Chemists uncover new role of a key base in organic synthesis

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An international team of chemists has discovered a new piece to the puzzle of how a powerful base used in organic synthesis, cesium carbonate, plays a pivotal role during a catalytic reaction.

The research, published by the *Journal of the American Chemical Society*, was led by Jamal Musaev, a theoretical chemist at Emory University, and Ken Itami, an experimental chemist from Nagoya University in Japan. Sun Yat-Sen University in Guangzhou, China, also contributed to the findings.

Many organic chemistry reactions are acid/base reactions, involving the exchange of positively charged hydrogen atoms. Acids donate the positively charged hydrogen and bases accept it.

The current research focused on the use of cesium carbonate as a base. Cesium carbonate has recently been observed to accelerate a particular class of catalytic reactions, a phenomenon termed the "cesium effect."

The use of cesium carbonate base and carboxylic acids co-catalysts have been shown to be critical in a number of recent carbon-hydrogen (C-H) bond functionalization reactions. The full story behind the impact of this base was previously not clear. It was known that the cesium base removed hydrogen protons, or scavenged acidic acid, from the solution, and was also involved in the exchange of ligands during a reaction, but these two factors did not explain the acceleration seen.

This recent work offers a new explanation. The researchers found that cesium base can generate an aggregate state: The molecules come together creating a cluster that is actually the starting point for the catalytic reaction, and not the discreet carboxylic acids and carbonate complexes as was previously thought.

"One-by-one, we are identifying key components of catalytic reactions and then putting them all together," Musaev says. "It's difficult work, but important, because the more your understand the reaction the better you can predict ways to modify it and control it."

The findings about how the base acts in these reactions has the potential to impact the development of not just new C-H functionalization reactions, but the way that catalytic reactions in general are considered.

Provided by Emory University

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