Recent Progress in THz Spectroscopy at Jet Propulsion Laboratory (JPL)

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Recent progress in astronomical observations in the frequency region of sub-millimeter to THz is remarkable. This frequency range is, however, opaque largely due to atmospheric water, oxygen and ozone, making astronomical observations from ground very challenging. The Herschel Space Observatory and the Stratospheric Observatory For Infrared Astronomy (SOFIA) opened up the terahertz/far-infrared region with unprecedented sensitivity, frequency coverage, and spectral resolution. The HIFI (The Herschel-Heterodyne Instrument for Far-Infrared) instrument on board the Herschel Space Observatory, in particular, has produced a large amount of high-quality spectroscopic data. Large portions of the THz region are swamped by known common molecules such as CH_3OH, C_2H_5CN, $HCOOCH_3$, CH_3OCH_3. Underneath the forest of lines from those common molecules, molecular ions such as CH^+, OH^+, H_2O^+, H_2Cl^+, HCl^+, and ArH^+ have been identified in interstellar space. For identification of these species, the laboratory data were indispensable. As a part of the on-going endeavor, we present some of the recent laboratory results. As examples, THz spectroscopy of CH^+ and D_2H^+ will be discussed.

The JPL millimeter and submillimeter spectrometer (FMSS) which was constructed using frequency mutiplier chains as THz radiation sources, developed at JPL or purchased from Virginia Diodes, was used to record terahertz transitions of these ions. It has been proven to have high sensitivity and fast-scanning capability.

The extended negative glow discharge apparatus (transferred from University of Waterloo, but originally made at Ibaraki University) was employed to generate these two ions. As examples, Figure 1 shows typical signals of CH^+ and D_2H^+ terahertz lines that are weak and have not been observed previously anywhere.

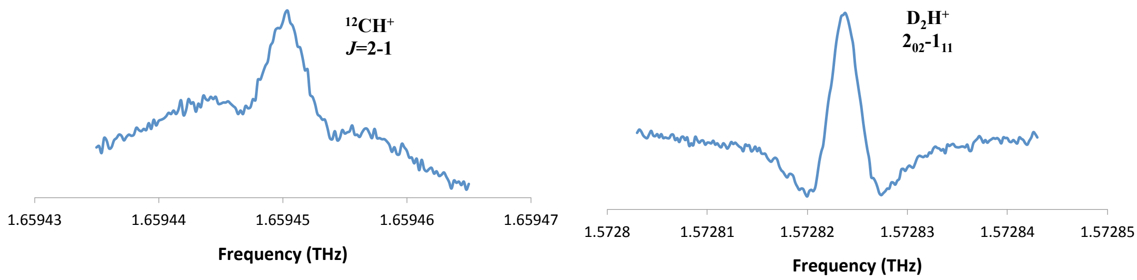

Figure 1: The $^{12}CH^+$ $J = 2 - 1$ line at 1.659 THz and the D_2H^+ $2_{02} - 1_{11}$ line at 1.573 THz, demonstrating the high-sensitivity of our JPL terahertz spectrometer. The frequency scan was made with a 200 kHz step size. A dwell time at each point was 150 ms.

1 CH^+

In 1937, Dunham detected a couple of unidentified lines in near-UV, and later Douglas and Herzberg identified them based on their laboratory observations to be low-J

electronic transitions of CH^+. This is one of the first interstellar molecules identified. The electronic spectra, in particular the $A^1\Pi - X^1\Sigma^+$ band, have been investigated extensively. On the other hand, the pure rotational transitions have not been studied as extensively. Only the lowest rotational transition, $J = 1 - 0$, was observed in the laboratory for the normal species, $^{13}CH^+$, and CD^+.[1] Based on the laboratory frequency, CH^+ was detected in star forming regions with the Hershel space observatory. Cernicharo et al identified pure rotational transitions from $J = 2 - 1$ to $J = 6 - 5$ in the far-infrared region in the ISO spectrum of the planetary nebula NGC 7027.[2] The ISO spectra, however, were of low-resolution, so high-resolution spectroscopic observation is highly desirable. In this presentation, we have extended the measurements to higher-J lines up to 2 THz.

For production of CH^+, an extended negative glow discharge in a gas mixture of CH_4 ($\sim$ 0.5 mTorr) diluted in He ($\sim$ 60 mTorr) was used. The optimum discharge current was about 15 mA and the axial magnetic field of 160 Gauss was applied. The discharge cell was cooled down to liquid nitrogen temperature. In this investigation, the $J = 2 - 1$ and $3 - 2$ lines were observed for $^{12}CH^+$ and $^{13}CH^+$. For CD^+, $J = 2-1$ to $J = 4-3$ were measured. These THz measurements are not only useful for providing better characterization of spectroscopic properties but also will serve as starting point for astronomical observations.

2 D_2H^+

Pure rotational transitions of D_2H^+ observed by high-resolution spectroscopy have been limited so far to the $J = 1_{10} - 1_{01}$ transition at 691.7 GHz[3] and $J = 2_{20} - 2_{11}$ at 1.370 THz, and $J = 1_{11} - 0_{00}$ at 1.477 THz.[4,5] As this ion is a light asymmetric-top molecule, spectroscopic characterization and prediction of other rotational transition frequencies are not straightforward. We present new measurements up to 2 THz by using the JPL frequency multiplier chains, and observed four new THz lines and re-measured the three known transitions.

D_2H^+ was generated in an extended negative glow discharge in a gas mixture of $H_2 \sim$ 2mTorr, $D_2 \sim$ 2 mTorr, and Ar$\sim$17 mTorr, and the cell was cooled to liquid nitrogen temperature. Although the line density was very sparse, careful chemical checks were carried out to ascertain that the lines observed were indeed the ones from D_2H^+.

The Watson Hamiltonian was employed for the analysis. For this type of light asymmeteric-top molecules, a relatively large number of higher-order centrifugal distortion constants are needed to fully characterize the rotational levels. Seven rotational transition frequencies together with the combination differences derived from three fundamental bands were subject to least square analysis to determine the molecular constants. The improved molecular constants provide better predictions of other unobserved rotational transitions.

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