National Aeronautics and Space Administration

Terahertz Spectroscopic Investigations of Diatomic Transition Metal Hydrides in Support of Next Generation Space/Balloon Borne Observatories

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Program: FY22 SURP

Strategic Focus Area: Origin, evolution, and structure of the universe

Objectives: The primary objective of this strategic partnership effort is to execute frequency modulated direct absorption spectroscopy of astrophysically relevant transient metal hydrides in the terahertz region (0.7 – 2 THz) of the electromagnetic spectrum in pursuit of observational quality rest frequencies. Experimental efforts in this spectral region are challenged by both the rare nature of tuneable narrow linewidth radiation sources and the large search bandwidths associated with the targeted transient species that lack direct laboratory observation. Such work is necessary; however, to facilitate new observational discoveries in the ISM and circumstellar environments. This technical effort requires both the custom glow discharge cells native to the Ziurys laboratory to generate these exotic transient species, and the high frequency source hardware of the JPL laboratory used to collect their rotational spectra in this valuable spectral region. The collected data is then analyzed with custom least-squares Hamiltonian software to allow for extraction of structural and electronic parameters and quantum assignment. These results along with observed rest frequencies are then made available to astrophysics research communities through publication in peer reviewed journals and cataloging in the JPL public access database.

Background: Hydride molecules of the general formula MH, MH_2, etc. play an important role in the chemistry of the interstellar medium, both in our Galaxy and external galaxies. Such species are thought to be among the first formed in chemical networks, created from relatively simple reaction schemes. As a consequence, a relatively simple interpretation of observed abundances is possible, enabling the determination of the physical characteristics of the gas in which hydrides are found. Until recently, our knowledge of interstellar hydrides was limited, primarily arising because of observational difficulties. Hydrides are typically light molecules with large rotational constants, such that their fundamental transitions lie in the sub-millimeter and the far-infrared wavelengths of the electromagnetic spectrum that are typically inaccessible by ground-based astronomy. The *Herschel Space Observatory* played a key role in changing this situation, with extensive space-born measurements that enabled the discovery of interstellar SH^+, HCl^+, H_2Cl^+ , H_2O^+ and ArH^+, as well as the first intensive studies of HF and OH^+. Fortunately, at the time of the launch of *Herschel*, rest frequencies were available for these molecules that made these new discoveries possible. This work aims to ensure new rest frequencies of desirable hydride species are available for future missions.

Approach and Results: Year one SURP efforts focused on the acquiring the first laboratory observation of FeH in 1 to 2 THz spectral region using frequency modulated direct absorption techniques. This first in class measurement required combining highly specialized laboratory capabilities and institutional knowledge associated with the Ziurys research group at the University of Arizona and the High-Resolution Molecular Spectroscopy Laboratory at JPL (Figure 1). UA graduate student Tyler Herman visited JPL where he received intensive training with the Herschel legacy GaAs-based cascaded multiple chain sub-mm and THz local oscillator hardware still maintained by group 329H (Figure 1b). Two source modules (0.7 and 1.0 THz) and a collection of ancillary hardware were then transferred to UA to be interfaced with specialized AC/DC glow discharge cells native to the Ziurys Group at UA (Figure 1c, Figure 2). This hardware set was used to record the Lambda split $\Omega = 3/2$; $J = 5/2$ <- $3/2$ transitions of FeH in direct absorption for the first time ever. This result serves as a significant scientific and programmatic accomplishment and a major stepping stone to future planned work at even higher frequencies.

Significance/Benefits to JPL and NASA: Science associated with the molecular astronomy has long been a Caltech/JPL hallmark, culminating in the highly capable Herschel/HIFI instrument which has left an unmatched legacy of THz hardware immediately useful for scientific research that supports the furthering of astronomical detections. Further explorations of interstellar and circumstellar chemistry are limited due to observational constraints including atmospheric opacity and state populations, leading to a need for additional space (Hercshel 2.0) and balloon (ASTROS-like) missions. Strategic support of new characterizations of relevant molecular spectra thus, by proxy, also strategically supports future mission concepts.

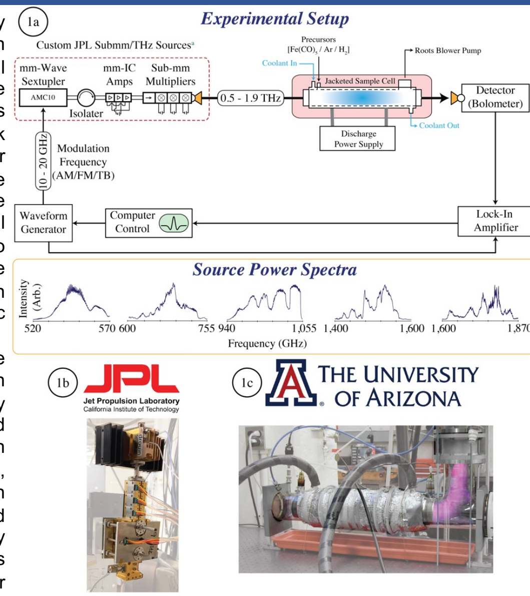

FIGURE 1: Experimental setup used for frequency modulated direct absorption of transient metal hydrides in block diagram format (1a). The THz radiation sources deployed are supplied by JPL (1b) and interfaced with custom AC/DC glow discharge cells maintained by the Ziurys Group at the University of Arizona (1c).

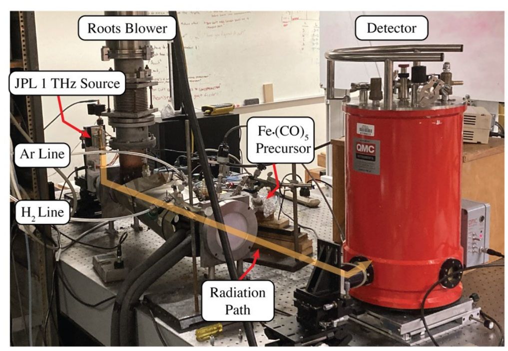

FIGURE 2: Photograph of the actual experimental setup at the University of Arizona after the JPL source hardware was transported and installed. Terahertz radiation is columnated with an off-axis parabola and directed through the discharge cell before detection with a liquid helium cooled bolometer detector.

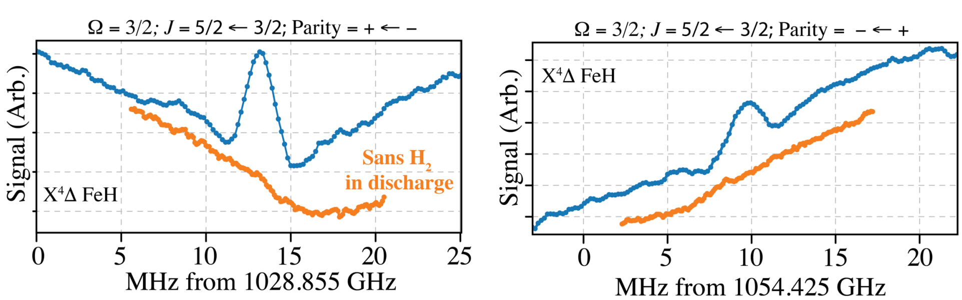

FIGURE 3: The first detection of the Lambda split $\Omega = 3/2$; $J = 5/2$ <- $3/2$ transitions of FeH ever recorded in direct absorption. This experimental observation constitutes a significant scientific and programmatic milestone. The new observations (blue traces) exhibit the classic expected second derivative lineshapes with spectral lines absent (orange traces) once a synthesis precursor agent is removed.

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