

ON THE SPECTROSCOPY OF ACYLIUM IONS: INFRARED ACTION SPECTROSCOPIC DETECTION OF NCCO^+

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The linear $\text{N}\equiv\text{C}-\text{C}\equiv\text{O}^+$ ion has been studied spectroscopically for the first time using the Free Electron Laser for Infrared eXperiments, FELIX, at Radboud University (Nijmegen, The Netherlands) in combination with the 4K 22-pole ion trap facility FELion.^a The vibrational spectrum of NCCO^+ was observed in the range from 500 to 1500 and 2000 to 2500 cm^{-1} using resonant photodissociation of the corresponding Ne-complex while monitoring the depletion of the ion-Ne cluster signal as a function of wavenumber. Spectroscopic assignment of vibrational bands relies on comparison against results from high-level quantum-chemical calculations performed at the CCSD(T) level of theory and very good agreement is found.

^aJusko et al. 2019, Faraday Discuss. 217, 172