INFRARED PREDISSOCIATION SPECTROSCOPY OF PROTONATED METHYL CYANIDE

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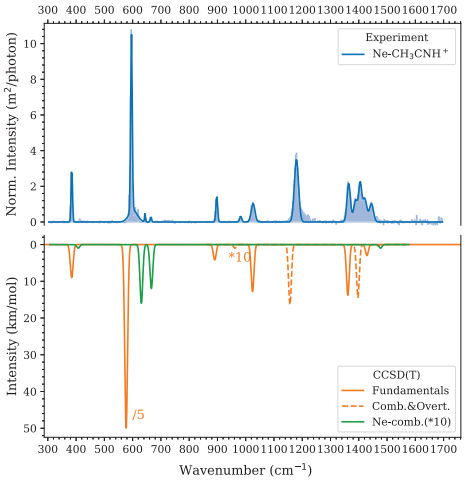
Methyl cyanide (CH_3CN) was among the first polyatomic molecules detected by radio-astronomical observations of the interstellar medium (ISM)[1]. As methyl cyanide has a proton affinity much larger than that of H_2, its protonated version (CH_3CNH^+) is postulated to form efficiently via exothermic proton transfer from H_3^+ to CH_3CN in the interstellar medium. In this talk, we present a comprehensive experimental and quantum-chemical study of the gas phase vibrational spectrum of CH_3CNH^+ [2]. We employed the widely tuneable free electron lasers for infrared experiments (FELIX) coupled to a cryogenic ion trap instrument [3] for our measurements. The spectrum was recorded in the 300-1700 and 2000-3300 cm^{-1} spectral regions using infrared predissociation (IRPD) action spectroscopy with neon as a weakly bound messenger atom. The assignment of the vibrational modes is based on anharmonic frequency calculations performed at the CCSD(T)/ANO2 level of theory. We demonstrate that the comparatively low-cost ANO0 basis-set provides accurate estimates on the influence of the weakly-bound neon atom as a tag in the IRPD experiments. The data presented here will support astronomical searches for the CH_3CNH^+ ion in space.



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