm{N})$ = 2.019(25) MHz.