ROTATIONAL SPECTRUM OF CYANOPHOSPHINE, H_2PCN

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The *a* type transitions of the microwave rotational spectra of cyanophosphine, H_2PCN, have been investigated in selected frequency regions between 10 and 42.5 GHz by Fourier Transformation Microwave (FTMW) spectroscopy. Rotational, centrifugal distortion and ^{14}N nuclear quadrupole coupling constants as well as the spin rotation coupling constants of phosphorus 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_2PCN equilibrium geometry.