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NEWS RELEASE

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Note to Journalists: An electronic copy of the research paper is available from Emil Venere, (765) 494-4709, venere@purdue.edu

'Buckyballs' have high potential to accumulate in living tissue

WEST LAFAYETTE, Ind. - Research at Purdue University suggests synthetic carbon molecules called fullerenes, or buckyballs, have a high potential of being accumulated in animal tissue, but the molecules also appear to break down in sunlight, perhaps reducing their possible environmental dangers.

Buckyballs may see widespread use in future products and applications, from drug-delivery vehicles for cancer therapy to ultrahard coatings and military armor, chemical sensors and hydrogen-storage technologies for batteries and automotive fuel cells.

"Because of the numerous potential applications, it is important to learn how buckyballs react in the environment and what their possible environmental impacts might be," said Chad Jafvert, a professor of civil engineering at Purdue.

The researchers mixed buckyballs in a solution of water and a chemical called octanol, which has properties similar to fatty tissues in animals. Jafvert and doctoral student Pradnya Kulkarni were the first to document how readily buckyballs might be "partitioned," or distributed into water, soil and fatty tissues in wildlife such as fish.

Findings indicated buckyballs have a greater chance of partitioning into fatty tissues than the banned pesticide DDT. However, while DDT is toxic to wildlife, buckyballs currently have no documented toxic effects, Jafvert said.

"This work points out the need for a better understanding of where the materials go in the environment," he said. "Our results show they are going to be taken up by fish and other organisms, possibly to toxic levels. This, however, indicates only the potential of buckyballs to bioaccumulate. They could break down in the environment or in an organism once taken up."

Researchers do not yet know whether buckyballs will break down in the environment or will be metabolized by animals, which would reduce the risk of accumulating in fatty tissues.

"For example, we don't bioaccumulate sugars because we process sugars, but we do bioaccumulate other compounds that we don't metabolize," Jafvert said. "If we have the ability to metabolize buckyballs, we won't bioaccumulate them."

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Findings were detailed in a research paper that appeared in August in the journal Environmental Science and Technology. The paper was written by Jafvert and Kulkarni.

The researchers determined the "octanol-water partition coefficient," which enables them to show how readily buckyballs would be partitioned.

"The bottom line is, if buckyballs partition favorably from water to octanol, they are also likely to partition favorably from water to fatty tissues," Jafvert said.

The researchers also are investigating whether sunlight breaks down buckyballs and other structures called carbon nanotubes, which also could have widespread industrial applications.

"We need to learn how reactive these materials are in the environment," Jafvert said. "Do they break down? What kinds of products do they form? We have learned so far that buckyballs absorb light, and they do photoreact. That's potentially a good thing because it means it won't hang around for a long period of time, reducing the exposure concentration, which would then reduce any potential toxicity that it may or may not have."

Named after architect R. Buckminster Fuller, who designed the geodesic dome, buckminsterfullerenes, or buckyballs, are soccer-ball-shaped molecules containing 60 carbon atoms. A buckyball has a width of about 1 nanometer, or one-billionth of a meter, which is roughly 10 atoms wide.

The researchers determined precisely how soluble the buckyballs are in water and confirmed that the molecules form clusters, which complicates efforts to understand how they might be dispersed by water in the environment.

"Typically, buckyballs are not found in water because their solubility is so low, but the same could be said of DDT," Jafvert said. "DDT is found in sediment, so you would assume buckyballs would also end up in sediments. That means there is also a chance that marine organisms, like worms that are eating sediment, are going to be potentially accumulating buckyballs unless they break down in the environment."

The research is affiliated with the Center for the Environment and the Birck Nanotechnology Center at Purdue's Discovery Park and is funded by the Environmental Protection Agency and the National Science Foundation through the NSF's Nanoscale Interdisciplinary Research Team, or NIRT. The work is part of a larger NIRT project at Purdue involving researchers in agronomy, civil engineering, agricultural and biological engineering, mechanical engineering, food science, and earth and atmospheric sciences.

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ABSTRACT

Buckminsterfullerene's (C60) Octanol-Water Partition Coefficient (Kow) and Aqueous Solubility

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To assess the risk and fate of fullerene C60 in the environment, its water solubility and partition coefficients in various systems are useful. In this study, the log Kow of C60 was measured to be 6.67, and the toluene-water partition coefficient was measured at log Ktw) 8.44. From these values and the respective solubilities of C60 in water-saturated octanol and water-saturated toluene, C60's aqueous solubility was calculated at 7.96ng/L(1.11°—10-11M) for the organic solvent-saturated aqueous phase. Additionally, the solubility of C60 was measured in mixtures of ethanol-water and tetrahydrofuran-water and modeled with Wohl's equation to confirm the accuracy of the calculated solubility value. Results of a generator column experiment strongly support the hypothesis that clusters form at aqueous concentrations below or near this calculated solubility.The Kow value is compared to those of other hydrophobic organic compounds, and bioconcentration factors for C60 were estimated on the basis of Kow.