Ultrafast Molecular Dynamics of 2-Bromothiophene

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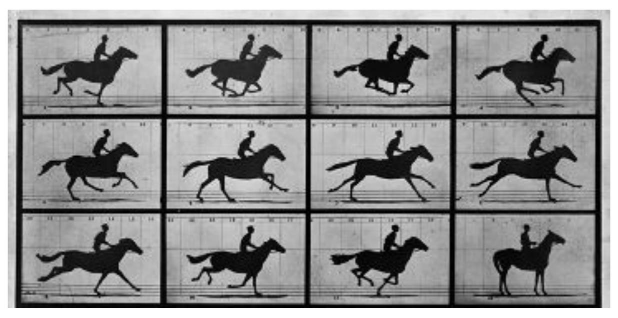
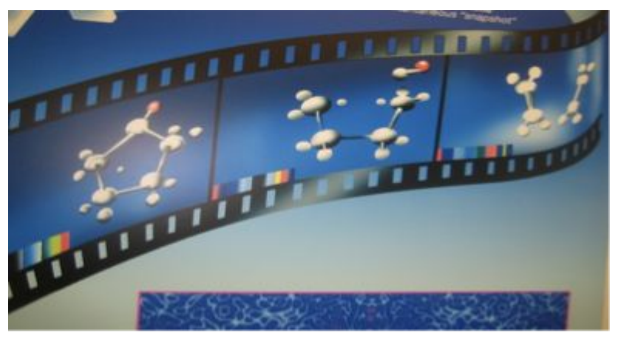
Introduction

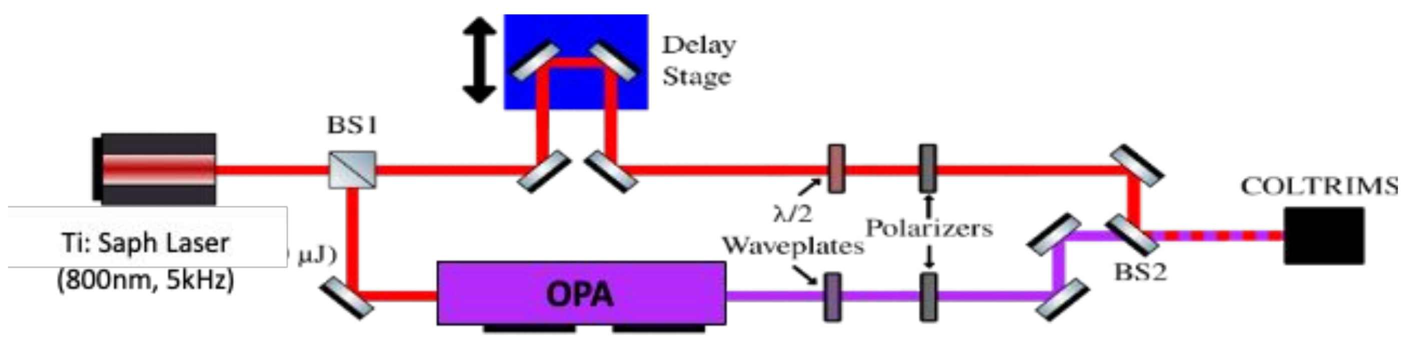
Ultrafast molecular dynamics can be likened to creating a movie at the molecular level. To make a conventional movie, individual frames are captured quickly enough to be seamlessly combined, allowing smooth depiction of movement. Similarly, to visualize ultrafast molecular dynamics, such as those in 2-bromothiophene, we must capture images at the molecular timescale—taking snapshots faster than the molecules rotate, which occurs on the order of 10^-12 seconds, and faster than they bend or stretch, which happens on the order of 10^-15 seconds. This enables us to observe the swift, intricate movements within molecular structures.





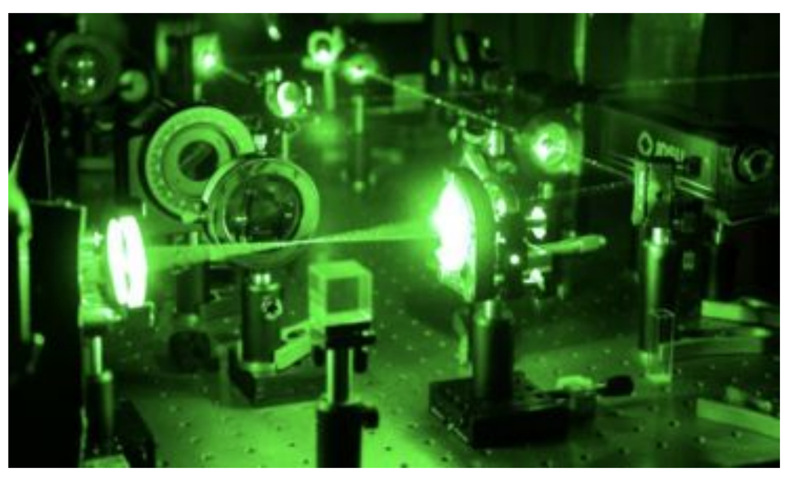
Experimental Setup

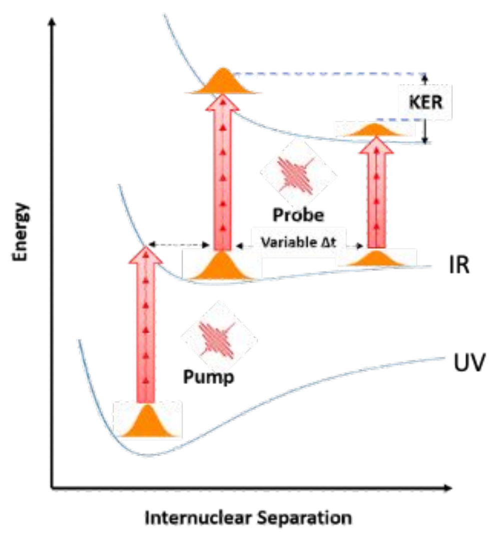
To achieve the ability to track 2-bromothiophene molecular dynamics, a specific experimental set-up is required. An ultrafast table top laser that enables pump probe spectroscopy as well as a COLd Target Recoil-Ion Momentum Spectroscopy (COLTRIMS) apparatus utilizing coincident coulomb explosion imaging was used.



Pump-Probe Spectroscopy

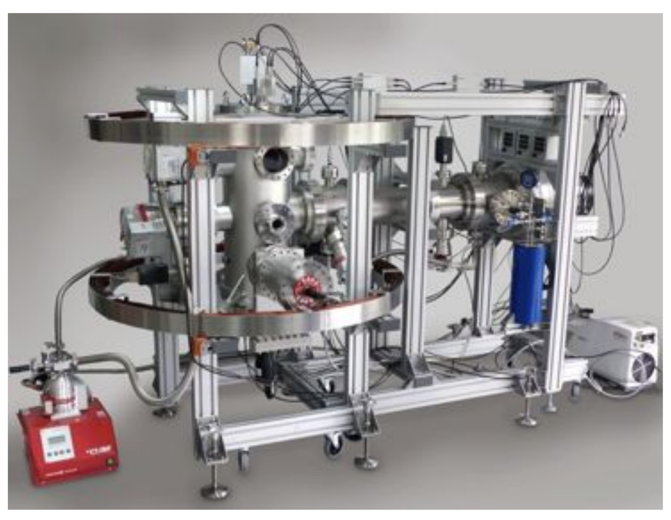
Pump-probe spectroscopy is an advanced technique that uses a pair of laser pulses to explore dynamic processes within molecules or materials. The first laser pulse (the "pump") excites the system to a higher energy state, and a subsequent laser pulse (the "probe") interrogates the system after a precise delay. By varying this delay, the technique captures and measures fast reactions and changes, offering a detailed, time-resolved view of molecular dynamics and energy transfer processes as they unfold.

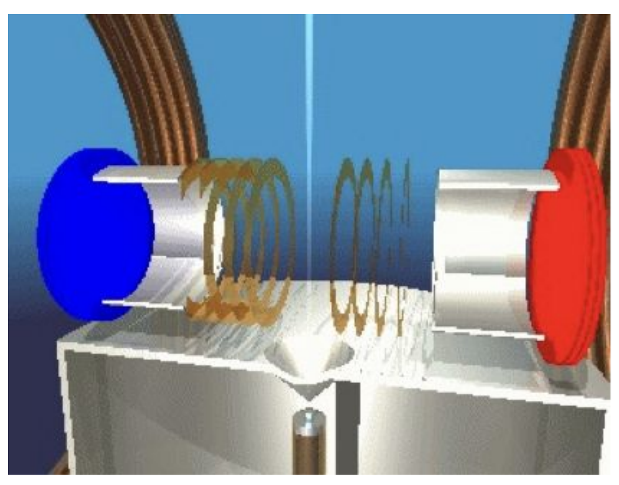




COLd Target Recoil-Ion Momentum Spectroscopy

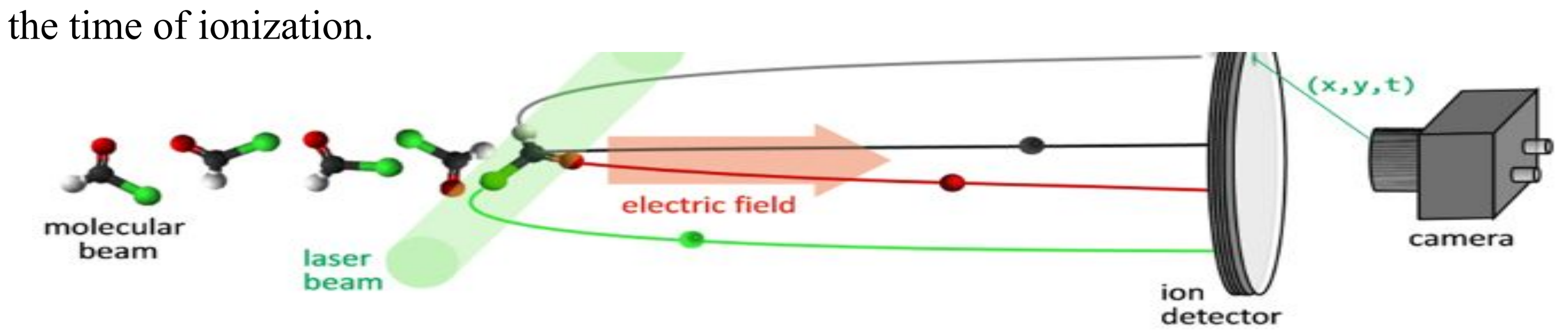
A COLTRIMS apparatus, or COLd Target Recoil-Ion Momentum Spectroscopy, is designed to precisely measure the momentum of ions and electrons ejected from atoms or molecules during ionization. It uses electric and magnetic fields to guide these particles to detectors, collecting two key pieces of information: the time of flight, which refers to how long it takes for the particles to reach the detector from the point of ionization, and the ion impact position, which is the exact location where the particles hit the detector. These measurements enable the accurate calculation of the particles' momentum, providing valuable insights into molecular dissociation and the fundamental processes of chemical and physical transformations.



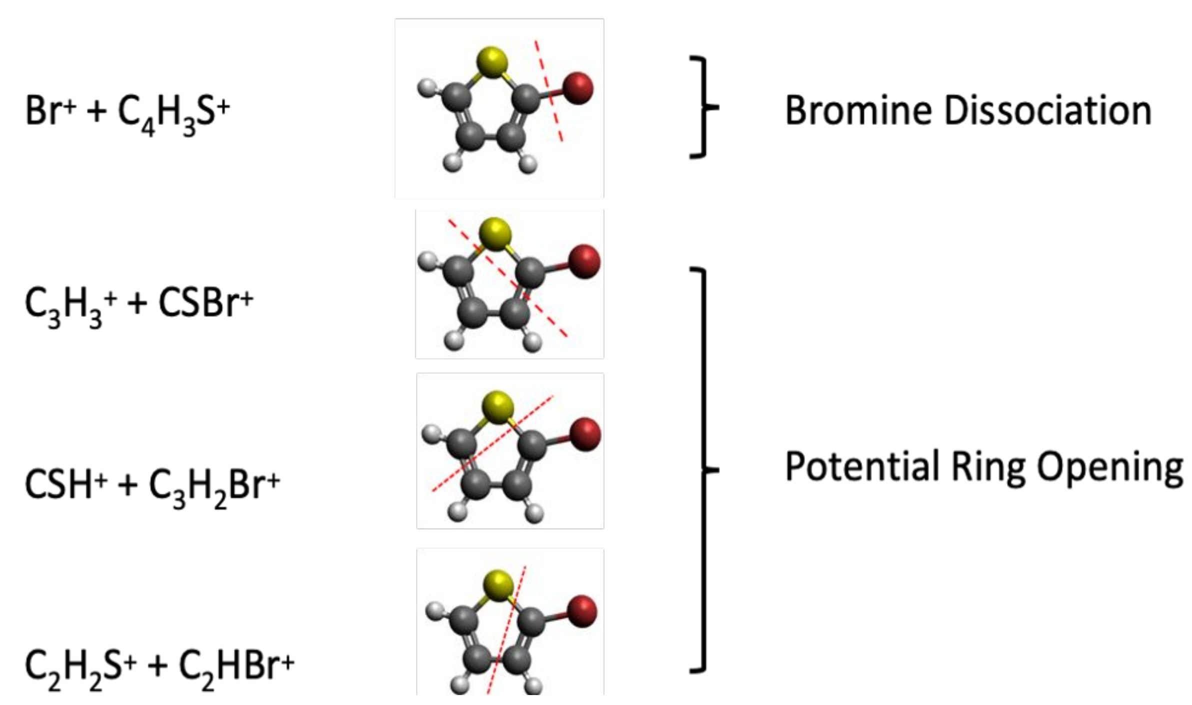


Coincident Coulomb Explosion Imaging

Coulomb explosion imaging is a technique used to study the structure and dynamics of molecules by inducing their disassembly through the Coulomb force, which arises when a molecule is ionized and its constituent charged particles repel each other. This process rapidly drives the particles apart, and by measuring the momentum of these fragments, scientists can reconstruct the original molecular structure and gain insights into the molecular dynamics at the time of ionization.

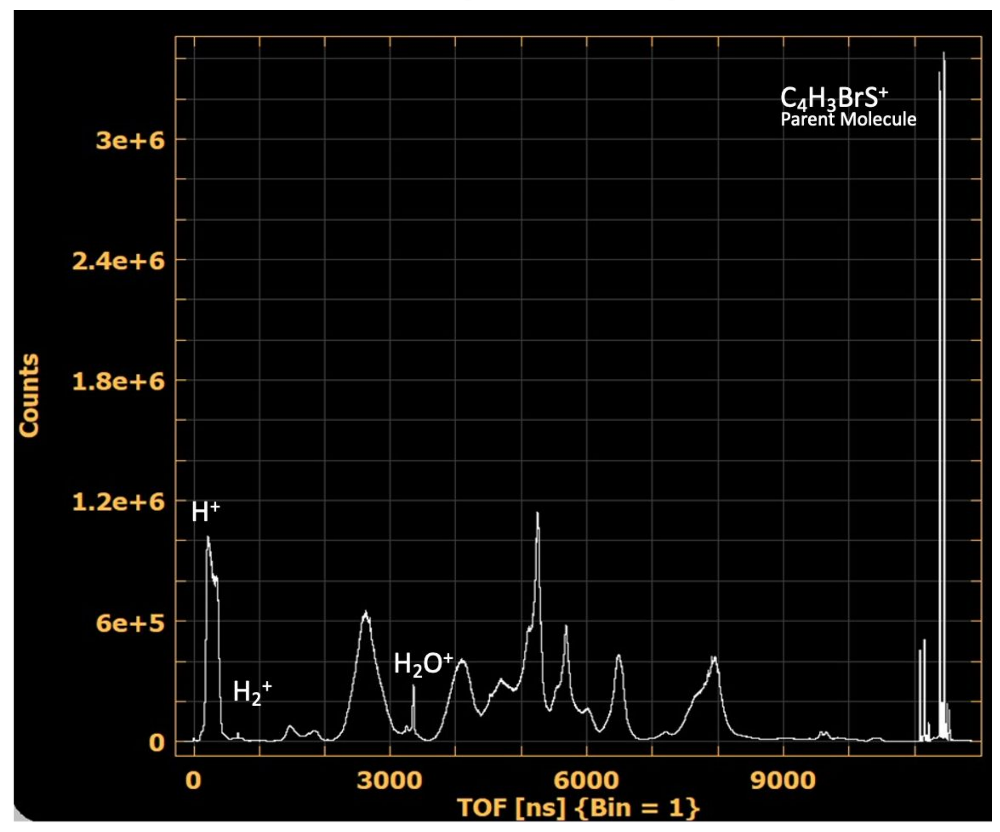


Two Body Coincidences



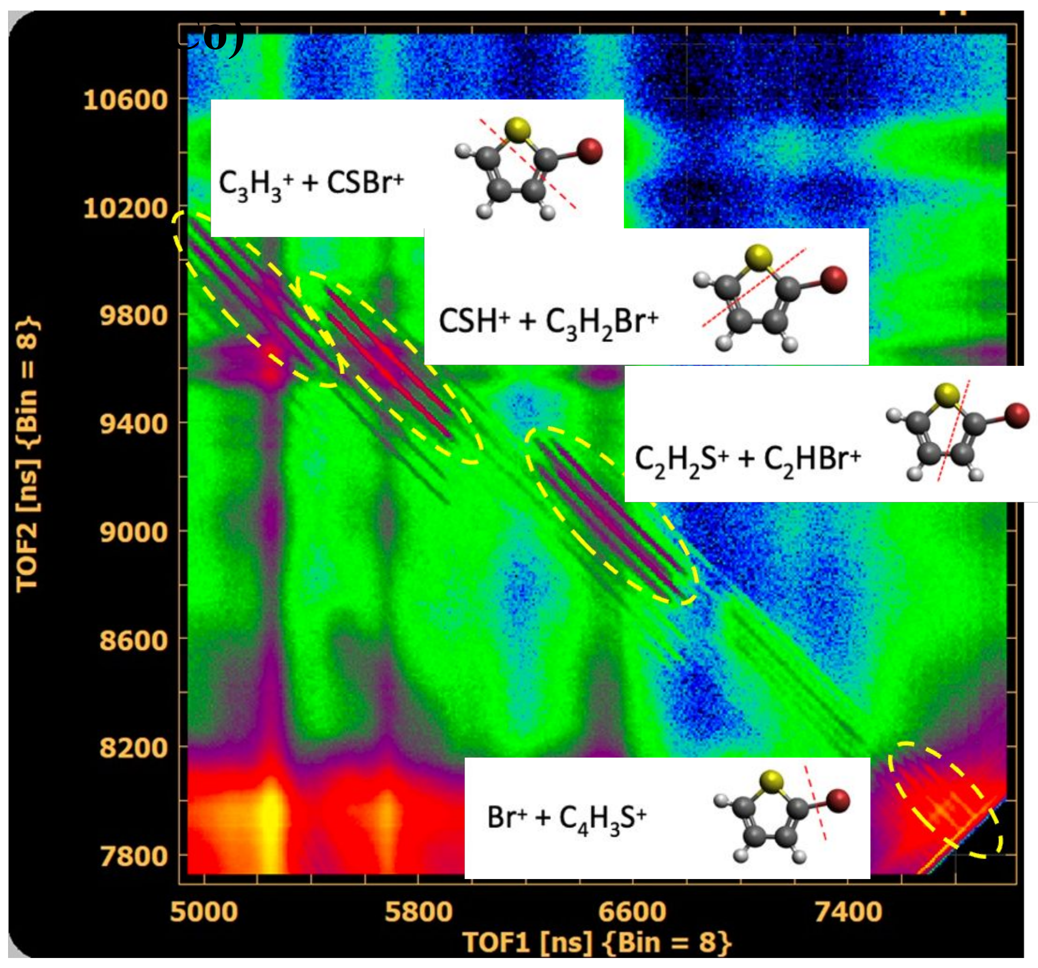
Here is the list of the two-body coincidences 2-bromothiophene undergoes during its ultrafast molecular dynamics. There are two main types of dynamics present, ring-opening and bromine dissociation

Time-of-Flight Histogram



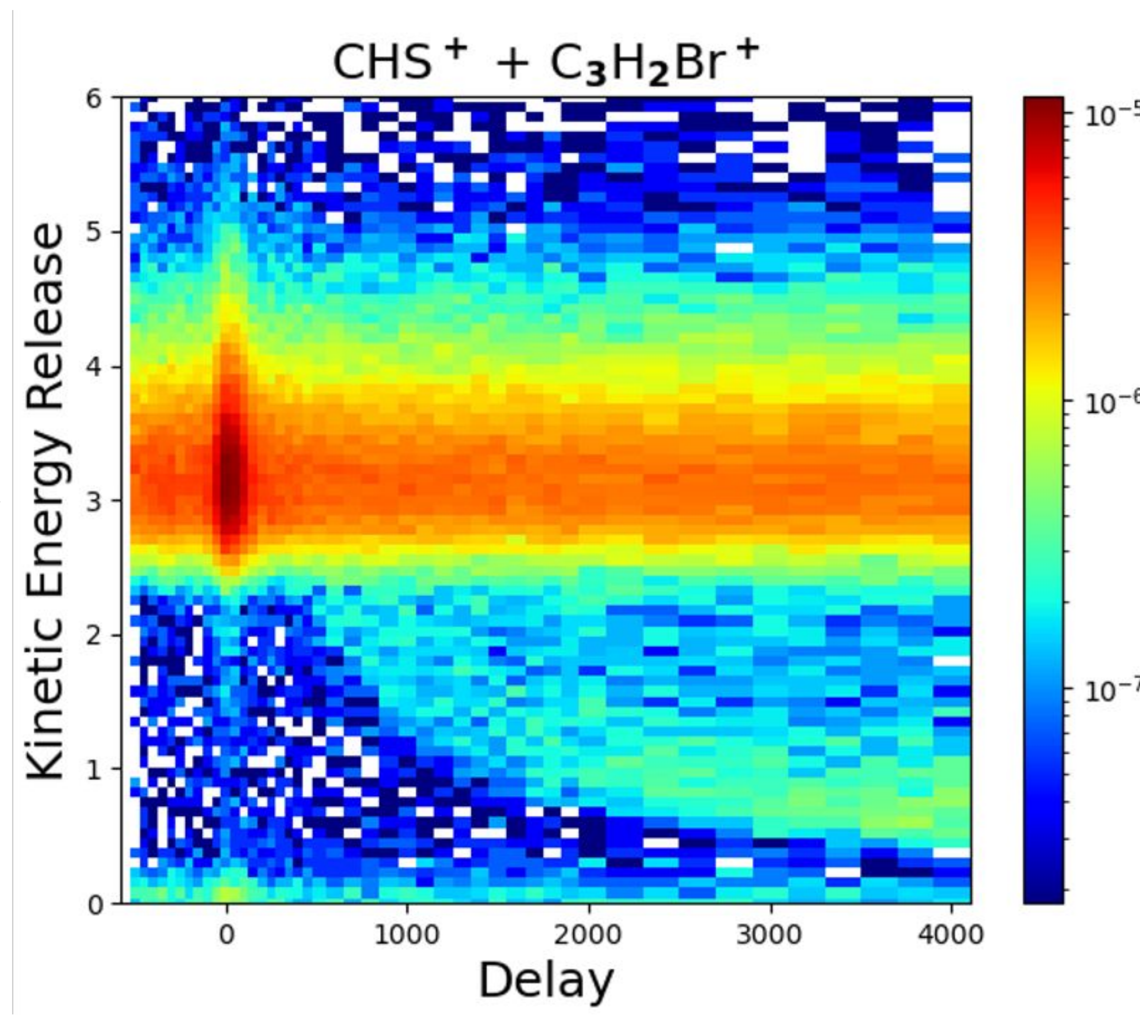
Histogram detailing the time is takes various particles to reach the detector after fragmentation

Photoion-Photoion Coincidence Map



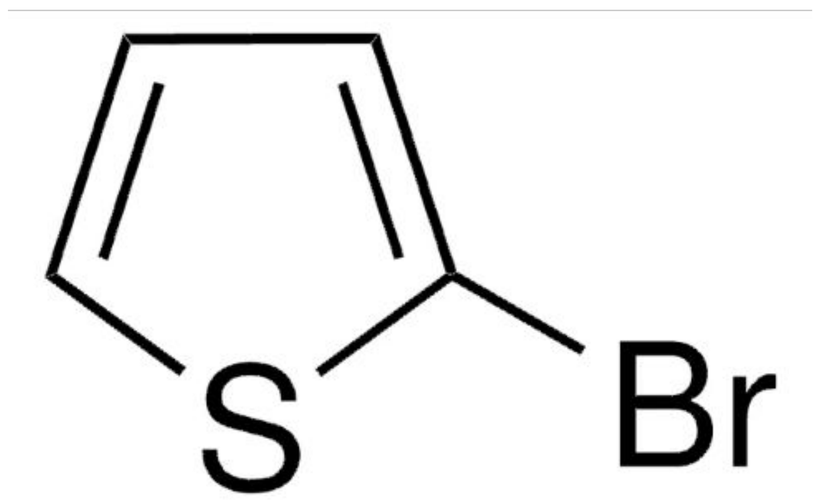
Angled lines = coincidence channels
Intense color = more prominent channel

Kinetic Energy Release Plot

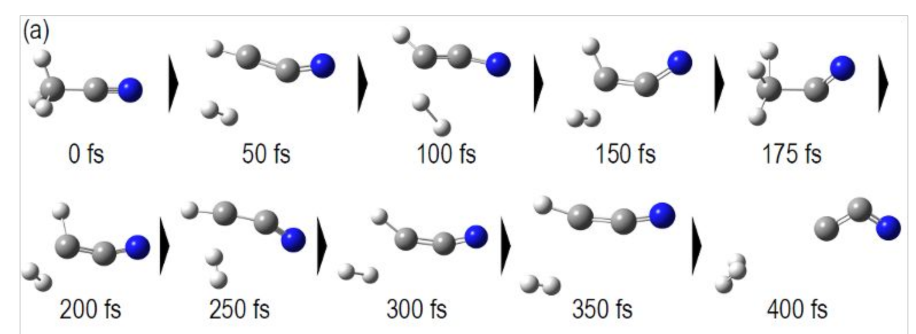


The curved wing of the plot indicates a variable about of energy being released during the fragmentation of 2-bromothiophene. This indicates that molecular dynamics are taking place.

2-Bromothiophene



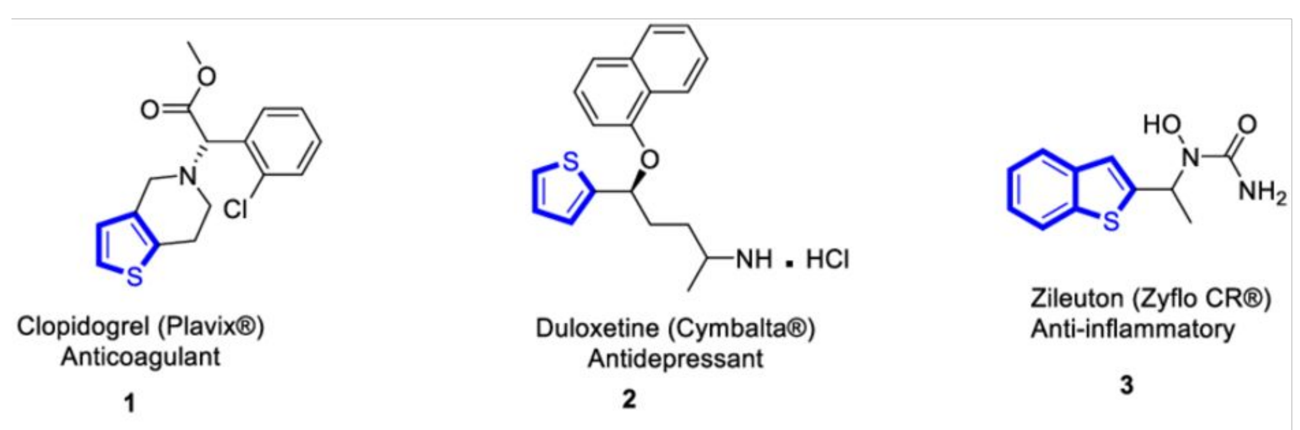
H_3^+ Migration in Acetonitrile (Dynamics every 50fs)



Example, from another experiment, of ultrafast molecular dynamics over time of H_3^+ migration

Why 2-Bromothiophene

Studying the ultrafast molecular dynamics of 2-bromothiophene is significant due to its relevance in various fields. As a ring-opening molecule, understanding its behavior under light exposure can lead to breakthroughs in creating more efficient organic semiconductors, which are critical for advancing OLED and OPV technologies. Thiophenes and their derivatives are pivotal in these devices for their conductive properties. Furthermore, insights gained from these studies can also influence drug design and biochemistry, where thiophene structures play a role in designing new pharmaceuticals, potentially leading to better medical treatments and therapeutic strategies.



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