Phantom parent molecule of important class of chemical compounds isolated for first time

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A team of scientists from the University of Georgia and two European universities has, for the first time, synthesized and characterized the elusive parent molecule of an important class of chemical compounds.

The discovery, reported today in the journal *Nature*, involves trapping the carbene hydroxymethylene (HCOH) in a matrix of argon at 11 degrees Kelvin—just above absolute zero (.67 degrees F)—where it was observed to decay, over a period of a few hours, to formaldehyde in a process that bears resemblance to the radioactive decay of nuclei.

While chemists had theorized for some years that HCOH should be isolable, this is the first time it has been achieved, and the accomplishment provides a greater understanding of the behavior of a class of compounds extremely important to organic and organometallic chemistry.

"It took a perfect match between experimental observations and theoretical predictions for us to say we have this molecule for the first time," said UGA chemist Wesley Allen, "but it worked beautifully, and this method can work for other elusive molecules as well."

Co-authors with Allen on the paper were Peter Schreiner and Hans Peter Reisenauer of Liebig University in Germany; Edit Mátyus and Attila Császár of Eötvös University in Hungary; and Frank Pickard and Andrew Simmonett, who along with Allen are with the department of chemistry at UGA. Schreiner received his doctoral degree from UGA and was on the faculty for several years before returning to Germany.

While the capture of HCOH is important, just as interesting is the team's unexpected discovery that the molecule decays to formaldehyde near absolute zero through "quantum tunneling," one of the more mystifying aspects of quantum theory. In quantum tunneling, a particle passes through a barrier that is impenetrable by normal standards.

"This kind of tunneling happens all the time with electrons, because they are so light," said Allen, "but for it to happen for heavier particles such as hydrogen atoms, the barriers must be more modest. In this case, the HCOH molecule tunnels under an enormous barrier, perhaps the most spectacular example of this process known in chemistry."

The reason why the group was studying HCOH at all began with a NASA project, since scientists at the space agency wanted to see if the elusive molecule existed in space but first needed to know what it would look like. Unfortunately, no one had been able to isolate and characterize it until the current research.

Allen and his UGA colleagues, who are theoretical chemists—studying chemistry by large-scale computations based on the laws of physics—say that it's now highly unlikely that free HCOH will be found in space.

"One of the most gratifying parts of this work is that we made the predictions of the tell-tale signatures of the molecule prior to the actual laboratory studies, which were done in Europe," said Allen, "so to us it helps prove the value of quantum chemistry in finding solutions in the lab."

While the signatures of HCOH were predicted, the quantum tunneling aspect came completely out of left field, Allen said, surprising everyone involved.

"Peter [Schreiner] called me up and said the decay mechanism was tunneling, because the molecule was perfectly stable when a heavy hydrogen isotope was inserted," said Allen. "I initially laughed at this idea. But I did the theory to see if it could be quantum tunneling, and sure enough we found out that it is what was happening in all likelihood. It was amazing."

Source: University of Georgia

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