

Infrared spectroscopy of protonated fullerenes

J. Palotás^{1*}, J. Martens¹, G. Berden¹ and J. Oomens¹

¹*FELIX Laboratory, IMM, Radboud University, Nijmegen, the Netherlands*

**julianna.palotas@ru.nl*

We investigate protonated fullerenes in ion trap mass spectrometer with IR multiple photon dissociation (IRMPD) spectroscopy using the wide wavelength tunability and high pulse energies of the FELIX free electron laser. For ionization, we use an atmospheric pressure chemical ionization (APCI) source which is efficient for less polar materials. With this measurement, we present interesting results for the gaseous IR spectra of $C_{60}H^+$.

When one proton attaches to the highly symmetrical neutral fullerene, its symmetry is significantly reduced causing many bands that were inactive in the unprotonated system to become IR-active, resulting in a rich vibrational spectrum. The spectra of the protonated species are therefore entirely different in appearance from the neutral C_{60} . Experimental data are supported by results from quantum-chemical calculations at the DFT level.

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