Chemical Evolution of Cometary Molecules Revealed through Mid-IR High-Dispersion Spectroscopy by *SPICA*

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ABSTRACT

Comets are thought to be remnants of the planetesimals in the proto-planetary disk so that cometary ices provide us with precious clues of physical and chemical conditions in the early solar system. The mid-IR region is a very fruitful window to study the cometary volatiles since numerous ro-vibronic bands of molecules are observed simultaneously, and symmetric molecules can be accessed. However, because of the strong atmospheric extinction and the capability of previous instruments, there are only a few studies of cometary molecules in mid-IR regions with discontinuous limited wavelength regions or with low-dispersion spectroscopy. The mid-IR high-dispersion spectroscopy with *SPICA* could make a breakthrough discovery in the cometary volatiles like aliphatic hydrocarbons (e.g., C_2H_2, C_2H_4, C_2H_6), PAHs as well as the pre-biotic molecules (e.g., PH_3). In this study, we discuss the feasibility to find new molecular species and to identify previously unidentified emission lines and the composition of those new species.

1. INTRODUCTION

Comets are thought to be aggregates of planetesimals that were remnants of the early solar system. The volatiles incorporated into the comets are precious clue to the physical and chemical evolution of molecules. Parent volatiles that are directly released from the cometary nucleus such as H_2O, CO_2, and CO are usually studied in near-IR region or radio domain. However, those observations are severely affected by telluric absorption. The space telescopes like *AKARI* and *SPICA* are powerful tools to study such volatiles. In particular, although there are transitions of C-H, N-H, C-O bending modes of many molecules, the mid-IR region could not be fully accessed from ground based observatories. Moreover, the high-dispersion spectroscopy provides us the rotational temperature of volatiles. Chemical compositions of cometary organic volatiles are particularly important to study the chemical evolution of our solar system.

2. FLUORESCENCE EXCITATION MODELS

In order to determine the chemical composition of cometary coma, we need the g-factors for the molecular species. Here, we introduce the fluorescence excitation models of the volatiles that could be observed in mid-IR region. Cometary volatiles are assumed to be excited by the solar radiation field in the model. We also assumed that the rotational population distribution follows the Boltzmann distribution that is maintained by inter-molecular collisions in the inner coma. Downward transitions into vibrational states from highly excited states are neglected in this study. Only direct pumping from the ground state is considered (see Figure 1 as an example). The balance equations for each energy level are solved numerically to determine the population in each level. Then the g-factor is calculated as a product of the population and the relevant Einstein A coefficient. Einstein A coefficients necessary to build the equations are basically taken from the HITRAN database (Rothman et al. 2008). High-resolution solar spectrum is taken from Kurucz (2005) and the results based on his stellar model.

3. RESULTS

We constructed fluorescence excitation models of the aliphatic hydrocarbons (C_2H_2, C_2H_4, and C_2H_6), PH_3 and NH_3. Here we show a case when we assumed a rotational temperature of 100 K and the comet at 1 AU from the Sun in Figure 2–4 and give some description of each molecule below.

3.1. Aliphatic Hydrocarbons (C_2H_2, C_2H_4, and C_2H_6)

In the case of aliphatic hydrocarbons, emission lines appear around 10 to 14 μm region. In particular, cometary C_2H_4 is one of key species for the chemical reactions related to the formation of C_2H_6. Moreover, C_2H_4 has never been detected in comets by previous studies. It will be a candidate of the species newly detected in comets. Although CH_4 is another aliphatic hydrocarbon, the emission lines appear in 7 μm region. The abundances of CH_4 and C_2H_6 are important for comparisons with ISM. The near-IR observations are also needed to investigate the CH_4. Thus, the 10 μm region is so important.

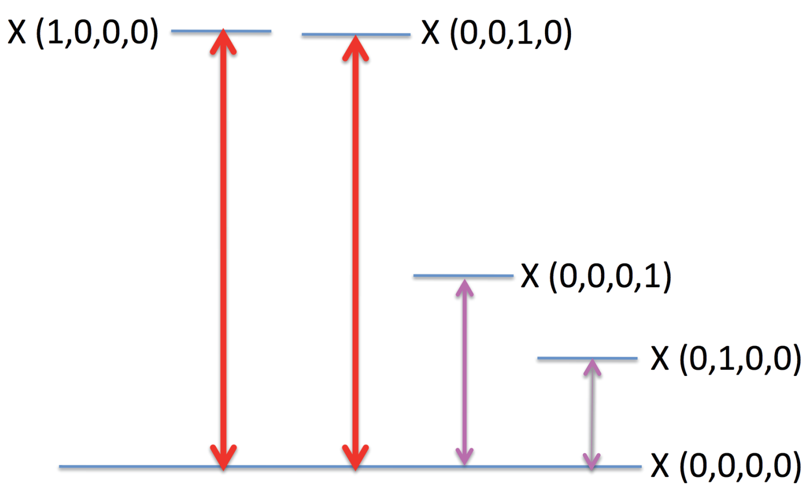

Figure 1. Fluorescence excitation model of NH_3 as an example. The fluorescence excitation model of each molecular species includes its fundamental transition. The solar radiation field is considered as the main energy source for pumping from the ground state.

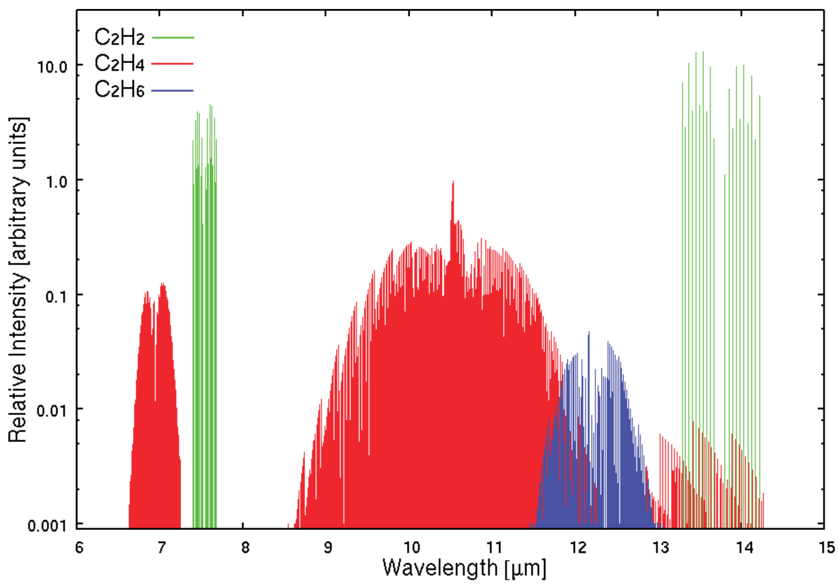

Figure 2. The synthesized spectra of the hydrocarbon molecules that have fundamental vibrational transitions around 10 μm region. We expect strong fluorescence emission lines of C_2H_2, C_2H_4 and C_2H_6 in this wavelength region. C_2H_4 has especially strong emission bands while this molecule has never been detected in comets in the near-infrared wavelength region.

3.2. PH_3

Phosphorus "P" is one of the important species for biology and PH_3 has never been found in cometary coma or ices. Recently, 103P/Hartley 2 showed the D/H ratio in H_2O similar to that of VSMOW (Hartogh et al. 2011). This result indicates that the pre-biotic molecules are possibly brought by the comets to the early Earth. Our calculation show the strongest line is found at 10 μm if the molecule exists. However, *SPICA*/MCS (high-dispersion spectrograph) cannot cover around the 10 μm regions. We propose the 10 μm region high-dispersion spectrograph with *SPICA*. Also, we need the laboratory measurements of PH_3 and chemical evolutionary models including phosphorus atoms.

3.3. NH_3

Ammonia has been previously well studied in both near-IR regions and radio domain. However, in the near-IR region, the line intensity is relatively weaker than in the mid-IR region. The nuclear spin isomers ratio of ammonia is one of the important metrics to investigate the formation temperature of the species. In a previous study, Shinnaka et al. (2011) reported the nuclear spin temperature of ammonia as ~30 K, higher than the typical dark molecular cloud (~10 K). If we try to observe NH_3 in the mid-IR region, the 10 μm region is also important.

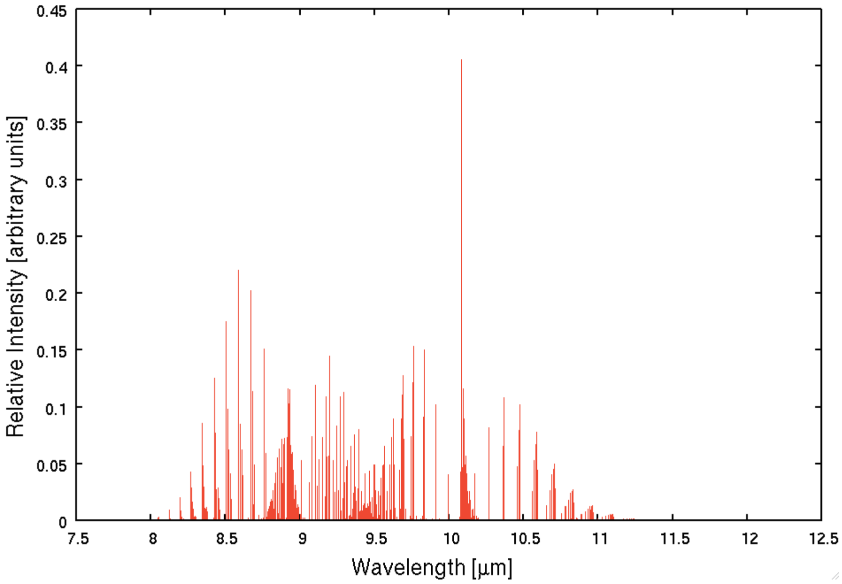

Figure 3. Same as Figure 2 but for PH_3. The strong Q-branch for the vibrational band at $\sim$10 μm is the candidate for the detection in comets.

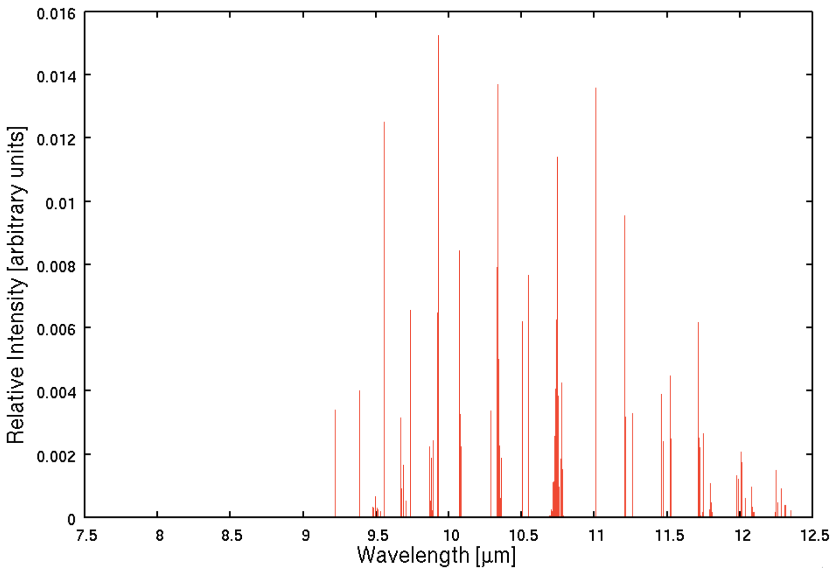

Figure 4. Same as Figure 2 but for NH_3. The spectrum of NH_3 shows the inversion doublet for each rotational line.

4. SUMMARY

SPICA will provide us with the precious opportunities to investigate comets in the mid-infrared wavelength region. The success of the high-dispersion spectroscopic observations for the molecules proposed here will shed light on the origin of the solar system and it also makes clear view on the delivery of organic molecules into the early Earth as the origin of life. As far as molecules we studied in this paper, the capability for spectroscopy down to 10 μm region (at least) is desired.

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