Researchers use neutrons to spy on the elusive hydronium ion

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A Los Alamos National Laboratory research team has harnessed neutrons to view for the first time the critical role that an elusive molecule plays in certain biological reactions. The effort could aid in treatment of peptic ulcers or acid reflux disease, or allow for more efficient conversion of woody waste into transportation fuels.

In a paper appearing this week in Angewandte Chemie International Edition, Los Alamos researchers join an international team in describing the role played by the elusive hydronium ion in the transfer of protons during enzyme-catalyzed reactions.

Prior to this research, no one has ever directly witnessed the role of the hydronium ion, a water molecule bound to an additional hydrogen ion, in macromolecular catalysts—the catalytic mechanisms of enzymes.

Researchers took an interest in an enzyme that has the potential to allow conversion of sugars in woody biomass into alcohol, a potential alternative fuel, because the enzyme loses its effectiveness when the pH value of the milieu is lowered—a common occurrence in the interior of industrial yeast cells fermenting alcohol. As it turns out, this biochemical reaction also has ramifications for the activation of proton pumps in the stomach, which produces excess acid in those afflicted by gastric diseases.

The scientists sought to figure out the mechanism behind these reactions. Neutrons from the Los Alamos Neutron Science Center provided a

possible tool for unveiling the secret agent at the heart of the chemistry.

Hydronium ions had not been seen before by researchers who attempted to use X-rays to understand the chemical mechanism of enzymes. This is because tiny hydrogen atoms are essentially invisible under X-rays. To help make things visible, the researchers substituted hydrogen in their enzyme samples with deuterium, an isotope of hydrogen that behaves chemically identical to its nonisotopic counterpart. Deuterium yields a clear signal when bombarded with neutrons. Therefore, neutrons provided a perfect method for uncloaking the elusive hydronium ions, which appeared as a pyramid-shaped mass in the enzyme's active site where the chemical reaction occurs.

The researchers discovered a crucial change as the system they were studying fell into the acidic range of the pH scale (below 6). The hydronium ion that could be seen facilitating the binding of a metal ion cofactor crucial to the conversion of the sugar molecule into its fermentable form suddenly became dehydrated—think of water, H_2O, being removed from hydronium, H_3O+. The space occupied by the relatively large hydronium ion collapsed into a tiny volume occupied by the remaining proton (a positively charged hydrogen ion, H+). This spatial change in the molecular structure prevented the sugar from being attacked by the enzyme.

The observed phenomenon provided an answer about why pH plays such an important role in the process and renders the enzyme inactive under acidic conditions. More important, it definitively illustrated that the hydronium ion plays a key role in the transport of protons in these types of biochemical systems.

"This is something that has never been seen before," said Los Alamos researcher Andrey Kovalevsky, principal author of the paper. "This proves that hydronium is the active chemical agent in our studies of the

catalytic mechanism of enzymes."

The research has broad implications for the possible role of hydronium ions in other biological systems. In addition to acid reflux disease, the research may help provide a better understanding of metabolic transfer of energy in living cells or living organisms.

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