MILLIMETER/SUBMILLIMETER SPECTRUM OF THE CCP ($X^2\Pi_r$) RADICAL

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The pure rotational spectrum of the CCP radical ($X^2\Pi_r$) has been measured using millimeter-wave direct absorption techniques. This work is the first high-resolution data for this radical. This species was created by the reaction of gas-phase phosphorus and acetylene in the presence of argon carrier gas and an AC glow discharge. Twenty-four rotational transitions were measured in the frequency range of 120 to 413 GHz. Each transition is separated into two spin-orbit components; however, only the Ω = 1/2 component has been observed to date. This spin component is additionally split into lambda-doublets. Below 209 GHz, hyperfine interactions due to the phosphorus nuclear spin of I = 1/2 are evident, spitting each lambda-doublet into two lines. The data were fit with a case (c) Hamiltonian, and effective rotational, lambda-doubling, and phosphorus hyperfine constants were determined. Additional searches are being conducted for the Ω = 3/2 component. These data prove that CCP has a linear geometry in its ground state. This structure is similar to other MC_2 species, such as CCS and CCCl, in contrast to NaC_2, MgC_2, AlC_2, and SiC_2. The change in structure from T-shaped to linear is caused by a increase in the covalent bonding interactions between the C_2 moiety and the heteroatom.