Pitt scientists help bring world's smallest test tubes 'From the Lab to the Fab'

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Just by picking up the phone, Nobel Laureate and nanotube pioneer Richard Smalley convinced University of Pittsburgh R.K. Mellon Professor of Chemistry and Physics John T. Yates Jr. to enter the field of nanotube surface chemistry. "Rick Smalley's phone call resulted in six years of exciting work," says Yates, who will present highlights of research done at Pitt during a Presidential Event honoring Smalley Sept. 11 at the 232nd American Chemical Society National Meeting in San Francisco, Calif.

In collaboration with J. Karl Johnson, who is the William Kepler Whiteford Professor of Chemical Engineering at Pitt, Yates has extensively investigated the use of single-walled carbon nanotubes (SWNTs) as tiny test tubes. SWNTs are cylindrical molecules with a diameter equivalent to about three atoms. The tube walls are made of a single curved sheet of carbon atoms. Experimenting at such a small scale presents many challenges, but offers big rewards: "Doing chemistry inside of nanoscale test tubes allows one to probe the role of extreme molecular confinement on chemical behavior," says Yates, who also directs Pitt's University Surface Science Center.

In the mid-1990s, Smalley recognized that SWNTs would likely be excellent adsorbents because of the enhanced attractive forces expected for molecules located inside the nanotubes. Yates has developed novel methods to measure the relative number of inside and outside molecules attracted to the nanotubes, while Johnson checks experimental results and provides more details through theoretical molecular modeling than could be provided by experiments alone.

Yates and Johnson, along with their students and postdoctoral fellows, obtained a striking result for water molecules confined inside SWNTs, as reported in a recent paper in the Journal of the American Chemical Society. The water molecules inside nanotubes bond together into rings made of seven water molecules. Yates and Johnson, who also are researchers in Pitt's Gertrude E. and John M. Petersen Institute of NanoScience and Engineering, found that these rings stack like donuts along the nanotube. The rings themselves are bound together by a new type of hydrogen bond that is highly strained compared to the hydrogen bonds within each molecular "donut."

The researchers first detected this novel hydrogen bond experimentally by its unusual singular vibrational frequency and later deduced its character by modeling. "The behavior of water as a solvent inside of nanotubes will probably differ strongly from its behavior in ordinary water based on the donut configuration and the new kind of hydrogen bond discovered in this work," says Yates.

In another development, research showed that reactive molecules confined inside nanotubes are well shielded by the nanotube walls from reacting with active chemical species like atomic hydrogen, one of the most aggressive chemical reactants in the chemist's toolbox. The work suggests that chemists could keep certain molecules from reacting by storing them inside nanotubes, while molecules outside the tube are free to react. "This could provide a new tool for focusing reactive chemistry in the laboratory to select one molecule and exclude another one, tucked away inside of a nanotube," Yates says.

The researchers' pioneering work could lead to future SWNT-based technologies such as time-release medications and highly efficient gas masks to decontaminate toxic gases. In addition, their research promises to yield new insights into basic chemistry. "Confining matter inside of nanotubes could lead to a range of new chemical and physical properties for the confined molecules, allowing chemists a higher degree of control of molecular behavior," says Yates.

Source: University of Pittsburgh