FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY OF HCCNSi AND NCNSi

S. THORWIRTH, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; R. I. KAISER, *Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, U.S.A.*; M. C. MCCARTHY, K. N. CRABTREE, O. MARTINEZ, JR., *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, U.S.A. and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138, U.S.A.*

By means of Fourier transform microwave spectroscopy of a supersonic jet, the pure rotational spectra of the silicon-bearing chain molecules silaisocyanoacetylene, HCCNSi, and cyanosilaisocyanide, NCNSi, have been studied for the first time. The molecules were observed in low-current dc discharges through appropriate gas mixtures comprising CH_3CN/SiH_4 and cyanogen/SiH_4 heavily diluted in neon. Spectroscopic searches and identification were based on predictions from high-level quantum-chemical calculations at the CCSD(T) level of theory in combination with large basis sets. Excellent agreement between experimental and calculated molecular parameters is found. In addition to the parent isotopic species, rotational lines of rare isotopologs were also observed.
Because of the close relationship of these two species to known astronomical molecules and due to their sizable dipole moments of $\mu = 1.4\,\mathrm{D}$ (HCCNSi) and $\mu = 5.4\,\mathrm{D}$ (NCNSi) both are plausible targets for future astronomical searches using large radio telescopes.