【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Mathematical and physical sciences)

Title of Project：Isotopomer Material Cycle Analysis

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Research Area：Environmental chemistry, Geochemistry, Environmental behavior analysis
Keyword：material cycle analysis, isotopomer

【Purpose and Background of the Research】

Global environmental issues are caused mostly by anthropogenic disturbances to the natural cycles of environmental materials. The cycle of such materials need be analyzed quantitatively and precisely to help understanding the natural and anthropogenic processes regarding their cycles. We proposed the use of 'isotopomers' which are known to be powerful tracers to reduce the uncertainties regarding the biological, chemical, and physical source and sink processes of environmental materials.

'Isotopomers' are defined as isotopically substituted molecules of a molecular species. Bio-elements such as hydrogen and sulfur have one to four isotopes. And there are numerous isotopomers for each molecule with different sites and different combinations of isotopes. We have dedicated ourselves to the analysis of the cycle of greenhouse gases in terms of their own isotopomers, their source materials and their sink products to reduce uncertainties concerning their sources and sinks.

During the past years the following technologies have been developed in the field of isotopomer analysis:

1) Measurements for mass-independent fractionation (MIF) in some compounds containing oxygen and sulfur.

2) Precise measurements of molecules containing more than one rare isotope (clumped-isotope), which potentially may be used as a new thermometer and atmospheric tracer.

3) Position-specific isotopic analysis (PSIA) for some structurally-complex biomolecules.

Our final goal is the generation of a novel isotopomer material cycle analysis which is applicable to all environments from cells to the Earth system.

【Research Methods】

We advance the formulation of new material cycle analysis by integrating cutting-edge measurement technologies, theoretical calculations, and numerical models.

Our main focus includes:

1) Analytical development for isotopomers of biomolecules such as acetic acid using mass spectroscopy and NMR, and its application to environmental and microbial samples.
2) Analytical development for MIF and clumped-isotope of gaseous and aerosol species relevant to climate change.
3) Theoretical calculation of rate constants for the atmospheric reactions of isotopomers
4) Clarification of N_2O cycle and sulfur cycle using isotopomer models and available data.

【Expected Research Achievements and Scientific Significance】

The generation of a new material cycle analysis is expected to refine the estimation of global cycles of greenhouse gases and related materials. The new isotopomer material cycle analysis will be effective not only for refinement of greenhouse gas cycles but also for better understanding of biogeochemical processes.

【Publications Relevant to the Project】

Yoshida, N., and S. Toyoda, Constraining the atmospheric N_2O budget from intramolecular site preference in N_2O isotopomers, *Nature*, **405**, 330-334, 2000.

Ueno, Y., M. S. Johnson, S. O. Danielache, C. Eskebjerg, A. Pandey, and N. Yoshida, Geological Sulfur Isotopes Indicate Elevated OCS in the Archean Atmosphere, Solving Faint Young Sun Paradox, *Proc. Nat. Acad. Sci., USA.*, **106**, 14784-14789, 2009.

【Term of Project】 FY2011-2015

【Budget Allocation】 160,300 Thousand Yen

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