MILLIMETER-WAVE SPECTROSCOPY AND COUPLED CLUSTER CALCULATIONS FOR NCCP

L. BIZZOCCHI, C. D. ESPOSTI, *Dipartimento di Chimica "D. Ciamician", Università di Bologna, Via F. Selmi 2, I-40126 Bologna, Italy*; P. BOTSCHWINA and B. SCHULZ, *Institut für Physikalische Chemie, Universität Göttingen, Tammannstrasse 6, D-37077 Göttingen, Germany*.

The rotational spectrum of the unstable NCCP molecule has been investigated in the millimeter wave region. The ground state spectra of the most abundant isotopomer and of the ^{13}C and ^{15}N containing species were studied, and lines in the ν_2, ν_3, ν_4, and ν_5 vibrationally excited states were detected for the normal isotopomer. Electric quadrupole and magnetic spin-rotation coupling constants of the nitrogen nucleus were also determined. The experimental work was assisted by high level CCSD(T) calculations with the large cc-pVQZ basis, which provided accurate predictions for the vibration-rotation coupling constants and the ground state rotational constants of the less abundant isotopic species. r_0 and r_s molecular structures of NCCP were derived directly from the experimental ground state rotational constants of four different isotopomers, and an accurate equilibrium structure could be evaluated by combining theoretically computed vibration-rotation coupling constants with experimental ground state rotational constants.