Scientists develop a unique approach for splitting water into hydrogen and oxygen

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The design of efficient systems for splitting water into hydrogen and oxygen, driven by sunlight is among the most important challenges facing science today, underpinning the long term potential of hydrogen as a clean, sustainable fuel. But man-made systems that exist today are very inefficient and often require additional use of sacrificial chemical agents. In this context, it is important to establish new mechanisms by which water splitting can take place.

Now, a unique approach developed by Prof. David Milstein and colleagues of the Weizmann Institute's Organic Chemistry Department, provides important steps in overcoming this challenge. During this work, the team demonstrated a new mode of bond generation between oxygen atoms and even defined the mechanism by which it takes place. In fact, it is the generation of oxygen gas by the formation of a bond between two oxygen atoms originating from water molecules that proves to be the bottleneck in the water splitting process. Their results have recently been published in *Science*.

Nature, by taking a different path, has evolved a very efficient process: photosynthesis - carried out by plants - the source of all oxygen on Earth. Although there has been significant progress towards the understanding of photosynthesis, just how this system functions remains unclear; vast worldwide efforts have been devoted to the development of artificial photosynthetic systems based on metal complexes that serve as catalysts, with little success. (A catalyst is a substance that is able to increase the rate of a chemical reaction without getting used up.)

The new approach that the Weizmann team has recently devised is divided into a sequence of reactions, which leads to the liberation of hydrogen and oxygen in consecutive thermal- and light-driven steps, mediated by a unique ingredient - a special metal complex that Milstein's team designed in previous studies. Moreover, the one that they designed - a metal complex of the element ruthenium - is a 'smart' complex in which the metal center and the organic part attached to it cooperate in the cleavage of the water molecule.

The team found that upon mixing this complex with water the bonds between the hydrogen and oxygen atoms break, with one hydrogen atom ending up binding to its organic part, while the remaining hydrogen and oxygen atoms (OH group) bind to its metal center.

This modified version of the complex provides the basis for the next stage of the process: the 'heat stage.' When the water solution is heated to 100?C hydrogen gas is released from the complex - a potential source of clean fuel - and another OH group is added to the metal center.

'But the most interesting part is the third 'light stage,'' says Milstein. 'When we exposed this third complex to light at room temperature, not only was oxygen gas produced, but the metal complex also reverted back to its original state, which could be recycled for use in further reactions.'

These results are even more remarkable considering that the generation of a bond between two oxygen atoms promoted by a man-made metal complex is a very rare event, and it has been unclear how it can take place. Yet Milstein and his team have also succeeded in identifying an unprecedented mechanism for such a process. Additional experiments have indicated that during the third stage, light provides the energy required to cause the two OH groups to get together to form hydrogen peroxide (H_2O_2), which quickly breaks up into oxygen and water. 'Because hydrogen peroxide is considered a relatively unstable molecule, scientists have always disregarded this step, deeming it implausible; but we have shown otherwise,' says Milstein. Moreover, the team has provided evidence showing that the bond between the two oxygen atoms is generated within a single molecule - not between oxygen atoms residing on separate molecules, as commonly believed - and it comes from a single metal center.

Discovery of an efficient artificial catalyst for the sunlight-driven splitting of water into oxygen and hydrogen is a major goal of renewable clean energy research. So far, Milstein's team has demonstrated a mechanism for the formation of hydrogen and oxygen from water, without the need for sacrificial chemical agents, through individual steps, using light. For their next study, they plan to combine these stages to create an efficient catalytic system, bringing those in the field of alternative energy an important step closer to realizing this goal.

Source: Weizmann Institute of Science (news : web)

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