MILLIMETER/SUBMILLIMETER SPECTRUM OF THE CCP (X^2Π_g) RADICAL

D. T. HALFEN, Steward Observatory, University of Arizona, Tucson, AZ, 85721; D. J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY, 40506; and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ, 85721.

The pure rotational spectrum of the CCP radical (X^2Π_g) 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 \( \Omega = 1/2 \) 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, splitting 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 \( \Omega = 3/2 \) component. These data prove that CCP has a linear geometry in its ground state. This structure is similar to other MC₂ species, such as CCS and CCCI, in contrast to NaC₂, MgC₂, AlC₂, and SiC₂. The change in structure from T-shaped to linear is caused by a increase in the covalent bonding interactions between the C₂ moiety and the heteroatom.