Enrichment and Spectroscopy of CH_3OD as a Step Toward the First Characterization of CH_2DOD

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In the interstellar matter (ISM), various complex organic molecules (COMs) have been identified. Among them, methanol (CH_3OH) is an important molecule for understanding chemical reactions related to the formation of COMs, as it has been considered as a seed molecules of COMs. Nevertheless, spectroscopic measurements of many CH_3OH isotopologue are still lacking. In particular, methanol exhibits significant variations in dipole moment depending on the transition, making it essential to determine transition intensities in terms of the dipole moment function. Thus, both frequencies and intensities of spectral lines must be measured. In this study, we carried out laboratory measurements of CH_3OD using the high-sensitivity emission-type spectrometer SUMIRE, developed at RIKEN.

A key experimental challenge is that, during vaporization, the hydrogen atom of the OH group in CH_3OD readily exchanges with residual water molecules inside the spectrometer. Therefore, highly deuterium-enriched samples are required. We established a simple method to prepare CH_3OD-enriched samples by repeated substitution of the OH hydrogen atom of CH3OH with deuterium in D_2O, followed by distillation. While the distillation technique itself is not novel, it provides a practical means of producing isotopically enriched samples suitable for spectroscopy. From the obtained spectra, we derived column densities of CH_3OH, CH_3OD, D_2O, and HDO, and determined their relative abundances. The results show that the abundance of CH_3OD increases with repeated distillation, whereas CH_3OH decreases. The CH_3OD fraction relative to total methanol increased from about 27% after the first distillation to 41% after the third (Figure 1).

In the future, we aim to apply the same methodology to synthesize CH_2DOD from CH_2DOH and D_2O Importantly, no spectroscopic measurements or molecular constants of CH_2DOD have ever been reported. Therefore, our planned measurements could represent the first spectroscopic characterization of this doubly deuterated isotopologue, providing highly novel and unique insights into the isotopic chemistry of methanol in star-forming regions.

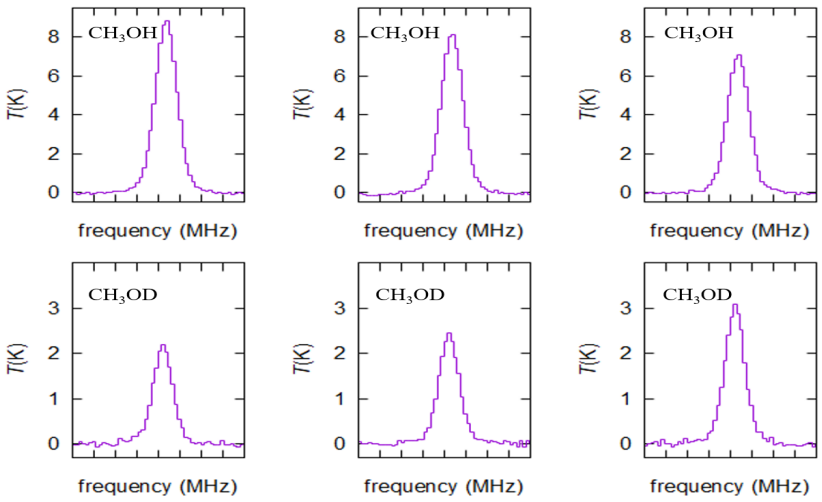

Figure 1. Top: Spectra of CH_3OH (5_0–4_0 E $v_t = 0$, 241700.16 MHz), from left to right: 1st, 2nd, and 3rd distillation. Bottom: Spectra of CH_3OD (5_0–4_0 A^+ $v_t = 0$, 226538.60 MHz), from left to right: 1st, 2nd, and 3rd distillation.