

ROTATIONAL SPECTRUM OF CYANOPHOSPHINE, H₂PCN

LU KANG, STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*;
M. C. McCARTHY, and P. THADDEUS, *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138*; and *Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138*.

The *a* type transitions of the microwave rotational spectra of cyanophosphine, H₂PCN, have been investigated in selected frequency regions between 10 and 42.5 GHz by Fourier Transformation Microwave (FTMW) spectroscopy. Rotational, centrifugal distortion and ¹⁴N 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 ¹³C and ¹⁵N isotopomer transitions were also observed. The derived *r*₀ structure is quite comparable to the calculated H₂PCN equilibrium geometry.