

$\nu_1+\nu_5$ OF HCCN: DETERMINATION OF THE ν_5 VIBRATIONAL ENERGY

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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 $\nu_1+\nu_5$ of the quasilinear molecule HCCN with the origin at 3355.510(9) cm^{-1} . Based on information from the $\nu_1+\nu_5-\nu_5$ spectrum^[1], the energy of the lowest excited state with angular momentum about the a-axis, ν_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^[2] [145(15) cm^{-1}] or from similar relative intensity measurements on the IR spectra^[1] [187(20) cm^{-1}]. The present value of the energy for ν_5 predicts a barrier to linearity similar to that obtained from the corresponding band of DCCN^[3] and is higher than that found by McCarthy et al.^[2].

^[1] C. L. Morter, S. K. Farhat and R. F. Curl, *Chem. Phys. Lett.* 207, 153(1993); ^[2] M. C. McCarthy, C. A. Gottlieb, A. L. Cooksy and P. Thaddeus, *J. Chem. Phys.* 103(18), 7779(1995); ^[3] Fuge Sun, A. Kosterev, G. Scott, V. Litosh, and R. F. Curl, *J. Chem. Phys.* 109(20), 8851(1998).