【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Interdisciplinary Science and Engineering)

Title of Project： Creation and Development of Nanoscale Laboratory

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Research Project Number：17H06119　Researcher Number：40314273
Research Area：　Organic Chemistry
Keyword：　Nanocarbon

【Purpose and Background of the Research】

Organic reactions are usually conducted in a vessel made of glasses or metals, by mixing substrate and reagent molecules in liquid solvents. There is a huge number of molecules, as many as the Avogadro constant, in such a reaction system. Therefore, a substrate molecule, for example, encounters other molecules and collides with them including solvent molecules, reagent molecules, and another substrate molecules, with interaction each other. One of the major purpose of organic chemistry is directed to a desired reaction to take place under such complicated conditions.

However, an interaction with one molecule to another is not always well understood because experimental studies are usually done by observing averaged molecular phenomena. Although gas-phase conditions are sometimes selected for studies on single molecular systems, high-vacuum conditions (10^{-10} Torr, 22.4 mL) even contain ca. 600 million molecules, rendering evaluation of pure molecular interaction rather difficult.

This research project aims to create a variety of nono-sized flasks and put one or two distinct chemical species into them in order to create basic science of the isolated materials. It will realize completely isolated single molecules and make it possible to study them under ambient conditions in solution. For the purpose, we need to construct suitable-sized and inert space which is completely isolated from outer condititons, i.e., the Nanospace Laboratory.

【Research Methods】

As shown in Figure 1, fullerenes, spherical clusters of carbon, have hollow space inside the carbon cages, which is suitable for accommodation of small molecules. Although several methods have been so far known for production of endohedral fullerenes encapsulating metal ions or atoms of rare gases, no general method is available for selective encapsulation of a variety of chemical species as well as for desired fullerene cages. In this project, we are going to synthesize endohedral fullerenes encapsulating various chemical species by “molecular surgery”, which includes construction of an opening on the fullerene cage, insertion of a small molecule through it, and the following restoration of the opening by the technique of organic chemistry.

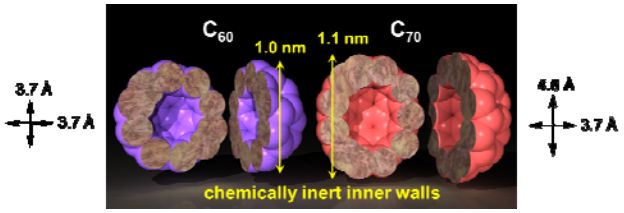

Figure 1 Structures of fullerene C_{60} and C_{70}

We expect encapsulation of a single molecule without any intermolecular interaction, a small molecule having an electronic or magnetic dipole, highly reactive chemical species, metal atoms, and several chemical species with combination of them. We need to develop rational synthetic routes for suitable openings (size, functional groups, and reality for restoration) and to realize the encapsulation for the Nanoscale Laboratory.

【Expected Research Achievements and Scientific Significance】

Taking advantage of completely isolated space, we expect that novel chemical species could be generated and that their properties should be unveiled. New properties of the isolated species that is different from those of bulk materials as well as unknown chemical species will provide great contribution toward new material science.

【Publications Relevant to the Project】

Endofullerenes: A New Family of Carbon Clusters, Edited by Akasaka, T. and Nagase, S., Springer Netherlands (2002).

【Term of Project】 FY2017-2021

【Budget Allocation】 160,100 Thousand Yen

【Homepage Address and Other Contact Information】

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