A VIBRATIONAL ACTION SPECTROSCOPIC STUDY OF THE RENNER-TELLER AND SPIN-ORBIT AFFECTED CYANOACETYLENE RADICAL CATION HC_3N^+ ($^2\Pi$)

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The linear radical cation of cyanoacetylene, HC_3N^+ ($^2\Pi$), is of fundamental spectroscopic interest due to its strong spin-orbit and Renner-Teller interactions, which have been investigated previously in several high-resolution photoelectron spectroscopic (PES) studies[a,b,c]. Here, we present the first broadband vibrational action spectroscopic investigation of this ion through the infrared pre-dissociation (IRPD) method using a Ne tag. Experiments have been performed using the FELion cryogenic ion trap instrument in combination with the Free Electron Lasers for Infrared eXperiments (FELIX) Laboratory at the Radboud University (Nijmegen, The Netherlands)[d]. The vibronic splitting patterns of the 3 interacting bending modes (ν_5,ν_6,ν_7), ranging from 180-1600 cm^{-1}, could be fully resolved revealing several bands that were previously unobserved. The associated Renner-Teller and cross-coupling constants were determined by fitting an effective Hamiltonian to the experimental data, and the obtained spectroscopic constants were in reasonable agreement with previous studies of the HC_3N^+ ion. The influence of the attached Ne atom on the infrared spectrum was investigated by *ab initio* calculations at the CCSD(T) level of theory, showing that the discrepancies between the IRPD and PES data can be explained by the effect of the Ne binding.

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