ROTATIONAL SPECTRA OF THE MOLECULAR IONS H_2NCO^+ AND NCO^-

VALERIO LATTANZI, CARL A. GOTTLIEB, PATRICK THADDEUS, and MICHAEL C. McCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138*; and SVEN THORWIRTH, *Max-Planck-Institut für Radioastronomie, Bonn, Germany, and I. Physikalisches Institut, Universität zu Köln, Germany*.

We report the first high resolution spectroscopic detection of H_2NCO^+, the protonated cation of isocyanic acid, in a discharge through HNCO heavily diluted in hydrogen in the throat of a supersonic nozzle. Spectroscopic constants derived from the two lowest rotational transitions agree very well with theoretical structure calculations of the ground state isomer, in which protonation occurs at the nitrogen atom, yielding an isomer of C_{2v} symmetry[a]. In the same molecular beam, the fundamental rotational transition of NCO^- was observed with well-resolved nitrogen quadrupole hyperfine structure. Detection of NCO^- in our beam was subsequently confirmed by observation of several millimeter-wave transitions in a low pressure discharge through cyanogen and water. The spectroscopic constants of NCO^- obtained earlier by infrared laser spectroscopy[b] are in good agreement with the highly accurate constants derived here. Owing to the high abundance of HNCO in many galactic molecular sources, both ions are excellent candidates for astronomical detection in the radio band.

[a] Structure calculated at the CCSD(T)/cc-pwCV5Z level of theory and zero-point vibrational effects at CCSD(T)/cc-pVQZ.

[b] M. Gruebele, M. Polak, and R. J. Saykally, *J. Chem. Phys.* **86**, 6631, (1987).