Sub-Millimeter Wave Detection of the D_2H^+ Ion: Precise Molecular Constants and Chemical Property.
（D_2H^+イオンのサブミリ波分光～正確な分子定数と化学的性質）

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Although the astrochemical significance of H_3^+ and its singly deuterated species, H_2D^+, are widely recognized and extensively investigated, there has been less spectroscopic information on the doubly deuterated species, D_2H^+. The first spectroscopic detection of D_2H^+ was made in the infrared region at NRC [1], followed by observations of two rotational transitions (2_{20}-2_{11} and 1_{11}-0_{00}) in the THz region [2]. Polyansky and McKellar derived more accurate molecular constants and term values by combining all the available data [3]. However, since the molecule is very light, even such revised molecular constants should better be subjected to critical tests.

The line position of only one accessible transition (1_{10}-1_{01}) to our sub-millimeter wave spectrometer was predicted to 691.705 GHz by using previous IR data [3]. Experimental setup used was described elsewhere [4]. The D_2H^+ molecules were generated in an extended negative glow discharge in the mixture of H_2 and D_2 with Ar as buffer gas near the liquid nitrogen temperature (77 K). The extended negative glow discharge condition that is the only way to maintain detectable concentration of the ion in the cell can be produced only when magnetic field (~200 G) is applied to the discharge plasma. Following numerous efforts, in the range of the expected spectral region, we discovered only one signal at 691.660400 GHz that is highly magnetic field sensitive. This absorption line vanishes by cutting off H_2 or D_2 gases, inducing tiny leak, or raising cell temperature. In contrast to H_2D^+, the mixing ratio of H_2 / D_2 is found to be less sensitive in producing D_2H^+. This behavior is similar to the findings in previous IR spectroscopy at NRC [1, 5], despite orders of magnitude of difference in gas pressures. The optimum mixing ratio of gases is found to be H_2 / D_2 / Ar = 4 / 2 / 17 mTorr and discharge current is about 8 mA. The observed line width (FWHM = 1.7 MHz) is comparable with the Doppler line width of the molecule (FWHM = 1.9 MHz), assuming that the temperature of the cell is 77 K. A set of the improved molecular constants is obtained by combining all available IR data.

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