Clean 3-way split observed

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In chemistry as in life, threesomes are not known to break up neatly. And while open-minded thinkers have insisted that clean three-way splits do happen, nobody had actually witnessed one – until now.

A paper in the Aug. 8 issue of *Science* provides the first hard evidence for the simultaneous break-up of a molecule into three equal parts.

Previous studies of so-called "concerted break-ups" had only suggested their existence, said co-author Anna Krylov, a theoretical chemist at the University of Southern California.

"The experiments by our collaborators (at the University of California, San Diego) demonstrated that this mechanism is present, and our theory explained why and how it happens," she said.

The breakthrough matters for two reasons. Concerted reactions have long been thought to play an important role in organic chemistry, and Krylov's theoretical model offers a framework for better understanding and perhaps manipulating such reactions.

In addition, important phenomena in the atmosphere and in combustion involve three-body reactions. Ozone forms when three molecules come together at exactly the same time – an event no different in theory from a simultaneous split.

Such events are relatively rare: Theory and experiment agree that in most cases a threesome will fall apart in steps, with one bond breaking before the next.

"Why would it happen simultaneously?" Krylov asked rhetorically.

But she and graduate student Vadim Mozhayskiy showed that if the electrons of the sym-triazine molecule are energized in a particular way, the whole flies apart into three identical and equally energetic parts.

Unraveling the mechanism has become possible only through the combined efforts of theoreticians and experimentalists.

Co-author Robert Continetti and his team at UCSD used electrical charges to energize molecules of sym-triazine to their breaking point. By separating the molecules in time and space, the researchers were able to identify the products from individual molecular events.

In some cases, the three parts from a single molecule had exactly the same energy and reached detectors at the same time, indicating that a simultaneous three-way split had occurred.

Even with this discovery, three-body reactions remain largely mysterious, Krylov said.

"The gap in understanding of single-bond and multiple-bond breaking processes is just incredible."

Krylov hopes to promote further work in the field through her iOpenShell Center, a USC-based institute supported by the National Science Foundation and created to foster collaborations between theoretical and experimental chemists.

"The center provides a framework for these interactions," she said.

Source: University of Southern California