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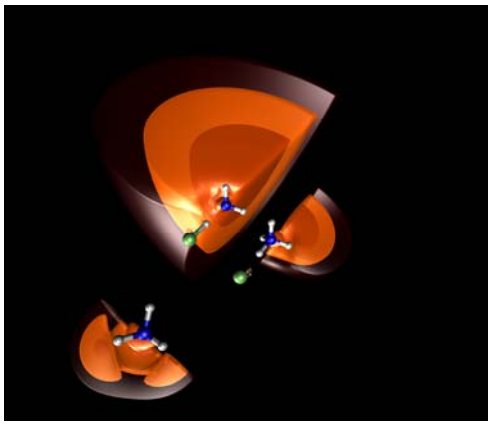
EMSL In Brief
Environmental Molecular Sciences Laboratory

All Alone, Ammonia and Hydrogen Chloride Use Negativity to Get Attached

Electrons spur the chemical reaction between hydrochloric acid and ammonia, users from the Department of Energy's Environmental Molecular Sciences Laboratory announced in a February 2008 cover article in *Science*. The findings may help scientists precisely control the chemistry in systems contained in hydrogen-powered cars.



An extra electron helps NH_3 bump up to an HCl (top middle) and pull the hydrogen from its chloride. This creates an electron-adorned ammonium chloride, an ionic salt (bottom right). The extra electron may find its way, temporarily, into the ammonium molecule (bottom left), forming a Rydberg radical. Credit: Maciej Haranczyk

The team of experimental and theoretical chemists from Johns Hopkins University, Heriot-Watt, University, and Pacific Northwest National Laboratory investigated how HCl and NH_3 react to form ammonium, NH_4^+, and chloride, Cl^- , ions without help from their surroundings. The result revealed that supplying or removing an extra electron—not one already residing in the molecules—can make the reaction go from acid and base to neutral molecule or back again.

Previous research has shown that when one ammonia molecule and one hydrogen chloride molecule are placed together, nothing happens. Researchers have long suspected additional electrons in the environment could aid the reaction.

To test the idea, the team conducted the reaction in reverse. First, they created a molecule of ammonium chloride adorned with an extra electron, representing an environmental electron. Using a beam of light, they then measured how easily different colors of light knocked off that electron. Losing the electron leaves behind an off-kilter $NH_4^+Cl^-$, which immediately rearranges into NH_3 and HCl.

With the data, electronic structure calculations were performed using EMSL computational resources. This let the team gauged the distance between chloride's hydrogen and ammonia's nitrogen when the extra electron is around. The results showed how losing the surplus electron can cause ammonia and hydrogen chloride to transform into ammonium chloride. Understanding the reaction brings hope that chemistry will have a clean future.

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