

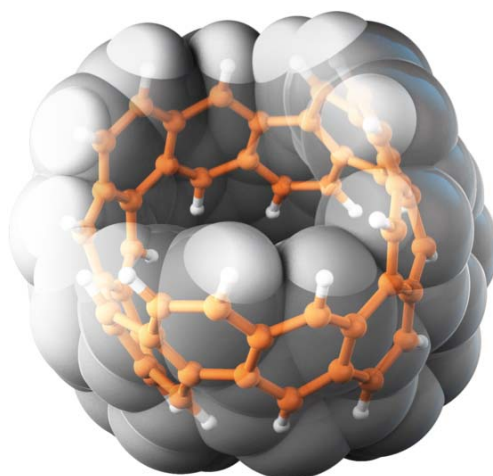
Press Release

At Last: Beautiful, consistent carbon belts

~ Synthesis of a carbon nanobelt with potential applications in nanotechnology ~

May 11, 2017

Nagoya, Japan – Chemists have tried to synthesize carbon nanobelts for more than 60 years, but none have succeeded until now. A team at Nagoya University reported the first organic synthesis of a carbon nanobelt in *Science*. Carbon nanobelts are expected to serve as a useful template for building carbon nanotubes and open a new field of nanocarbon science.



A carbon nanobelt, represented as a ball-and-stick model and space-filling model. Carbon atoms are colored in orange and gray and hydrogen atoms are colored in white.

The new nanobelt, measuring 0.83 nanometer (nm) in diameter, was developed by researchers at Nagoya University's JST-ERATO Itami Molecular Nanocarbon Project, and the Institute of Transformative Bio-Molecules (ITbM). Scientists around the world have tried to synthesize carbon nanobelts since the 1950s and Professor Kenichiro Itami's group has worked on its synthesis for 12 years.

"Nobody knew whether its organic synthesis was even possible or not," says Segawa, one of the leaders of this study who had been involved in its synthesis for 7 and a half years. "However, I had my mind set on the synthesis of this beautiful molecule."

Carbon nanobelts are belt-shaped molecules composed of fused benzene rings, which are aromatic rings consisting of six carbon atoms. Carbon nanobelts are a segment of carbon nanotubes, which have various applications in electronics and photonics due to their unique physical characteristics.

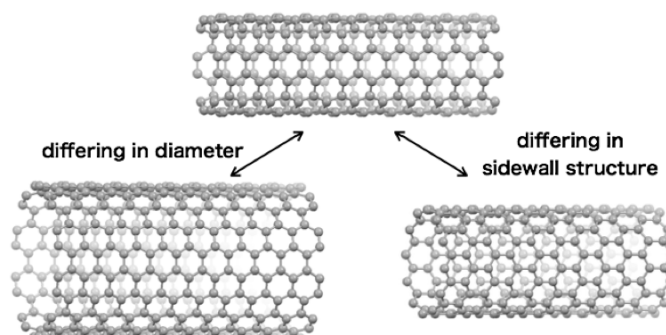


Figure 1. Carbon nanotubes that have different diameters and sidewall structures.

Current synthetic methods produce carbon nanotubes with inconsistent diameters and sidewall structures, which changes their electrical and optical properties. This makes it extremely difficult to isolate and purify a single carbon nanotube that has a specific diameter, length and sidewall structure. Therefore, being able to precisely control the synthesis of structurally uniform carbon nanotubes will help develop novel and highly functional materials.

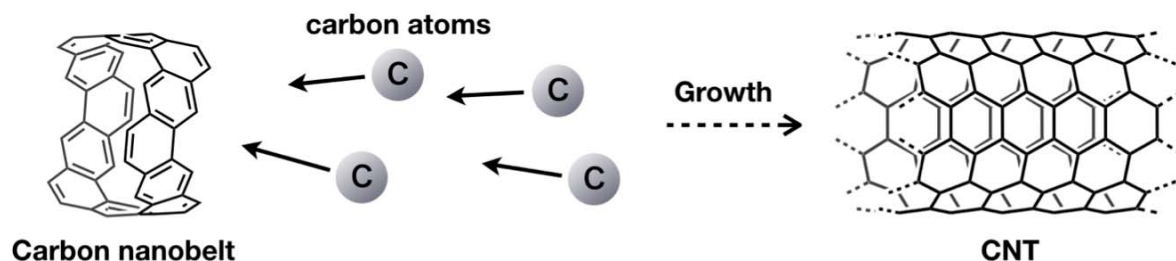


Figure 2. General strategy for carbon nanotube growth using a carbon nanobelt as a template.

Carbon nanobelts have been identified as a way to build structurally uniform carbon nanotubes. However, synthesizing carbon nanobelts is challenging due to their extremely high strain energies. This is because benzene is stable when flat, but becomes unstable when they are distorted by fusion of the rings.

To overcome this problem, Guillaume Povie, a postdoctoral researcher of the JST-ERATO project, Yasutomo Segawa, a group leader of the JST-ERATO project, and Kenichiro Itami, the director of JST-ERATO project and the center director of ITbM, have succeeded in the first chemical synthesis of a carbon nanobelt from a readily available precursor, *p*-xylene (a benzene molecule with two methyl groups in the 1,4- (*para*-) position) in 11 steps.

The key to this success is their synthetic strategy based on the belt-shaped formation from a macrocycle precursor with relatively low ring strain. In their strategy, the team prepared a macrocycle precursor from *p*-xylene in 10 steps, and formed the belt-shaped aromatic compound by a coupling reaction (Fig. 3). Nickel was essential to mediate the coupling process.

“The most difficult part of this research was this key coupling reaction of the macrocycle precursor,” says Povie. “The reaction did not proceed well day after day and it took me three to four months for testing various conditions. I have always believed where there’s a will, there’s a way.”



Figure 3. Synthetic approach towards the carbon nanobelt from *p*-xylene in 11 steps.

In 2015, Itami launched a new initiative in his ERATO project to focus particularly on the synthesis of the carbon nanobelt. At the so-called “belt festival,” various new synthetic routes for the carbon nanobelt were proposed and more than 10 researchers were involved in the project. On September 28, 2016, exactly a year after the start of the festival, the carbon nanobelt structure was finally revealed by X-ray crystallography in front of the Itami group members. Everyone held their breath while staring at the screen during X-ray analysis, and cheered when the cylindrical shape image of the carbon nanobelt appeared on the screen. Itami, Segawa and Povie expressed their joy with a high five (movie: <https://www.youtube.com/watch?v=cABZla9w0uo>).

“It was one of the most exciting moments in my life and I will never forget it,” says Itami. “Since this is the result of a decade-long study, I greatly appreciate all the past and current members of my group for their support and encouragement. Thanks to their skill, toughness, sense and strong will of all members, we achieved this successful result.”

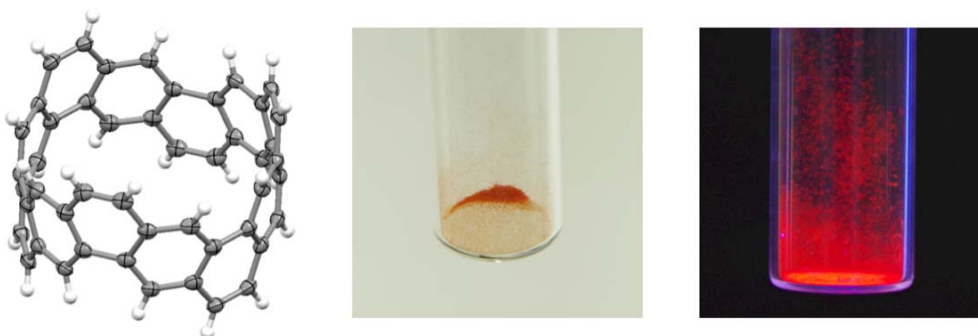


Figure 4. From the left: X-ray structure of carbon nanobelt, crystals of carbon nanobelt under room light, and under UV light.

The synthesized carbon nanobelt is a red-colored solid and exhibits deep red fluorescence. Analysis by X-ray crystallography revealed that the carbon nanobelt has a cylindrical shape in the same manner as carbon nanotubes (Fig. 4). The researchers also measured its light absorption and emission, electric conductivity and structural rigidity by ultraviolet-visible absorption fluorescence, and Raman spectroscopic studies, as well as theoretical calculations.

“Actually, the synthesis part was finished last August but I could not rest until I was able to confirm the X-ray structure of the carbon nanobelt,” says Povie. “I was really happy when I saw the X-ray structure.”

The carbon nanobelt will be released to the market in the future. “We are looking forward to discovering new properties and functionalities of the carbon nanobelt with researchers from all over the world,” say Segawa and Itami.

This article “Synthesis of a carbon nanobelt” by Guillaume Povie, Yasutomo Segawa, Taishi Nishihara, Yuhei Miyauchi and Kenichiro Itami is published online in *Science*. DOI: 10.1126/science.aam8158 (<http://dx.doi.org/10.1126/science.aam8158>)

JST-ERATO Itami Molecular Nanocarbon Project (<http://www.jst.go.jp/erato/itami/index.html>)

JST-ERATO Itami Molecular Nanocarbon Project was launched at Nagoya University in April 2014. This is a 5-year project that seeks to open the new field of nanocarbon science. This project entails the design and synthesis of as-yet largely unexplored nanocarbons as structurally well-defined molecules, and the development of novel, highly functional materials based on these nanocarbons. Researchers combine chemical and physical methods to achieve the controlled synthesis of well-defined uniquely structured nanocarbon materials, and conduct interdisciplinary research encompassing the control of molecular arrangement and orientation, structural and functional analysis, and applications in devices and biology. The goal of this project is to design, synthesize, utilize, and understand nanocarbons as molecules.

About WPI-ITbM (<http://www.itbm.nagoya-u.ac.jp/>)

The Institute of Transformative Bio-Molecules (ITbM) at Nagoya University in Japan is committed to advance the integration of synthetic chemistry, plant/animal biology and theoretical science, all of which are traditionally strong fields in the university. ITbM is one of the research centers of the Japanese MEXT (Ministry of Education, Culture, Sports, Science and Technology) program, the World Premier International Research Center Initiative (WPI). The aim of ITbM is to develop transformative

bio-molecules, innovative functional molecules capable of bringing about fundamental change to biological science and technology. Research at ITbM is carried out in a "Mix-Lab" style, where international young researchers from various fields work together side-by-side in the same lab, enabling interdisciplinary interaction. Through these endeavors, ITbM will create "transformative bio-molecules" that will dramatically change the way of research in chemistry, biology and other related fields to solve urgent problems, such as environmental issues, food production and medical technology that have a significant impact on the society.

About JST-ERATO (<http://www.jst.go.jp/erato/en/about/index.html>)

ERATO (The Exploratory Research for Advanced Technology), one of the Strategic Basic Research Programs, aims to form a headstream of science and technology, and ultimately contribute to science, technology, and innovation that will change society and the economy in the future. In ERATO, a Research Director, a principal investigator of ERATO research project, establishes a new research base in Japan and recruits young researchers to implement his or her challenging research project within a limited time frame.



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