THE PURE ROTATIONAL SPECTRUM OF THE PCN $(X^3\Sigma^-)$ RADICAL

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The pure rotational spectrum of the PCN radical ($X^3\Sigma^-$) has been measured using both millimeter-wave direct absorption and Fourier transform microwave techniques. This work is the first laboratory detection of this radical. In the millimeter/submillimeter region, this species was created by the reaction of gas-phase phosphorus and cyanogen in the presence of argon carrier gas and an AC glow discharge. In the microwave regime, it was produced from a mixture of PCl₃ vapor and cyanogen diluted in argon and a DC discharge. Twenty-four rotational transitions were measured in the frequency range of 137 to 413 GHz, as well as three rotational transitions from 19 to 34 GHz. Each transition is split into three fine-structure components, a result of spin-rotation and spin-spin interactions. Below 277 GHz, hyperfine interactions due to the phosphorus nuclear spin of I = 1/2 are evident, spitting each line into doublets. For the microwave data, nitrogen hyperfine structure additionally splits each line into three components. The data have been fit with a case (b) Hamiltonian, and rotational, fine-structure, and phosphorus and nitrogen hyperfine constants were determined. PCN is a possible interstellar/circumstellar species given the recent detections of HCP and CCP.