Heavy Hydrogen

Kentaro Sato

Isotope with Its Own Symbol

Discovering and naming a new element are one of scientists' biggest dreams. The name of an element that you coined would be used for generations to come, so it might be a greater honor than receiving a Nobel Prize. In the history of chemical elements, which we know a few more than a hundred today, there have been many disputes and confusions over claiming that honor. In fact, the number of the "phantom elements" – elements that were given a name once but removed from the periodic table after their identities were proven false - is said to equal that of the "real" elements.

Quite a few cases are known where an isotope of the same element was mistaken as a distinct element and given its own name. For example, thorium 227 and 230 were initially named radioactinium and ionium, respectively, and had their own atomic symbols. This kind of confusions were gradually sorted out, but there remain two isotopes of the same element which maintain own names and symbols. Of course, they are deuterium (atomic symbol D) and tritium (atomic symbol T).

The reason why these two names are still being used is because these isotopes have somewhat different physico-chemical properties from common "light hydrogen" (atomic symbol H) and their properties have useful applications. As you know, the properties of the isotopes of the same element are essentially equivalent. But for the smallest element in the periodic table, the difference in the number of neutron by just one has such a big relative impact to the whole elemental character that the differences in the properties between isotopes become tangible.

Deuterium was discovered in 1932. Harold Urey (who is also famous for the Urey-Miller experiment demonstrating the synthesis of amino acids in pre-biotic atmosphere) succeeded in concentrating deuterium by slowly distilling liquid hydrogen, relying on the small difference in boiling point. Urey was given the Nobel Prize in Chemistry just two years later, a testament to how highly his discovery was recognized.

Atomic Energy and Deuterium

An important application of newly isolated deuterium was in the development of nuclear energy. In order to sustain nuclear chain reactions of radioactive substances such as uranium, it was necessary to slow down the speed of released neutrons. In this purpose, deuterium had just the right property as a "neutron moderator." Even today, heavy water (also known as deuterium oxide) is used as a neutron moderator in nuclear reactors in countries such as Canada.

Deuterium was also used as a component of nuclear fusion and therefore in the development of hydrogen bombs. Deuterium and tritium are a combination which brings about nuclear fusion at the lowest temperature (which is still 100 million degrees Kelvin), so they are considered as the most promising "fuels" for nuclear fusion reactors. However, there are all too many issues to overcome before realizing practical implementation of the technology. Even after a few decades of research, nuclear fusion remains as a "potential future energy source."

In 1989, a report of "cold fusion" generated a controversy. The report was that anomalously high levels of heat and small amounts of nuclear radiation were detected in the electrolysis of heavy water using the electrodes made of palladium. It was claimed that the cause was the nuclear fusion of deuterium at room temperature! Nuclear fusion requires a huge plant and ultrahigh temperature otherwise, so if the finding were true it would revolutionize energy use. This experiment, known as the Fleischmann-Pons experiment after the names of the discoverers, became not only a scientific, but also an industrial and a political sensation.

Unfortunately though, the Fleischmann-Pons result could not be reproduced despite the replication experiments by many other scientists. The radiation levels measured in these experiments were minimally different from the background and far from sufficient to support the claim that nuclear fusion reaction was taking place. The research on cold fusion is still ongoing today, but few reports appear on reliable peer-reviewed scientific journals. Even with most optimistic perspective, it does not seem to become a hopeful energy source anytime soon.

Deuterated Solvents

For organic chemists, the most common application of deuterium is probably NMR solvent. Deuterated solvents such as d-chloroform, d6-DMSO, and D_2O are routinely used by chemists to prepare sample solutions for NMR measurements. Deuterated solvents are undoubtedly an essential part of chemistry research.

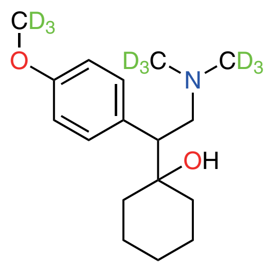
So how are these deuterated solvents synthesized? In electrolysis of water, H_2O reacts more easily than D_2O, releasing more of gaseous H_2 than D_2. As a result, this process increases the concentration of D_2O and this is currently the main way of how heavy water is produced.

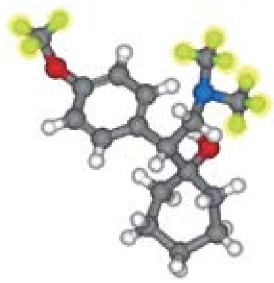
According to an old literature, deuterium can be synthesized by reacting hexachloroacetone with D_2O. Also reported is the synthesis of deuterated acetone by stirring acetone in alkaline heavy water. Deuterated DMSO can be made probably under similar conditions. It would be nice to know how deuterated solvents are produced commercially in these days, but most of it seems to be kept as corporate secrets. Nonetheless, we should be grateful to have an access to high quality deuterated solvents which once had to be prepared in our laboratories.

Deuterium and Life

How does deuterium behave in terms of biology? For instance, what biological effects would it have if you raise an animal with heavy water alone? Would it produce an animal with the same appearance but with 10% heavier weight? According to a report, if you give an animal heavy water, health defects such as muscle weakness start to show after 10–20% of the body fluids are replaced with heavy water and death is reached at 30–40%. As mentioned earlier, deuterium has different reactivities from common hydrogen. For example, carbon-deuterium (C-D) bond is famously known to be 6–10 times less reactive compared to carbon-hydrogen (C-H) bond. This deuterium isotope effect most likely disrupts important biological reactions and causes toxic effects.

The application of deuterium has been growing broader in recent years. The compounds which are "isotopically labeled" with deuterium are suited for detection by mass spectroscopy, making them useful in areas such as the study of biosynthetic pathway of natural molecules and the tracing of drug molecules inside the body. Though the detection sensitivity of deuterium is lower than tritium, deuterium is less expensive and easier to handle (not requiring any special facilities for handling of a radioactive isotope) therefore is a more popular choice.





Example of Deuterated Drugs "Venlafaxine-d6"

But the isotope effect of deuterium mentioned earlier has to be considered carefully. Pharmaceutical drug molecules are often metabolized in the liver through oxidative cleavage of their C-H bonds. Therefore, labeled compounds containing deuteriums in place of hydrogens may not necessarily behave the same as non-labeled counterparts do.

Then there came an idea that the isotope effect could be something positive if looked at from an opposite angle; if the incorporation of deuterium into a drug molecule increases its stability *in vivo*, it could increase the efficacy of existing drugs. There was a venture company which rattled the pharmaceutical industry by doing exactly that and starting to file new patent applications for one existing drug after another. If all these get approved as new patents, the venture would potentially take away the huge profits of major drug makers.

However, it seems that most of them have not been approved because simple deuteration of existing drug molecules has been judged insufficient to qualify as "inventiveness", which is an essential quality of new patents. Still, this idea has become one of standard means of drug design. The number of drug candidate molecules containing deuteriums for the aim of slowing down metabolism is increasing.

Also in recent years, there have been cases in the field of materials science where deuterium was used in the light emitting layer of OLED (organic light-emitting diode) to improve emission efficiency and durability. The cost of using deuterium is of course a concern, but this kind of high value added products may be able to counterbalance it. Being hydrogen but not exactly hydrogen at the same time, this interesting "element" deuterium has been kind of in the blind spot of scientists. It could very well have many more possibilities.

Introduction of the author :

Kentaro Sato

[Brief career history] He was born in Ibaraki, Japan, in 1970. 1995 M. Sc. Graduate School of Science and Engineering, Tokyo Institute of Technology. 1995-2007 Researcher in a pharmaceutical company. 2007-Present Freelance science writer. 2009-2012 Project assistant professor of the graduate school of Science, the University of Tokyo.
[Specialty] Organic chemistry
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Technical Glossary

Deuterium and Tritium

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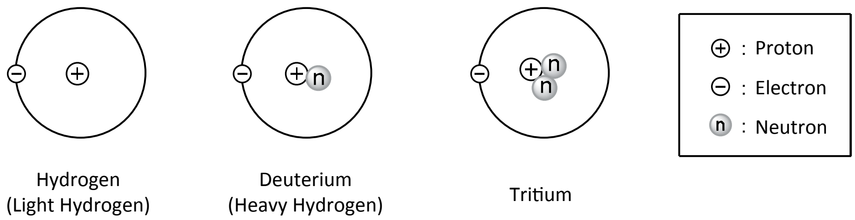
Deuterium is one of isotope of hydrogen and has a nucleus consisting of one proton and one neutron, and one electron out of the nucleus. Tritium is one of isotope of hydrogen and has a nucleus consisting of one proton and two neutrons, and one electron out of the nucleus.



Nuclear Fusion

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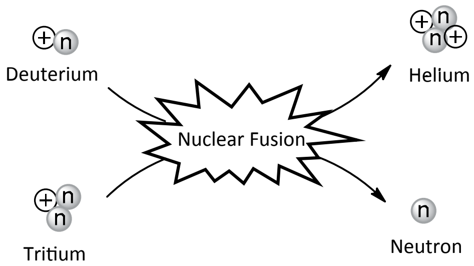
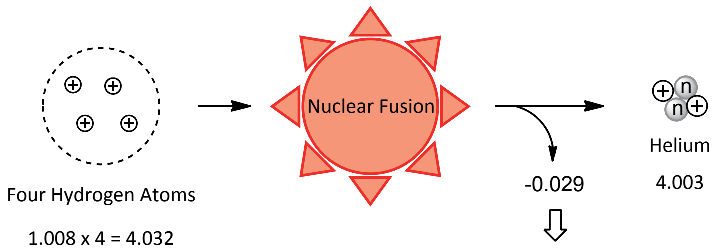
Nuclear fusion is a phenomenon in which two light nuclei fuse with each other to form a single heavier nucleus. As a typical example, one deuterium and one tritium transform into one helium and one neutron by nuclear fusion.



One actual example of nuclear fusion in our life is the sun. At the center of the sun, four hydrogen atoms fuse to form a helium atom. Enormous energy is generated in the nuclear fusion. How much energy would be produced by nuclear fusion?

The atomic weights of hydrogen and helium are 1.008 and 4.003 respectively. The total atomic weight of four atoms of hydrogen is calculated at 4.032. In fact, the actual atomic weight of helium is 4.003. It is suggested that the atomic weight of helium becomes lighter by 0.029 amu. As a matter of fact, the decreased amount of weight is transformed into energy. To calculate the energy we use Einstein's equation (i.e. $E = mc^2$). In the case of 1kg of hydrogen atom, 7.2 g of the weight will be decreased by nuclear fusion. So the amount of energy can be calculated by the following (shown below in an equation):



How energy is produced from 1kg of hydrogen?

$$E = mc^2 = 7.2 \times 10^{-3} \times (3.0 \times 10^8)^2 \fallingdotseq 6.48 \times 10^{14}\ \text{J}$$

We find an enormous amount of energy is released by nuclear fusion. It seems like great energy, but there are many problems to be solved for the technical and safety aspects. To be available to use that energy for our benefit, it will take more time.