Position specific analysis of nitrogen and carbon isotopes in molecules of biogeochemical interests

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Nitrous oxide (N_2O) is a trace but ubiquitous gas important in global warming and ozone levels and it is highly incorporated in the nitrogen biogeochemical cycles. It is one of the smallest molecules with asymmetric configuration, which was first studied by fragmentation in isotope mass spectrometer and recently by mid-IR laser spectrometer. The two nitrogens in the different positions have their own signatures of their origins and the reaction pathways. Nitrification, denitrification, and several microbial nitrogen process has each fractionation patterns in their position preferences of ^{15}N.

For some organic compounds, such as ethanol, acetic acid and vanillin, position-specific isotopic analysis (PSIA) has been available due to emergence of on-line pyrolysis-gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS) and quantitative isotopic ^{13}C NMR spectroscopy. We developed the measurement method of the molecular and intramolecular $\delta^{13}C$ value of ethanol in aqueous solution using an on-line pyrolysis-GC-C-IRMS. The ^{13}C values of the pyrolytic fragments (CO, CH_4) can be measured with high repeatable result using the system, allowing correcting factors to be applied in order to back-calculate the original $\delta^{13}C_{CH2OH}$ and $\delta^{13}C_{CH3}$ values of ethanol.

Other example of the popular and important chemical compounds is vinegar which is mainly consisting of acetic acid. The intramolecular $\delta^{13}C$ distribution of acetic acid can be very useful to avoid the poisonous agent, which can be mixed with the original materials. Acetic acid can be pyrolyzed and results in three main fragments (CO, CH_4, CO_2). CO_2 fragment corresponds to carboxyl part (COOH) while we expect the CH_4 fragment should correspond to methyl part (CH_3). Using five acetic acid standards to make the calibration curve and then we make the single injection with head space-solid phase micro-extraction (HS-SPME) into GC-Py-GC-C-IRMS system. This method will also be very useful for applications of acetic acid and many related studies. Some other applications will also be presented.