Pieces of Catalyst Puzzle Explained

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Catalysts speed up chemical reactions, as in your car's catalytic converter, and they even double as clichés, as in "catalyst for change," but how they work remains a mystery.

Enzymes — proteins that catalyze biological reactions — may be the least understood.

A popular explanation among chemists and biologists is the "strain hypothesis," which proposes that an enzyme molecule stretches the reacting bond like a spring, eventually breaking it.

Arieh Warshel, professor of chemistry in USC College, is a leading advocate of an alternate theory that could have wide implications.

Based on computer simulations, Warshel believes that enzyme catalysis relies on electrostatic energy to help sever chemical bonds.

His latest study, published last month in the *Proceedings of the National Academy of Sciences Early Edition*, proposes an electrostatic mechanism for catalysis of reactions in vitamin B12 enzymes.

Until this study, B12 enzymes represented what Warshel calls "the last bastion" for the strain hypothesis.

"B12 enzymes have been originally assumed to present what is perhaps the best support for the popular idea that strain energy contributes in a major way to enzyme catalysis," Warshel wrote in PNAS.

“To some people it was just a puzzle,” he said. “To me it was a major problem” that challenged Warshel’s own theory.

Warshel said he solved the problem by showing that B12 enzymes employ a “trick” that enables them to harness electrostatic energy.

He called this “a completely general approach” that could lead to new catalyst formulations for research or industry.

“The trick used by B12 enzymes may, in fact, be a very powerful new strategy in enzyme design,” he wrote.

The trick is a variation on the theory that Warshel previously proposed.

All reactions have an activation barrier, analogous to the resistance one feels when pulling apart two magnets. Catalysts lower the activation barrier dramatically.

They do this, according to Warshel’s computer models, by placing a negative charge on the positive end of a chemical bond, and a positive on the negative end.

The resulting electrostatic attraction between the enzyme and the two ends of the bond helps to overcome the force of the bond itself.

In B12 enzymes, the key bond between the two parts of the reacting molecule breaks in such a way that neither of the bonded atoms is electrically charged. That would appear to rule out an electrostatic intervention by the enzyme.

But Warshel showed that in B12 there is an additional partially charged group attached to one of the key bonded atoms. When the bond stretches, the partially charged group comes closer to an oppositely charged area elsewhere in the B12 enzyme.

The electrostatic force between the two charges then helps to cleave the bond.

The finding could have implications for research into biological processes, Warshel said, since “everything that happens in your body, everything, is catalyzed by enzymes.”

In particular, this is important for the understanding of so-called “radical reactions” when the bonded atoms are not charged.

The other authors on the study are Warshel’s graduate students Pankaz Sharma, Zhen Chu and Mats Olsson.

Source: USC College

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