Fuel cells might get hydrogen from water, organic material

August 31 2005

A novel technique for producing hydrogen from water and organic material has been found recently at Purdue University, a discovery that could help speed the creation of viable hydrogen storage technology.

Though the method has not yet been evaluated for economic feasibility on a large scale, chemist Mahdi Abu-Omar said it could offer solutions to several problems facing developers of fuel cells, which are looked upon as a potential replacement to fossil-fuel burning engines in automobiles. The technique requires only water, a catalyst based on the metal rhenium (REE-nee-um) and an organic liquid called an organosilane, which can be stored and transported easily.

"We have discovered a catalyst that can produce ready quantities of hydrogen without the need for extreme cold temperatures or high pressures, which are often required in other production and storage methods," said Abu-Omar, an associate professor of chemistry in Purdue's College of Science. "It is possible that this technique could lead to fuel cells that are safe, efficient and not dependent on fossil fuels as their energy source."

Abu-Omar's research team, which includes Purdue's Elon A. Ison and Rex A. Corbin, published their findings today (Wednesday, Aug. 31) in the Journal of the American Chemical Society.

Hydrogen is the most plentiful element on Earth and, once isolated, is a clean-burning fuel that produces neither greenhouse gases nor toxic emissions. Because hydrogen can be used for electricity production, transportation and other energy needs, many see a changeover to a "hydrogen economy" from our oil-based one as the solution to global energy problems. But before hydrogen can be used as fuel, it must be extracted from other substances that are often fossil fuels, and then stored safely in sufficient quantities. If these problems can be solved, hydrogen-powered generators, known as fuel cells, might replace internal combustion engines everywhere from electrical plants to cars.

Abu-Omar and his colleagues were not concentrating on these problems when they began studying organosilanes, a group of organic molecules that have been slightly modified in the laboratory. But as commonly happens in science, he said, a project often takes researchers in different directions than originally anticipated.

"Initially, we were concerned with finding useful catalysts to convert these silicon-based fluids into silanols, another type of substance that is valuable in the chemical industry," he said. "It's the sort of work chemists do all the time, and it's usually of interest only to other chemists. But sometimes the byproducts of conversions are as interesting as what you wanted in the first place."

Abu-Omar's team took a compound based on rhenium, a comparatively rare metal often obtained while mining copper, and added it to the organosilane in the presence of water. Over the course of an hour, the organosilane changed completely into silanol, leaving the water and rhenium catalyst unchanged. But the team also noticed there was a gas bubbling from the mixture.

"It turned out to be pure hydrogen," Abu-Omar said. "The reaction is not only efficient at creating silanol, but it also generates hydrogen at a high rate in proportion to the amount of water."

The team estimates that about 7 gallons each of water and organosilane could combine to produce 6 1/2 pounds of hydrogen, which could power a car for approximately 240 miles.

"The big question is, of course, whether it would be economically viable to create organosilane fuels in the quantities necessary to power a world full of cars," Abu-Omar said. "As of right now, there simply isn't enough demand to make more than small volumes of this liquid, and while it's a relatively easy process, it's not dirt cheap either."

But, Abu-Omar speculated, producing organosilanes in larger quantities would bring the price down, and the byproduct – silanol – also could be recycled or sold to lessen the overall cost.

"On today's chemical market, silanol is even more expensive than organosilanes are, but their value would of course decline as well if there were suddenly millions of gallons of them on the market," he said. "These are the sorts of questions that economists would have to look at, and we have other questions of our own, such as whether these reactions can be carried out on naturally occurring hydrogen sources."

Abu-Omar said this question might prove to be the more relevant one as investigations continue.

"I think the big point here is that hydrogen can be produced from water and a form of organic matter," he said. "If this rhenium-based catalyst can do the trick on organosilanes, perhaps we can find other catalysts that can generate hydrogen from garbage, or from biomass left over from the harvest."

The current findings, he said, demand that the method be scrutinized more carefully.

"For now, we've demonstrated the initial premise that we can produce and store hydrogen on demand with this method," he said. "It's a great start, but we need to know more about the economic and ecological price of doing this on a larger scale."

Abu-Omar is affiliated with Purdue's new Energy Center in Discovery Park. The center will focus on developing economically and environmentally sound energy sources, and on helping to change policies and perceptions about the way we use energy. More than 75 campus experts in disciplines from engineering, science, agriculture and liberal arts will contribute to the effort.

ABSTRACT

Hydrogen production from hydrolytic oxidation of organosilanes using a cationic oxorhenium catalyst

Elon A. Ison, Rex A. Corbin and Mahdi Abu-Omar

We describe herein the novel application of a transition metal oxo complex, a cationic oxorhenium(V) oxazoline, in the production of molecular hydrogen (H2) from the catalytic hydrolytic oxidation of organosilanes. The main highlights of the reaction are quantitative hydrogen yields, low catalyst loading, ambient conditions, high selectivity for silanols, water as the only co-reagent, and no solvent requirement. The amount of hydrogen produced is proportional to the water stoichiometry. Thus, reaction mixtures of polysilyl organics such as HC(SiH3)3 and water contain potentially > 6% by weight hydrogen. Kinetic and isotope labeling experiments have revealed a new mechanistic paradigm for the activation of Si-H bonds by oxometalates.