ROTATIONAL SPECTRUM OF CYANOPHOSPHAACETYLENE, H_2P-C≡C-C≡N

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The *a* type transitions of the microwave rotational spectra of cyanophosphaacetylene, H_2P-C≡C-C≡N, have been investigated in the frequency region between 5 and 26.5 GHz by Fourier Transformation Microwave (FTMW) spectroscopy. Rotational, centrifugal distortion and ^{14}N nuclear quadrupole coupling constants have been determined. Density functional theory level *ab initio* calculations were performed to predict the molecular constants, and the predicted values are in good agreement with our experimentally determined results. The ^{13}C and ^{15}N isotopomer transitions were also observed. The derived r_0 structure is quite comparable to the calculated H_2P-C≡C-C≡N equilibrium geometry.