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News Item

Buckyballs in Disguise Take to the Water

Water solubility might greatly extend the range of reactions of the football-shaped carbon molecules known as fullerenes. But until now it has not been possible to make these hydrophobic, or water-hating, molecules dissolve in water.

Now a team of Swedish researchers claims to have solved the problem. Olof Wennerström and his colleagues at the Chalmers University of Technology in Göteborg, Sweden, enclosed fullerene molecules in a large water-soluble host molecule and so made them soluble in water. For the host, they used doughnut-shaped, cyclic molecules known as cyclo-dextrins (*Journal of the Chemical Society, Chemical Communications*, 1992, p. 604).

Wennerström's team first planned to make a complicated synthetic host molecule for C_{60} with the aim of dissolving it in water. However, two of his graduate students, Gunnar Westman and Thomas Anderson, hit on the idea of using the well known cyclodextrin molecule.

Cyclodextrins consist of six, seven or eight sugar molecules joined together in a ring. They are produced naturally by some bacteria when they metabolise starch. The molecule chosen by Wennerström and his colleagues, γ-cyclodextrin, has eight sugar units in its ring. It is highly polar on the outside, which makes it soluble. But it has a hydrophobic cavity, which means that organic molecules prefer to sit in this hole rather than roam free in a water solution. Because the fullerene molecules are very non-polar, they too prefer to sit inside the cavity, says Wennerström.

The researchers have used a computer to model the possible structure of the cyclodextrin–fullerene complex. Their results seem to indicate that the fullerene might be sandwiched between two cyclo-dextrin molecules in aqueous solution (a 2 : 1 complex).

However, Wennerström's colleague Mikael Sundahl suggests that the physical properties of the complex point more towards a 1 : 1 complex rather than a sandwich. Knowing the structure will be essential in order to understand the mechanisms of reactions of fullerenes in water.

According to Wennerström: "Many reactions with C_{60} in water should be tried." Water solubility might greatly extend the range of reactions of the molecule. "The most urgent problem is just how the cyclo-dextrin binds to and dissolves C_{60}," he says.

He believes that in water fullerenes will react differently to the way they would in organic solvents. The change could lead to interesting and potentially useful new products not possible in organic solvents. He also thinks that C_{60} might act as a catalyst for oxidation reactions in water.

Meanwhile, the group of chemists at the University of Sussex that co-discovered fullerenes have also carried out two new reactions on fullerenes. Roger Taylor and Harry Kroto and their colleagues at the Universities of Southampton and Leicester

have investigated the reactions of fluorinated fullerenes with water, and have found that a rather unusual reaction occurs.

The team first reported that they could make a fully fluorinated fullerene molecule $C_{60}F_{60}$ last year (*New Scientist*, 6 July 1991, p. 25). At the time, it was hoped that fluorinated fullerenes might make good 'superlubricants'. However, the researchers have found that such compounds react with water to release hydrogen fluoride. Not only would they be very impractical as lubricants, they would be dangerous as well.

This discovery led the researchers to look at how the hydrophobic, fluorinated fullerene reacts with water. Although the reaction is slow, the chemists found that by adding an organic cosolvent such as tetrahydrofuran or acetone there was an instantaneous and heat-generating reaction of the molecule with water. Such a reaction is not common in organic chemistry.

Fluorinated organic compounds, generally known as alkyl fluorides, are normally very resistant to attack from so-called nucleophilic groups, which seek out regions of positive charge in a molecule. The researchers say that the large cage structure of the fullerene molecule prevents nucleophiles, such as water, from attacking.

The chemists add that nucleophilic reactions of fluorinated fullerenes could open up yet more routes to novel fullerene materials by allowing the attachment of functional groups to the fullerene cage (*Journal of the Chemical Society, Chemical Communications*, 1992, p. 665).

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