

Halogenated Hydrocarbons

Tarnovsky team leverages lasers to control chemical reactions

A research team at Bowling Green State University has been employing Ohio Supercomputer Center systems to better understand the photochemistry of halogenated hydrocarbons.

Their study will contribute to a general understanding of solvent environmental effects on chemical reactions and, perhaps, to the ability to control chemical reaction pathways using ultrafast laser techniques.

"The core of photochemistry is molecular dynamics in excited electronic states," said Alexander N. Tarnovsky, Ph.D., the leader of the research team, an associate professor of chemistry at Bowling Green and a member of the university's Center for Photochemical Sciences. "Understanding electronic and structural changes throughout the course of a photo-induced process in the liquid phase, where the most chemistry occurs, is of fundamental and practical importance."

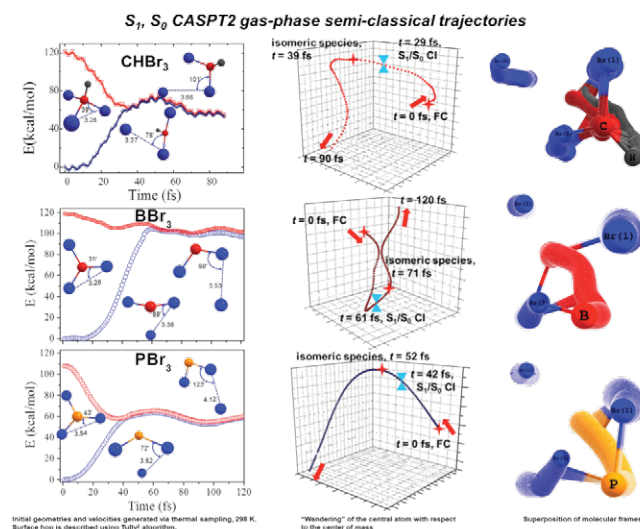
Polyhalogenated alkanes are compounds with more than one halogen atom that replaces a hydrogen atom attached to the carbon in a hydrocarbon chain. These substances have characteristic physical and chemical properties unique to them, such as their ability to act as solvents able to nonpolar and slightly polar substances.

Apart from their importance to photosynthetic and environmental chemistry, polyhalogenated alkanes also serve well as model systems because of their relatively simple structure (five atoms at minimum) and easily altered carbon-halogen bonds. Their short-lived intermediates and photoproducts are detectable by several established time-resolved experimental methods, such as the ultrafast pump-probe methods used throughout this project. And, in a practical sense, several of these molecules are considered to be important sources of reactive halogens in the atmosphere, playing a role in ozone-depletion in the troposphere.

Tarnovsky's group leverages OSC's Oakley Cluster to generate calculations with an assortment of scientific applications, including Guassian, NAMD, Amber, Q-Chem and Molcas 07. Their results aid in explaining the team's ultrafast femtosecond pump-probe spectroscopy

experiments, where the system response to excitation pulsed light ("the pump") is studied by examining the absorption/amplification of a monitoring pulse ("the probe") delayed in time from the initiating "pump" pulse.

"Small polyatomic solutes have density of states non-prohibitive for the tools of high-level computational photochemistry and detailed ultrafast time-resolved experimental studies," said Tarnovsky. "Gaining the atomic-level understanding of the photochemical reaction dynamics in these systems can be essential, per se, but it also provides the basis for a deeper understanding of photochemical reactions in more complex systems in condensed-phase environments." •



► Above: As a part of its study of halogenated hydrocarbons, members of the Tarnovsky group performed electronic structure calculations for phosphorus tribromide and boron tribromide.

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Research Title: Tracing ultrafast photoinduced rearrangement and energy flow in polyatomic molecules in solution

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