The microwave rotational spectrum of the Ne-HCCCN van der Waals complex

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We report the results of the first rotational spectroscopic investigation of the Ne-HCCCN van der Waals complex. The measurements were carried out in the frequency range from 4 to 26 GHz using a molecular beam Fourier transform microwave spectrometer. HCCCN was prepared from ethyl propiolate in the usual way, and for our investigation we used a dilution of 0.2% ethynyl cyanide in neon at a total pressure of 3 to 4 atm.

Strong $b$-type and weaker $a$-type transitions were observed. The spectra are consistent with a (vibrationally averaged) T-shaped geometry of the complex. The $^{14}$N nuclear quadrupole hyperfine components of the rotational transitions were resolved. The spectral analyses yielded rotational, centrifugal distortion, and $^{14}$N nuclear quadrupole coupling constants which were used to derive structural parameters and information about the large amplitude intermolecular motion.

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