MICROWAVE SPECTRUM AND STRUCTURE DETERMINATION OF THE CCAs RADICAL ($X^2\Pi_r$)

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The microwave spectrum of the CCAs radical $(X^2\Pi_r)$ has been measured using Fourier transform (FTMW) techniques. This species were created in a supersonic expansion by the reaction of arsenic trichloride, AsCl₃, and acetylene, C₂H₂, diluted in argon carrier gas, using a pulsed nozzle coupled with a DC discharge. Three rotational transitions of CCAs were measured in the frequency range of 12 to 32 GHz, in which both lambda-doubling and hyperfine interactions were observed, the latter due to the arsenic spin of I = 3/2. In addition, four rotational transitions for ¹³C¹³CAs were measured in the frequency range of 11 to 38 GHz, as well as several transitions arising from ¹³C¹²CAs and ¹²C¹³CAs. In these three species, hyperfine splittings were also observed due to the ¹³C nuclei, creating complex patterns for these isotopologues. These data were analyzed with a Hamiltonian incorporating the appropriate number of nuclear spins, and effective rotational, lambda-doubling, and arsenic and carbon-13 hyperfine constants were determined. From the effective rotational constants, bond lengths for this linear species have been established. The distribution of electrons in this radical has also been inferred from the hyperfine constants.