$\nu_1 + \nu_5$ OF HCCN: DETERMINATION OF THE $\nu_5$ VIBRATIONAL ENERGY

JIAXIANG HAN, P. Y. HUNG, JOHN DeSAIN, W. E. JONES, and R. F. CURL, Chemistry Department and Rice Quantum Institute, Rice University, Houston, Texas 77251.

The high resolution infrared spectrum of HCCN in the region 3338-3382 cm$^{-1}$ has been observed by infrared kinetic spectroscopy. The spectrum is assigned as the combination band $\nu_2 + \nu_5$ of the quasilinear molecule HCCN with the origin at 3355.510(9) cm$^{-1}$. Based on information from the $\nu_2 + \nu_5$ spectrum\textsuperscript{[3]}, the energy of the lowest excited state with angular momentum about the $a$-axis, $\nu_5$, is determined to be 128.913(9) cm$^{-1}$. This value is lower than the results obtained by means of relative intensity measurements on the millimeter-wave spectra\textsuperscript{[2]} [145(15) cm$^{-1}$] or from similar relative intensity measurements on the IR spectra\textsuperscript{[2]} [187(20) cm$^{-1}$]. The present value of the energy for $\nu_5$ predicts a barrier to linearity similar to that obtained from the corresponding band of DCCN\textsuperscript{[3]} and is higher than that found by McCarthy et al.\textsuperscript{[2]}