

Chemists identify organic molecules that mimic metals

A limitation in using hydrogen as a fuel in hydrogen-powered vehicles is the difficulty involved in storing it in a cost-effective and convenient manner. While it is possible to store hydrogen using metals, the resulting products often can be prohibitively expensive and cause environmental problems.

Chemists at UC Riverside now offer a possible solution. A class of carbenes – molecules that have unusual, highly reactive carbon atoms – can mimic, to some extent, the behavior of metals, the chemists have found. Called cyclic alkyl amino carbenes or CAACs, these organic molecules, the researchers report, could be used to develop carbon-based systems for storing hydrogen.

Study results appear in the April 20 issue of *Science*.

In their experiments, the researchers found that the CAACs can split hydrogen under extremely mild conditions, a behavior that has long been seen in metals reacting with hydrogen.

"The mode of action of these organic molecules, however, is totally different from that of metals," said Guy Bertrand, a distinguished professor of chemistry who led the research. "Moreover, the CAACs are able to split ammonia as well – an extremely difficult task for metals."

Bertrand explained that such a splitting of ammonia, under certain conditions, can pave the way for transforming abundant and inexpensive ammonia into useful amino compounds used to make pharmaceuticals and bulk industrial materials. "This is one of the top challenges for the 21st century," he said.

According to the UCR research team, the metal-mimicking carbenes offer another low-cost and low-toxicity benefit: Scientists now may be able to use non-metallic catalysts for a reaction, called "hydrogenation reaction," which plays a critical role in the food, petrochemical and pharmaceutical industries.

In their study, the researchers exposed a solution of CAACs to both gaseous hydrogen and liquid ammonia. "We used nuclear magnetic resonance spectroscopy to analyze the products," said Guido Frey, the first author of the research paper and a postdoctoral fellow, supported by the Alexander von Humboldt Foundation, in Bertrand's lab. "And we used single crystal X-ray diffraction analysis to confirm the structure of the products."

A carbene is a molecule that has a carbon atom with six electrons instead of the usual eight. Because of the electron deficiency, carbenes are highly reactive and usually unstable in nature.

Source: University of California - Riverside

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