HIGH-RESOLUTION SPECTROSCOPIC STUDIES OF THE ν_5 BENDING FUNDAMENTAL OF HCCN

M. D. ALLEN, K. M. EVENSON, *Time and Frequency Division, National Institute of Standards and Technology, Boulder, CO 80303-3328*; and J. M. BROWN, *The Physical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom*.

A high-resolution spectroscopic study of the ν_5 bending fundamental of HCCN has been carried out using far-infrared laser magnetic resonance (FIR LMR) spectroscopic techniques. This study has provided an accurate determination of the ν_5 separation 3,864,563.78(11) MHz (128.9079721(37) cm^{-1}), a more accurate determination of the spin-spin parameters, an improved set of molecular g-factors, and the first observation of hyperfine splittings in the ν_5 = 1 levels. The analysis of the HCCN radical was done using an 'A' reduced asymmetric rotor Hamiltonian and included the FIR LMR data (this work), microwave data [a], and millimeter-wave data [b]. A fit was performed including ΔK = 2 matrix elements and no improvement was observed compared with the fit using ΔK = 0. Thus, in this analysis there is no support for a slightly bent structure. We can now accurately predict zero field transitions which will be valuable for conducting searches for the ν_5 fundamental transition in stellar and interstellar sources.

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[a] Y. Endo and Y. Ohshima, *J. Chem. Phys.* **98**, 6618 (1993).

[b] M. C. McCarthy, C. A. Gottlieb, A. L. Cooksy, and P. Thaddeus, *J. Chem. Phys.* **103**, 7779 (1995).