FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY OF NCCO AND NCCCO

YOSHIHIRO SUMIYOSHI, HIDEYUKI TAKADA, AND YASUKI ENDO, *Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8902, Japan*.

Pure-rotational transitions of the NCCO and NCCCO radicals have been observed by Fourie-transform microwave spectroscopy. The radicals were produced in a supersonic jet by a pulsed electric discharge of 0.3% of pyruvonitrile ($CO(CN)(CH_3)$) in Ar for NCCO and a 0.3%/0.3% mixture of HC_3N and O_2 in Ar for NCCCO. Rotational transitions from $N = 1 - 0$ to $N = 3 - 2$ for NCCO, and those from $N = 2 - 1$ to $N = 6 - 5$ for NCCCO were observed. The rotational, fine and hyperfine constants for both of the radicals have been precisely determined. According to $ab\ initio$ calculations at the RCCSD(T)/cc-pVTZ(or -VQZ) level of theory, the radicals are found to have bent structures in the ground state, which are in good agreement with the results of the present observations. Discussions on the geometrical and electronic structures based on the determined molecular constants and results of the $ab\ initio$ calculations are given. The present results are compared with those of the related carbon-chain series, NC_nS.