

QUANTUM CASCADE LASER-BASED INFRARED PHOTODISSOCIATION ACTION SPECTROSCOPY OF HYDRATED AMINO ACIDS FOR PLANETARY SCIENCE IN SITU SENSING APPLICATIONS

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In the search for life on other worlds in our solar system, overlooked approaches to in situ sensing instrumentation can increase science return relating to the detection of prebiotic molecules such as amino acids, lipids, and nucleic acids at low size, weight, and power cost. Ongoing work at Caltech and the Jet Propulsion Laboratory (JPL) aims to explore how moderate power, continuous wave (CW) laser sources can be leveraged to execute single- and multi-photon photodissociation schemes adaptable to mass spectrometer (MS)-based in situ sensing platforms. These techniques could serve as potent analysis tools that provide unambiguous molecular identification through combined initial m/z , the IR or UV/Vis spectrum, as well as the photofragment mass spectrum. This talk will present an initial study of a low-power CW variant of messenger-assisted infrared photodissociation (IRPD) spectroscopy of singly hydrated, protonated phospho-tyrosine ($p\text{TyrH}^+(\text{H}_2\text{O})$) generated from an electrospray source with both complexation and analysis performed in a single stage linear ion trap MS. The room temperature IRPD spectrum of $p\text{TyrH}^+(\text{H}_2\text{O})$ was recorded by monitoring the loss of water tag when irradiated with a moderate power (<100 mW) quantum cascade laser (QCL) source in the fingerprint region ($865\text{-}950\text{ cm}^{-1}$ and $1000\text{-}1670\text{ cm}^{-1}$). Findings are compared against literature analog spectra collected using a free electron laser radiation source with presented results constituting a dramatic reduction in experimental complexity. Discussions will be aided with the support of quantum chemical calculations (DLPNO-CCSD(T)-F12/cc-pVTZ-F12// ω B97X-V/def2-QZVPP). Additionally, this presentation will briefly describe efforts to adapt flight heritage MS hardware at JPL to execute similar analysis schemes. Overall, the current study is the first demonstration of using low-power, CW QCL-based action spectroscopy for the goal of analyzing a broad range of prebiotic molecules on future search for life missions.