FIRST INFRARED PREDISSOCIATION SPECTRA OF He-TAGGED PROTONATED PRIMARY ALCOHOLS AT 4 K

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Cryogenic multipole ion traps have become popular devices in the development of sensitive action-spectroscopic techniques. The low ion temperature leads to enhanced spectral resolution, and less congested spectra. In the early 2000s, a 22-pole ion trap was coupled to the Free-Electron Laser for Infrared eXperiments (FELIX), yielding infrared Laser Induced Reaction (LIR) spectra of the molecular ions $\mathrm{C_2H_2}^+$ and $\mathrm{CH_5}^{+b}$. This pioneering work showed the great opportunities combining cold mass-selected molecular ions with widely tunable broadband IR radiation.

In the past year a cryogenic (T>3.9 K) 22-pole ion trap designed and built in Cologne (FELion) has been successfully coupled to FELIX, which in its current configuration provides continuously tunable infrared radiation from 3 μm to 150 μm, hence allowing to probe characteristic vibrational spectra in the so-called "fingerprint region" with a sufficient spectral energy density also allowing for multiple photon processes (IR-MPD). Here we present the first infrared predissociation spectra of He-tagged protonated methanol and ethanol ($\mathrm{MeOH_2}^+$/$\mathrm{EtOH_2}^+$) stored at 4 K. These vibrational spectra were recorded with both a commercial OPO and FELIX, covering a total spectral range from 3700 $\mathrm{cm}^{-1}$to 550 cm^{-1}at a spectral resolution of a few cm^{-1}. The H-O-H stretching and bending modes clearly distinguish the protonated alcohols from their neutral analoga. For $\mathrm{EtOH_2}^+$, also IR-MPD spectra of the bare ion could be recorded. The symmetric and antisymmetric H-O-H stretching bands at around 3 μm show no significant shift within the given spectral resolution in comparison to those recorded with He predissociation, indicating a rather small perturbation caused by the attached He. The vibrational bands were assigned using quantum-chemical calculations on different levels of theory. The computed frequencies correspond favorably to the experimental spectra. Subsequent high resolution measurements could lead to a better structural characterization of these protonated alcohols.

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[b] Asvany et al.: Phys. Rev.Lett. 94, 073001 (2005), Asvany et al.: Science 309, 1219-1222 (2005)