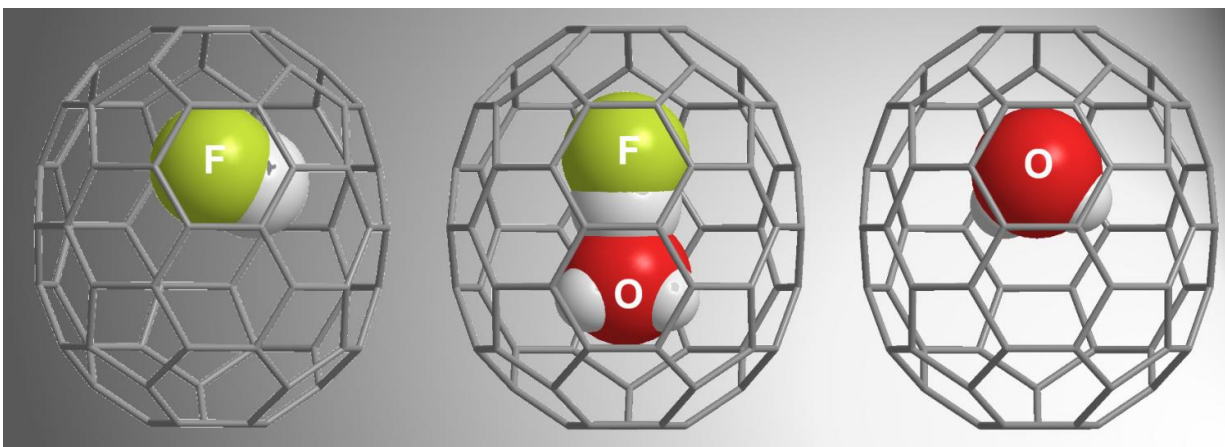


Researchers isolate hydrogen fluoride and water to understand acid dissolution

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Credit: Zhang et al.

(Phys.org)—Beginning level chemistry classes learn about Brønsted-Lowry acids. These acids dissociate in water to form an H^+ ion and a negatively charged counterion. While this is a fundamental lesson, the actual mechanism of dissolution is a bit of a mystery. The H^+ molecule combines with water to form H_3O^+ , but the number of water molecules needed to hydrate the simplest acid, HF, is unknown. Attempts to isolate HF and H_2O are difficult, largely because of the high reactivity of HF and the tendency of water to form hydrogen bonds.

To understand the fundamental mechanism behind acid dissolution,

Zhang et al. from the Institute for Chemical Research at Kyoto University encapsulated HF, as well as $\text{HF}\cdot\text{H}_2\text{O}$ and H_2O within a C_{70} fullerene. They found that in order to force the molecules into the open fullerene cavity, the molecules required "pushing from the outside" using [high pressure](#) conditions, and "pulling from the inside" via molecular interactions between HF and H_2O . They were able to identify how hydrogen bonding occurred between these two molecules. Their work appears in *Science Advances*.

Prior work by Zhang et al. showed that the C_{70} fullerene could be opened in a three-step process that involved the addition of a pyridazine derivative either to the alpha or beta bonds on the C_{70} . This created a 13-member ring opening that formed slightly different compounds, denoted by α -13mem and β -13mem. Dehydration of both compounds resulted in a 16-member ring opening. The ring could be closed again via hydrolysis and a two-step process.

β -16mem was large enough to capture H_2O , but α -16mem was not. Given these results from previous studies, for the current study, Zhang et al. used α -16mem to try to encapsulate HF. Instead, they found three different possibilities within the fullerenes: $\text{HF}@C_{70}$, $(\text{HF}\cdot\text{H}_2\text{O})@C_{70}$, and $\text{H}_2\text{O}@C_{70}$.

Their reaction conditions required high pressure (9000 atm) to "push" the guest molecule into the α -16mem cavity. Time-dependent studies showed that HF filled the cavity first, followed by $\text{H}_2\text{O}\cdot\text{HF}$, and then H_2O . Notably, the open cage did not entrap H_2O when HF was not present, indicating that the interaction between H_2O and HF prompted H_2O encapsulation. Further studies showed that HF is "pulling" H_2O into the cavity while the high pressure environment "pushes" it into the cavity.

This process allowed the authors to study the interaction between H_2O

and HF within a confined environment using ^1H NMR. NMR analysis showed that the $(\text{H}_2\text{O}\cdot\text{HF})@\text{C}_{70}$ was down-shifted from $\text{H}_2\text{O}@\text{C}_{70}$ and $\text{HF}@\text{C}_{70}$, which indicated hydrogen bonding. Furthermore, shift and coupling values indicated that oxygen was acting as the hydrogen-bond acceptor.

Using single-crystal x-ray diffraction, Zhang et al. demonstrated the structure of the $(\text{HF}\cdot\text{H}_2\text{O})@\text{C}_{70}$, and report the first x-ray structure for doubly encapsulated C_{70} . These analyses and experimental studies confirmed that the H^+ ion in HF forms a linear hydrogen bond with the O in H_2O . Additionally, compared to theoretical calculations of free H_2O and HF, the studies of the encapsulated [molecules](#) revealed close contact with hydrogen and oxygen that may be characteristic of $\text{H}_3\text{O}^+\cdot\text{F}^-$.

The C_{70} fullerene derivative provides an excellent nanoenvironment for studying isolated chemical species, something that has not been available to chemists in the past. This isolated environment allowed the authors to investigate the interactions of two compounds without interference from the surrounding environment and provided important insights into a ubiquitous chemical process.

More information: Rui Zhang et al. Isolation of the simplest hydrated acid, *Science Advances* (2017). [DOI: 10.1126/sciadv.1602833](https://doi.org/10.1126/sciadv.1602833)

Abstract

Dissociation of an acid molecule in aqueous media is one of the most fundamental solvation processes but its details remain poorly understood at the distinct molecular level. Conducting high-pressure treatments of an open-cage fullerene C_{70} derivative with hydrogen fluoride (HF) in the presence of H_2O , we achieved an unprecedented encapsulation of $\text{H}_2\text{O}\cdot\text{HF}$ and H_2O . Restoration of the opening yielded the endohedral C_{70} s, that is, $(\text{H}_2\text{O}\cdot\text{HF})@\text{C}_{70}$, $\text{H}_2\text{O}@\text{C}_{70}$, and $\text{HF}@\text{C}_{70}$ in

macroscopic scales. Putting an H₂O·HF complex into the fullerene cage was a crucial step, and it would proceed by the synergistic effects of "pushing from outside" and "pulling from inside." The structure of the H₂O·HF was unambiguously determined by single crystal x-ray diffraction analysis. The nuclear magnetic resonance measurements revealed the formation of a hydrogen bond between the H₂O and HF molecules without proton transfer even at 140°C.

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