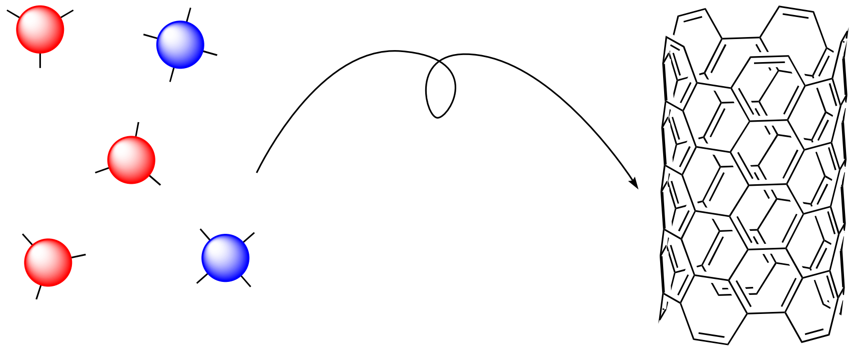
Carbon network synthesis: Designing smallest blueprints

Hideaki Nishina



Now, you can see many things around you. These things are made of very tiny parts, called "molecules", and properties of things such as color or hardness result from molecules. Molecules can be separated into two types, organic molecules such as sugar, and inorganic molecules such as water. The organic molecule has a structure mainly constructed of carbon atoms, and the inorganic molecule doesn't. So, the development of molecular materials is one of the essential parts of recent science technology.

But, making a molecule is not easy like making a papercraft, and its difficulty increases as the target molecule is big and complicated. That's not only because the number of procedures increases, but also there is no assurance that "divided molecular parts" in the procedure are stable, and molecules have their own three-dimensional body that prohibits some types of reaction.

Recently, in the field of organic chemistry, carbon-only molecules such as carbon nanotube or fullerene, a tube-like and soccer ball-like structure made of pentagonal or hexagonal patterns of carbon atoms, have been studied. Ordinally, a carbon atom has four "hands" to connect with other atoms, but in some types of structures, it has only three hands. Graphite which is the main material of pencil lead, and Carbon nanotube, fullerene, are made of only this "three-hands carbon atom." (in contrast, diamond is made of only "four-hands carbon")

Because of this property, they have unique and useful features of electrics or photonics. This feature can be changed by a small difference in molecular structure, such as replacing one hexagonal carbon pattern with pentagonal one. Of course, to study such types of molecules, they must be synthesized, which makes organic chemists spend a lot of time determining the synthetic pathways.

In my research, one solution to problems in synthesis is using "aromatic ring with three-hands" as a "three-hands carbon". An aromatic ring is a very stable hexagonal structure made of six "three-hands carbon", and there are several reactions that easily connect two rings compared to connecting two carbon atoms. Then, we can tackle the main question, "how to determine synthetic route efficiently?".

Of course carbon atom and aromatic ring is different, so even if my research succeeded it might not be applied directly in the synthesis of carbon nanostructure. However, thinking way of systematic synthetic route determination from target molecule structure can be used. Now, my research target is only carbon nanomaterials with high symmetry, but this doesn't mean other target molecules can't be synthesized in different types of systematic pathways. I believe this will result in one of the roadmaps in synthesis, and reduce time we use in synthetic route determination to some extent. It means that organic chemists can use more time on other things, such as designing molecules, thinking new hypotheses or applications.

Even if my research can't apply to ordinal carbon structure, nanocarbon material with large aromatic rings network will show interesting properties, and can be used as a new type of carbon nanomaterials.

I think there are also other possibilities in this. Recently, AI has been developing greatly, and using AI in chemical synthesis has been investigated. Systematic determination of synthetic routes will suit this trend. Since AI can be used with small requirements of the field, and "experiment robots" that synthesize molecules following route generated by AI would be made before long, much wider types of people can synthesize molecules. I think this could be a new form of "How to engage with science".

Of course, I didn't think about all of these things before I started my research. Also, the reason for entering this field is seemingly unconnected. In my case, I decided to study carbon-based organic chemistry because of my personal interest in electronic circuits. You may think "Then why didn't you go to the faculty of engineering?". As I mentioned at first, things we can touch are made of molecules, and their property is controlled by molecules. This appears in electronic circuit elements too, and the development of materials leads development of engineering. In the past, the invention of filament made it possible to change electricity to light, and the study of silicon expanded the possibility of controlling electricity. Nowadays, circuit elements are made of inorganic materials like metals, but recently there is also organic materials are used. For example, a new type of light called organic EL (organic electron-luminescence) used in TV is made of several organic molecules with roles. Applications to circuit elements of carbon-based materials, especially carbon nanotubes have also been studied, because they can change properties including electric resistance or so by structure although they are not metal. So, I thought "studying chemistry might result in making completely new types of electronic elements, and it must be fun!"

The reason for study is not necessarily concrete. If you enjoy making things, it might be a good idea to think about studying chemistry. "Making new things" is not unique to chemistry. But I think chemistry is one of the bases of making things because we can manipulate, assemble the smallest units currently, and it has a different interest compared to that of making things upon these bases.

856 words

I did not use any AI-related software for writing this essay, but used Grammarly to check grammar.