

模擬分子雲環境下で合成した有機化合物のLC/MS分析 A LC/MS analysis of organic matter produced in the laboratory simulating interstellar molecular clouds

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Chemical and isotopic compositions of organics in astrophysical environments are important information not only to understand their origins and evolution, but one of key topics to discuss the origin and evolution of the solar system. This study focuses on the early step of the chemical evolution in interstellar molecular clouds, from primitive gaseous molecules to ice with organics, which is thought to be one of the precursors of extraterrestrial organic matter in the solar system.

Photochemical synthesis experiments were conducted using a high vacuum chamber “Photochemistry in Interstellar Cloud for Astro-Chronicle in Hokkaido University” (PICACHU). In the chamber, a gold substrate (30 x 40mm) was set and cooled down to about 15K. Gaseous mixtures, prepared in a dedicated line, were admitted onto the surface of the substrate where they condensed forming ice samples. During the deposition the ice on the substrate was simultaneously irradiated UV light emitted from a deuterium lamp. After the photochemical process, the ice sample was warmed-up to room temperature, leading to form refractory organic residue that remained on the surface of the substrate. Then the substrate was stored in a sealed sample container under atmospheric air.

Each sample residue on the substrate was extracted with about 50μL of CH₃OH (LC grade reagent) to analyze the contained organics by liquid chromatography coupled to mass spectrometry (LC/MS), using “Ultimate 3000” LC and “Q Exactive” MS (Thermo Fisher Scientific). 1 to 10μL of sample solution was injected to electrospray ionization (ESI) source. Both positive and negative mass spectra were acquired in the range of m/z 80 to 800 with its resolution (M/ΔM) is 140,000 at m/z 200. The mass accuracy is generally less than ~0.001Da (1mDa) for positive ion.

This paper reports the results of 3 samples; A(H₂O : CH₃OH : NH₃ = 2 : 1 : 1, UV 71hours), B(H₂O : CH₃OH : NH₃ = 10 : 1 : 1, UV 165hours), and C(H₂O : CO : CH₃OH : NH₃ = 10 : 2 : 1 : 1, UV 240hours). All samples contained more than 1000 ion masses in the range of m/z 80 to 800. Major 1000 peaks were extracted using “Xcalibur” software (Thermo Fisher Scientific) for further data processing. The procedural background was calibrated using the mass spectra of CH₃OH extracted from the blank surface of the other gold substrate which are not exposed to both gases and UV, but kept about 15K for 3days in PICACHU. 700 to 900 ion peaks less than m/z 700 were distinguished. About 70 to 80% of the mass spectra can be grouped in various series of alkyl homologues consisting of CHN, CHNO and CHO. The alkyl homologues are discrete with the interval of 14.0156Da that infers methylene chains (-CH₂-)_n. Various alkyl homologues were also reported in the literature, e.g. Danger *et al.* (2013).

The stoichiometric composition was estimated for each ion peaks by Xcalibur, and most of them have less than C₃₀. More than a half of estimated C contained formulae also have both O and N. On the other hand, those without hetero elements (O and N) were minor. The distribution of m/z values of the mass spectra and their corresponding stoichiometric formula were different for each sample. That is due to both the composition of gaseous mixture, especially the existence of CO, and the duration time of UV irradiation.

Reference:

Danger *et al.* (2013) *GCA* **118**, 184.

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