

The 'missing link' in conducting molecules, butadiene—solved

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Linear polyenes are hydrocarbon chains with unusual optical and electrical properties. They have become a paradigm for studying photoisomerization—when molecular structures rearrange from absorbing light—because of their straightforward molecular structure, potential for electrical conductivity, and role in vision. Understanding how these molecules simultaneously rearrange through photoisomerization could advance materials science research by enabling artificial vision and producing wires from plastic, and new photovoltaic technologies.

Trans 1,3-butadiene, the smallest polyene, has challenged researchers over the past 40 years because of its complex excited-state electronic structure and its ultrafast (femtosecond, 10^{-15} s) dynamics. Butadiene remains the "missing link" between ethylene (C₂H₄,), which has only one double bond, and longer linear polyenes with three or more double bonds.

Now, an experimental team headed by Albert Stolow at the University of Ottawa and the National Research Council of Canada has solved trans 1,3-butadiene's electronic-structural dynamics. The researchers recently reported their findings in *The Journal of Chemical Physics*.

Stolow's group developed an ultrafast laser spectroscopy called timeresolved photoelectron-photoion coincidence spectroscopy (TRPEPICO) to conduct this research. The method involves a femtosecond pumpprobe process wherein an emitted photoelectron is measured as a



function of time. The photoelectron spectrum and angular distribution is sensitive to the electronic and structural dynamics of molecules. Over the past 20 years, Stolow has applied his method to a broad range of problems, including the ultraviolet stability of DNA bases and intramolecular proton transfer.

"We've shown over many years that our approach works and have provided lots of examples," Stolow said. He previously studied under John C. Polanyi and Yuan T. Lee, two Nobel Prize winners who researched molecular collision dynamics.

"Many of us thought that if we could understand ethylene, the basic building block, we would be able to understand the longer linear polyenes," Stolow said. "But butadiene is the 'missing link.' It didn't seem to behave like either case."

Stolow's team discovered that trans 1,3-butadiene behaves, simultaneously, like both ethylene and longer polyenes. Specifically, there is an ultrafast competition between ethylenelike dynamics and polyenelike dynamics.

The research team's experimental results were independently modeled and confirmed computationally by Todd J. Martínez's research team. Martinez is a researcher and professor of chemistry at Stanford University, who specializes in molecular quantum dynamics. Michael S. Schuurman of the NRC, a theorist specializing in quantum dynamics, also helped confirm this work.

"This collaboration is key. We each independently came up with the same results," Stolow said. "Dramatic technical advances in both experiment and theory have allowed us to finally solve the long-standing puzzle of electronic dynamics in butadiene, the 'missing link' of polyene photophysics."



More information: "Excited state non-adiabatic dynamics of the smallest polyene - trans 1,3-Butadiene. 1. time-resolved photoelectron-photoion coincidence spectroscopy," *Journal of Chemical Physics* (2018). DOI: 10.1116/1.5016452

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