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RPPR Final Report
as of 24-Apr-2019

Agency Code:

Proposal Number: 64598CH **Agreement Number: W911NF-14-1-0244**

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Report Date: 31-Aug-2018 Date Received: 07-Jan-2019
Final Report for Period Beginning 29-May-2014 and Ending 31-May-2018
Title: 7.1 Molecular Dynamics: Radical Reactions in the Decomposition of Geminal Di-Nitro Energetic Materials
Begin Performance Period: 29-May-2014 **End Performance Period:** 31-May-2018
Report Term: 0-Other
Submitted By: Laurie Butler Email: l-butler@uchicago.edu
Phone: (773) 702-7206
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 2 **STEM Participants:** 4

Major Goals: Radical intermediates are key players in chemical reaction mechanisms in synthetic chemistry, atmospheric chemistry, biological chemistry, and combustion. This work develops new methodology to detect and quantify radical intermediates, and to probe the elementary unimolecular reactions they undergo. The work also benchmarks new state-of-the-art electronic structure methods on open-shell systems.

Work beginning in the 1980's (Y. T. Lee, IRMPD of RDX) has sought to resolve the chemical mechanism of the decomposition of energetic materials. The new methods introduced in our work to probe the key radical intermediates along the energy release pathways should substantially contribute to the development of new energetic materials.

Accomplishments: The most important accomplishment was our Identification of the radical intermediates that lead to energy release in FOX-7. Indeed this work represent a paradigm shift in the study of the elementary decomposition mechanisms of energetic materials. Prior to this experiment focussed on the primary (first one or two) steps in the decomposition mechanism because the subsequent steps were extraordinarily difficult to characterize. Following our earlier experimental work on di-nitro energetic materials, we sought to computationally investigate the full decomposition pathways of FOX-7 to identify the portion of the decomposition mechanism that resulted in energy release (the primary steps typically require energy, they do not release energy). Our published work identifies the energy release mechanism for NO loss involving 3-member cyclic intermediates, rather than a nitro-nitrite isomerization, in particular the 1-amino-1-imino-2-nitro-2-ethyl and the 1,1-diamino,2-nitroethen-2-yl radical intermediates

The first of the two major experimental results was our crossed laser-molecular beam scattering study of the primary photodissociation channels of chloroacetaldehyde (CH2ClCHO) at 157 nm. We had used this precursor in the past to study the decomposition of the vinoxy radical intermediate to the two competing product channels H + ketene and methyl + CO, but the subsequent work in the ARO study revealed important complications. In addition to the C?Cl bond fission primary photodissociation channel, the ARO data evidenced two other photodissociation channels: HCl photoelimination and C?C bond fission. This is the first direct evidence of the C?C bond fission channel in chloroacetaldehyde, and we found that it significantly competes with the C?Cl bond fission channel. We determined the total primary photodissociation branching fractions for C?Cl fission : HCl elimination : C?C fission to be 0.65:0.07:0.28. The branching between the primary channels suggests the presence of interesting excited state dynamics in chloroacetaldehyde. Some of the vinoxy radicals from C?Cl photofission and most of the ketene cofragments formed in HCl photoelimination have enough internal energy to undergo secondary dissociation. While our previous velocity map imaging study on the photodissociation of chloroacetaldehyde at 157 nm focused on the barrier for the unimolecular dissociation of vinoxy to H + ketene, this work shows that the HCl elimination channel contributed to the high kinetic energy portion of the m/z = 42 signal in that study.

Our final experimental study continued our long term effort to establish quantitative photoionization cross sections for radical intermediates generated under collision-free conditions to allow unravelling the complicated decomposition channels of energetic materials. Our ARO experiment published in 2017 first identified the major dissociation channels of dichoromethane at 157 nm then determined the absolute photoionization cross section of the CH2Cl radical. The photoioinzation cross section allowed us to quantitatively determine the branching fraction to the newly identified C-C fission channel in chloroacetaldehyde producing HCO + CH2Cl.

Training Opportunities: Three Ph.D. students included ARO results in their dissertations, Ryan Booth, Preston Scrape and Jonathan Adams. Ryan Booth is now a researcher at Kirtland AFB, applying molecular beam methods he learned in my group to ionic liquids.

Results Dissemination: The results were reported in peer-reviewed journals, in international conferences, and in the ARO contractors meeting in Research Triangle Park, NC in August of 2017.

Honors and Awards: L. J. Butler was elected to the American Academy of Arts and Sciences in 2018.

Preston Scrape was awarded a NIST National Research Council Postdoctoral Research Associateship in 2017.

Protocol Activity Status:

Technology Transfer: Ryan Booth is now a researcher at Kirkland AFB.

PARTICIPANTS:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Chow-Shing Lam
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co-Investigator
Participant: Shih-Huang Lee
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co-Investigator
Participant: Shenshen Li
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

DISSERTATIONS:

Publication Type: Thesis or Dissertation
Institution: The University of Chicago
Date Received: 09-Feb-2017 Completion Date: 2/6/17 1:57PM
Title: Product Branching in the Photodissociation of Chloroacetaldehyde and the Incorporation of Angular Momentum in Statistical Predictions of Product Branching
Authors: Jonathan David Adams
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: The University of Chicago
Date Received: 31-Oct-2017 Completion Date: 7/21/17 8:04AM
Title: MOLECULAR BEAM EXPERIMENTS AND THEORETICAL STUDIES ON THE DYNAMICS AND PHOTOCHEMISTRY OF SEVERAL SMALL MOLECULES
Authors: Preston G. Scrape
Acknowledged Federal Support: **N**

Energetic Materials: Energy Release Pathways and Unstable Radical Intermediates

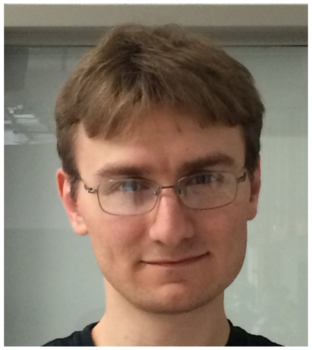
Laurie J. Butler, The University of Chicago

Ryan Booth, Ph.D. 2014

energy release in di-nitro compounds

Preston Scrape, Ph.D. 2017

Quantifying radical intermediates

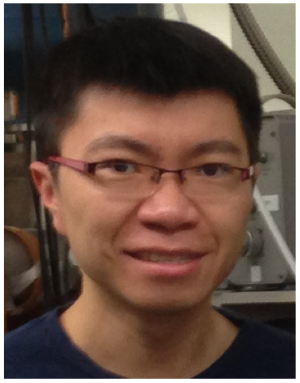


Jonathan Adams, Ph.D. 2017

developing photolytic precursors

Chow-Shing Lam, postdoc

vinoxy radical -> H + ketene



Radical Reactions in the Decomposition of Di-Nitro Energetic Materials

Laurie J. Butler, The University of Chicago

RESEARCH OBJECTIVE and CURRENT STATE-OF-THE-ART

Elucidate the energy release pathways in energetic materials

Tunable VUV photoionization detection of radical intermediates and their momentum-matched decomposition products allows one to resolve the complex decomposition pathways of energetic materials.

SCIENTIFIC OPPORTUNITY

- Due to their transient, reactive nature, radical intermediates have eluded detection and/or quantification.
- Developing new photolytic precursors for key radical intermediates and methods for the quantitative detection of radical intermediates facilitates studying their decomposition reactions.

TECHNICAL APPROACH:

- We use state-of-the-art experimental methods and high-level electronic structure theory. Our experiments include velocity map imaging and measurement of the velocities and angular distribution of radical intermediates and products in a crossed laser-molecular beam scattering apparatus. Tunable VUV photoionization at Taiwan's National Synchrotron Radiation Research Center probes radical intermediates in the chemical decomposition mechanism

RESEARCH ACCOMPLISHMENTS:

In our prior grant we elucidated key reactions in the decomposition of TNAZ, identifying a new transition state for exothermic NO loss in nitroalkyl radicals. Our computational study identified the energy release pathway in FOX-7.

In the current grant period we investigated the energetic onset of the H + ketene product channels of vinoxy radicals, measured the photoionization cross section of CH_2Cl radicals, and used that to determine the branching fraction to the C-C bond photofission channel of chloroacetaldehyde at 157 nm.

SCIENTIFIC IMPACT and ARMY/DoD RELEVANCE

Radical intermediates are ubiquitous in chemistry. From atmospheric processes to combustion to chemical synthesis and biological chemistry, radicals play a key role in rates and product branching. These studies provide new detection and dynamics probes of these reactive but transient species.

Energetic materials studied include the decomposition of FOX-7 and TNAZ.

INTERACTIONS, COLLABORATIONS, and TRANSITIONS

- Ryan Booth, Ph.D. 2014, is now a DoD researcher at Kirtland AFB. His research with Jamie Stearns uses molecular beam methods applied to ionic liquids

Our ARO supported program:

- Identify radical intermediates that lead to energy release in FOX-7
  Experiment and Theory
- Employ state-of-the-art techniques to probe nascent radical intermediates with high vibrational energies in the decomposition mechanism
- Develop appropriate photolytic precursors to generate radical intermediates under collision-free conditions to study their unimolecular dissociation channels

(Jim Parker once commented that a good photolytic precursor is worth its weight in gold. We initiated a new phase of our research program with this in mind.)

- Proposed work on NO_2 vs. NO Loss in Thermal vs. UV Initiation: New Ab Initio Theory (w. Mazziotti)

Progress and New Directions in our ARO supported program:

- Identify radical intermediates that lead to energy release in FOX-7
  Experiment and Theory

Completed: Theory identifying pathway to energy release in FOX-7 decomposition
Worth pursuing (w. Szpunar): Producing the 1,1-diamino,2-nitroethen-2-yl radical, and
measuring the predicted barrier to exothermic NO loss.
(but this requires a good photolytic precursor)
Comparison of the Internal State Signatures for the
Novel NO loss mechanism.

- Employ state-of-the-art techniques to probe nascent radical intermediates with high vibrational energies in the decomposition mechanism

Completed: Imaging experiment to resolve barrier to the H + ketene channel
in the competing dissociation channels of vinoxy.

- Develop appropriate photolytic precursors to generate radical intermediates under collision-free conditions to study their unimolecular dissociation channels

Completed: Study of the chloroacetaldehyde precursor to the vinoxy radical at 157 nm,
Measuring the branching between C-Cl photofission, HCl photoelimination,
and a new C-C photofission channel to produce CH_2Cl + HCO.

- NO_2 vs. NO Loss in Thermal vs. UV Initiation: New Ab Initio Theory (w. Mazziotti)

Ongoing collaboration, but direction now crafted by Mazziotti.

- **New Direction:** Establishing quantitative methods for detecting radical intermediates

Completed: The absolute photoionization cross section of the CH_2Cl radical.

Transformational and Evolutionary

Transformational Promise

Work beginning in the 1980’s (YT Lee, IRMPD of RDX) has sought to resolve the chemical mechanism of the decomposition of energetic materials. The new methods introduced in our work to probe the key radical intermediates along the energy release pathways should substantially contribute to the development of new energetic materials.

Evolutionary

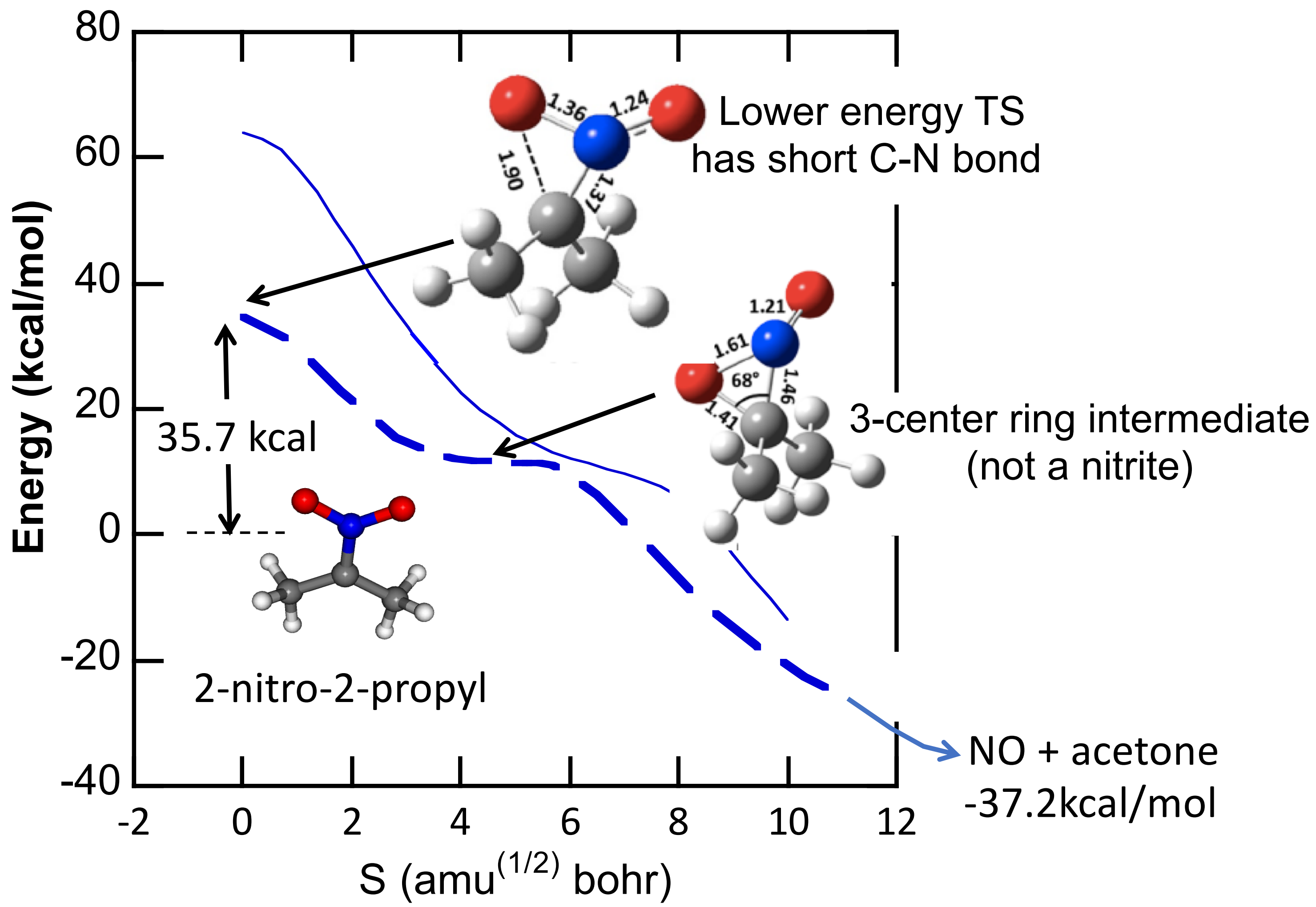
Radical intermediates are key players in chemical reaction mechanisms in synthetic chemistry, atmospheric chemistry, biological chemistry, and combustion. This work develops new methodology to detect and quantify radical intermediates, and to probe the elementary unimolecular reactions they undergo. The work also benchmarks new state-of-the-art electronic structure methods on open-shell systems.

Scientific Presentation: Progress in 2016-7

1. Review the predicted chemical mechanism for energy release in FOX-7
2. Scrape et al. experiment: Determination of the photoionization cross section of the CH_2Cl radical
3. Adams et al. experiment: Identify the three competing photodissocation channels of a photolytic precursor used to generate vinoxy radicals, and use the CH_2Cl photoionization cross section to complete our product branching determination to the CH_2Cl + HCO product channel .

Analog to TNAZ intermediate: New Low Barrier Pathway to the Exothermic Product Channel forming NO

The new 3-center ring pathway
has a barrier of only 35.7 kcal/mol



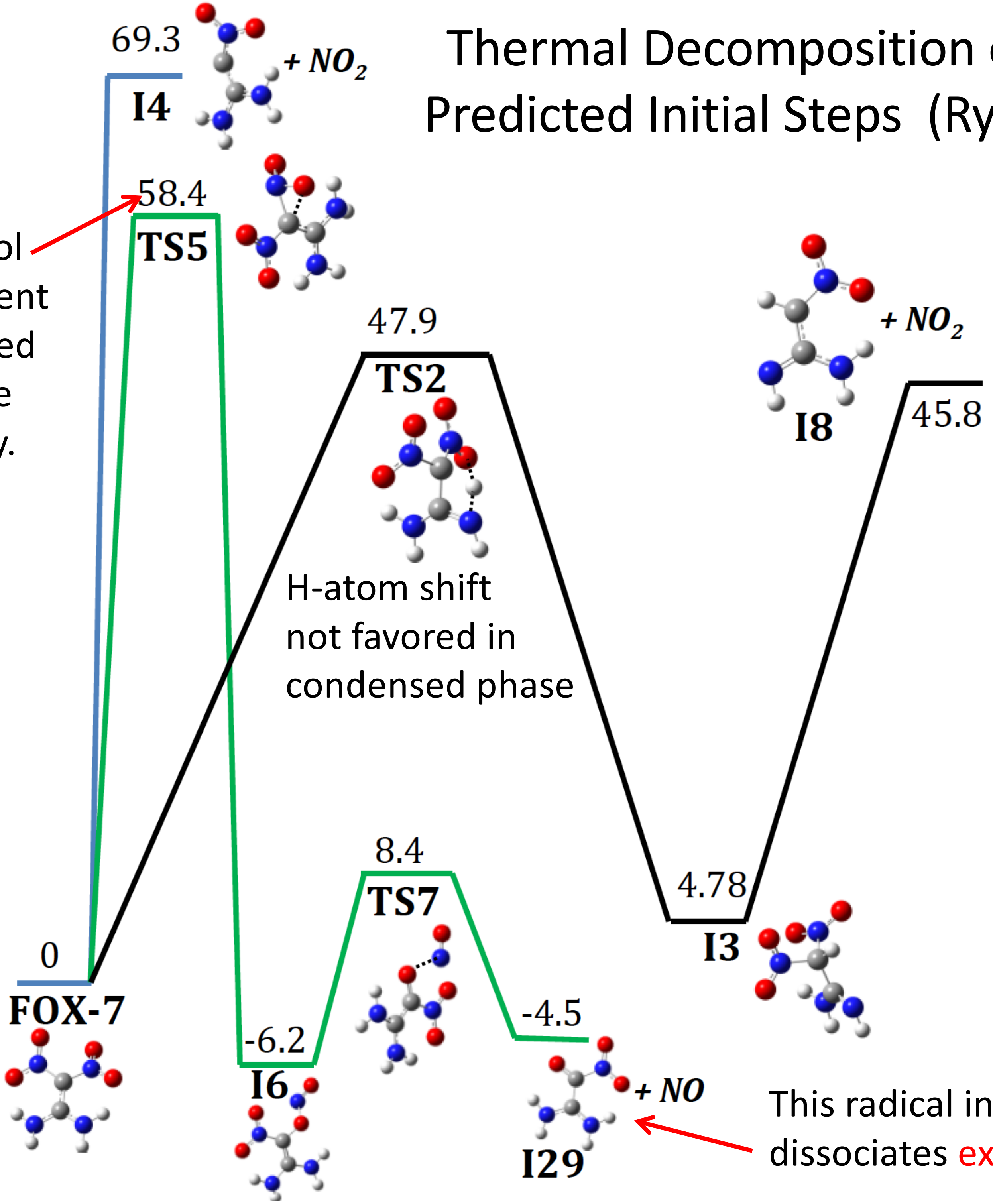
Lower energy TS
has short C-N bond

3-center ring intermediate
(not a nitrite)

2-nitro-2-propyl

NO + acetone
-37.2kcal/mol

Thermal Decomposition of FOX-7: Predicted Initial Steps (Ryan Booth)

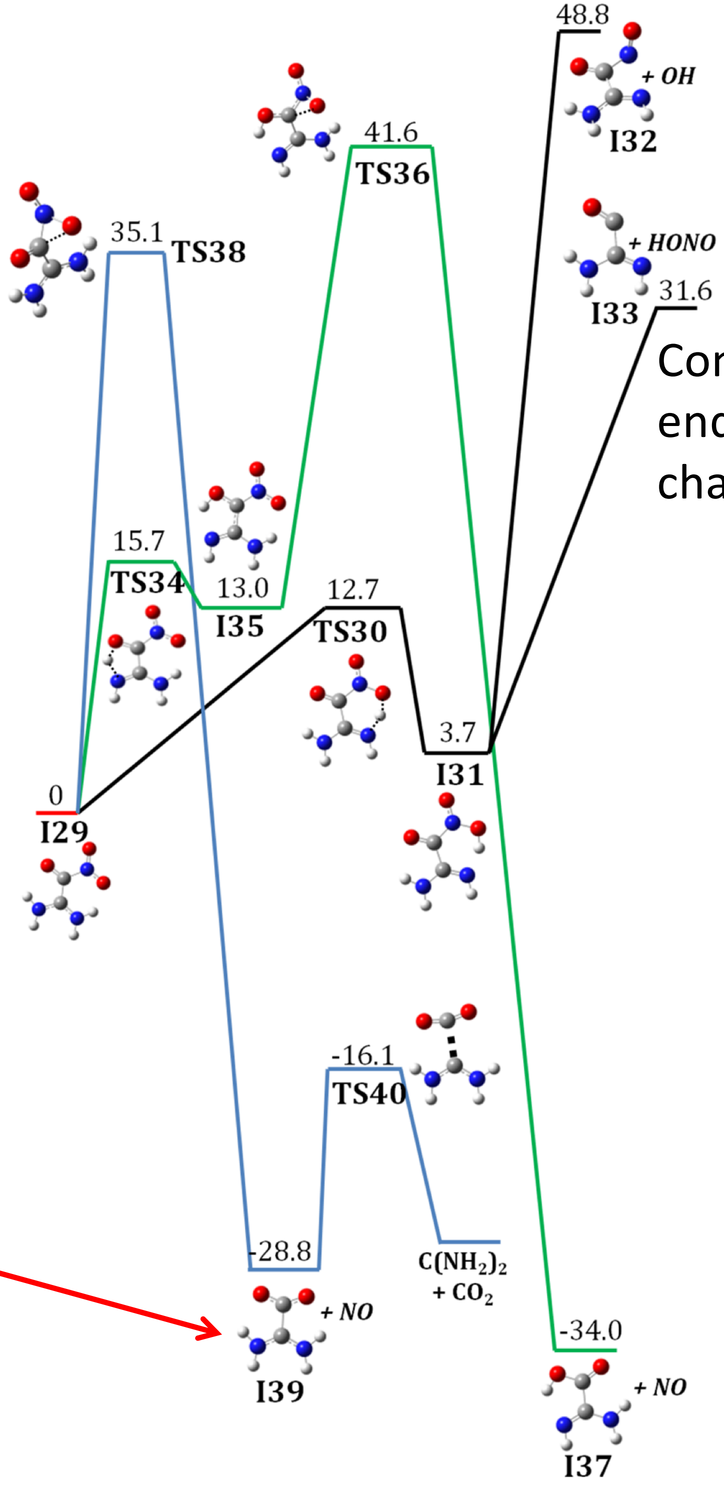


This 58.4 kcal/mol barrier is consistent with the measured condensed phase activation energy.

H-atom shift not favored in condensed phase

This radical intermediate dissociates exothermically.

After the first step, nitro-nitrite isomerization resulting in one NO product molecule, the radical intermediate (I29) has two highly exothermic decomposition routes available to it, both producing a second NO product molecule. A competing net endothermic channel produces HONO.



Competing endothermic channel

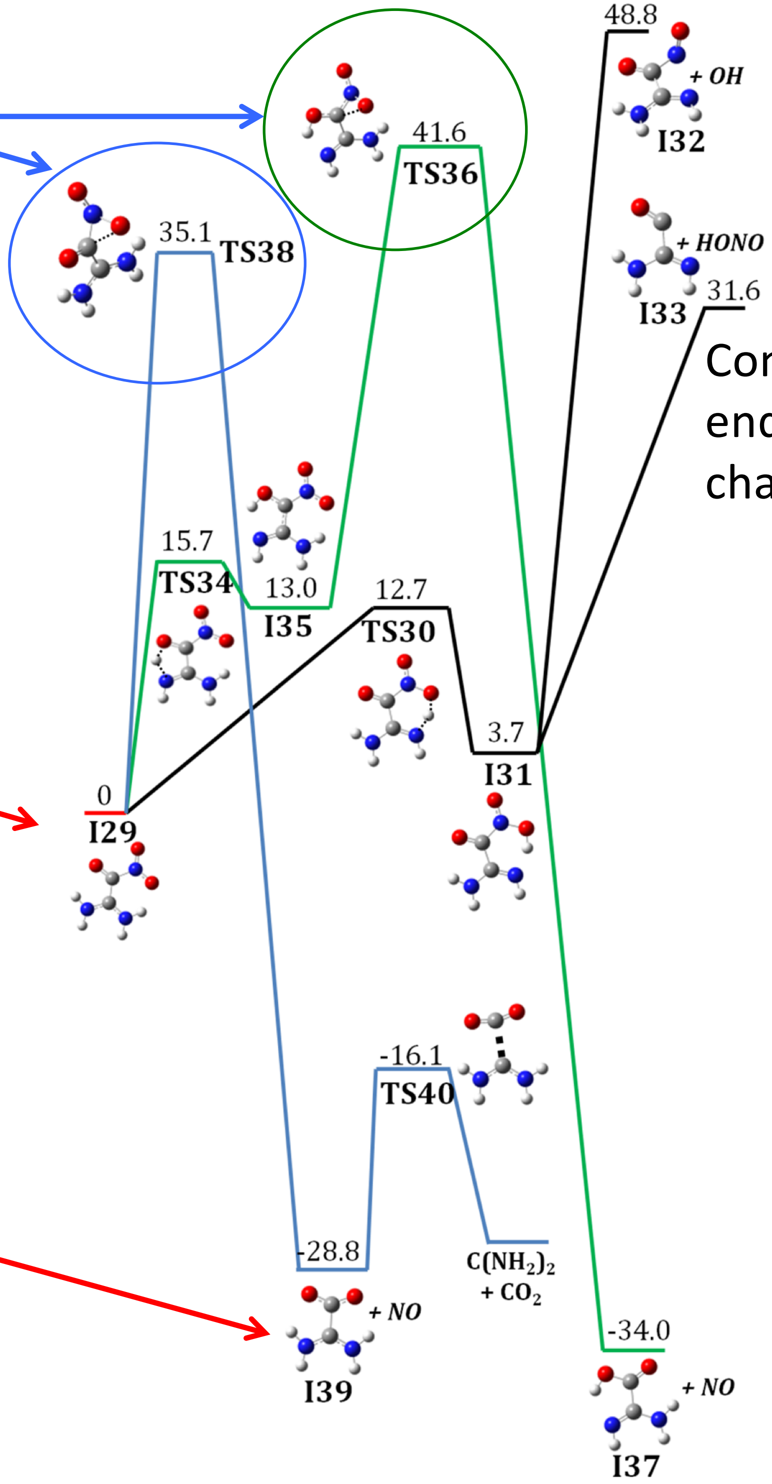
Radical intermediate produced in primary decomposition step

Exothermic product channels from the unimolecular dissociation of the I29 radical intermediate

THE TRANSITION STATES TO THE EXOTHERMIC PRODUCT CHANNELS ARE ANALOGOUS TO THE ONE DISCOVERED IN OUR PRIOR WORK ON THE 2-NITRO-2-PROPYL RADICAL.

Radical intermediate produced in primary decomposition step

Exothermic product channels from the unimolecular dissociation of the I29 radical intermediate



Competing endothermic channel

Measuring velocity distributions of radical products at Taiwan's National Radiation Research Center

Product identification:

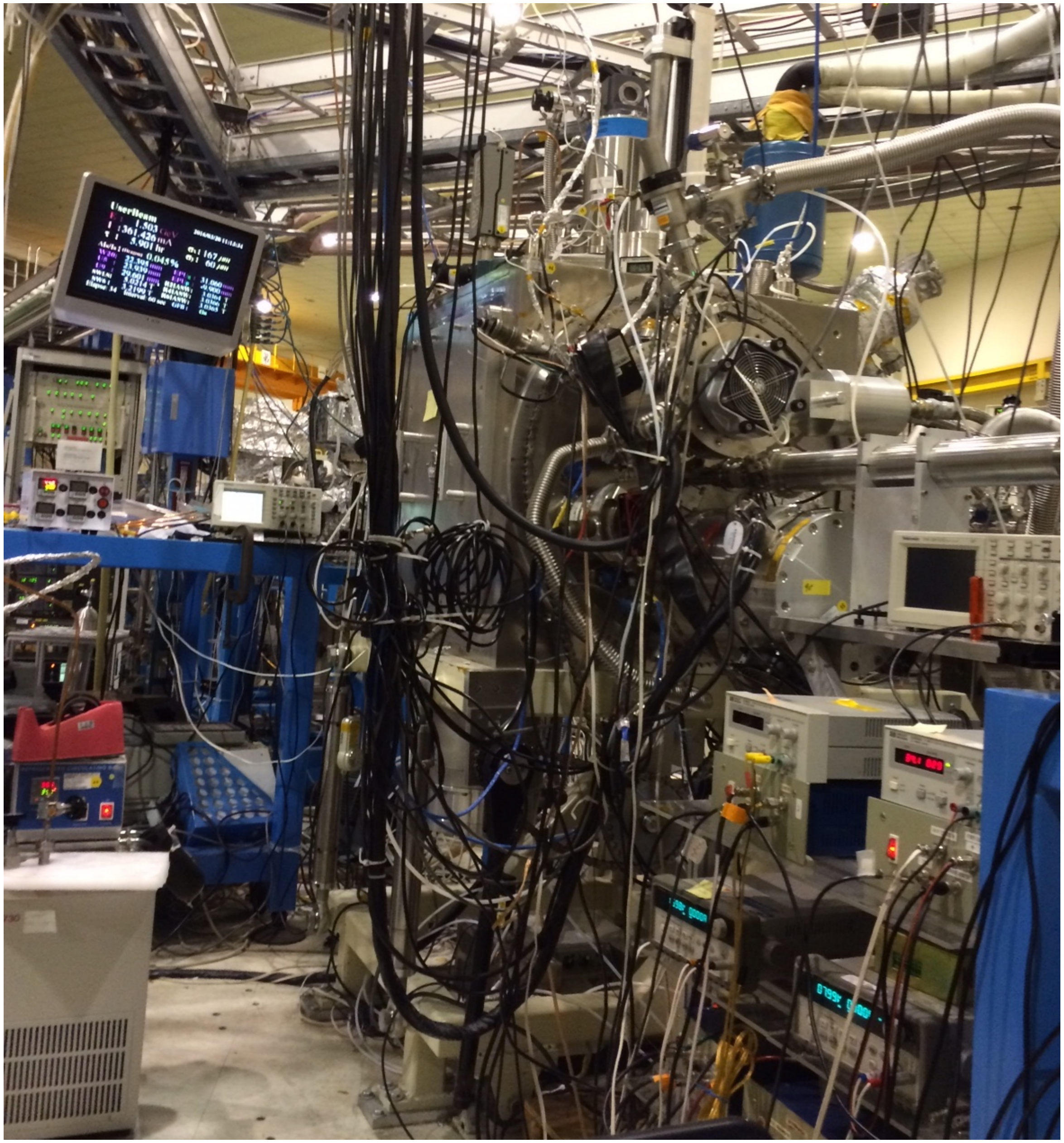
Mass to charge ratio m/z

AND

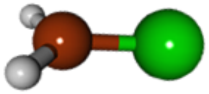
recoil velocity

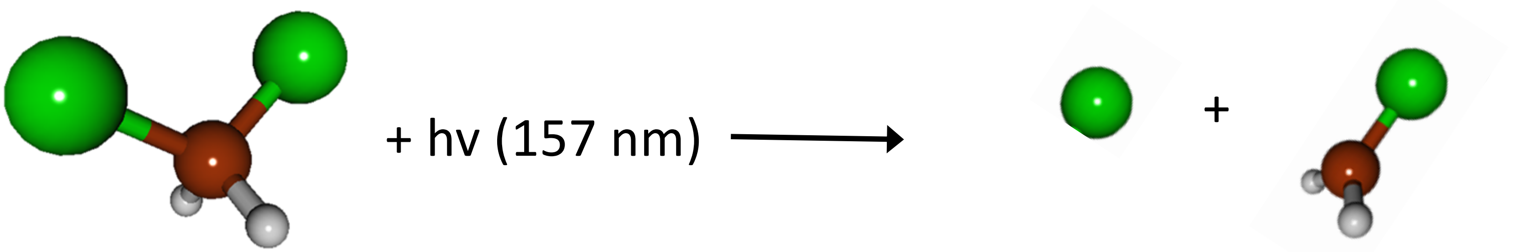
$$m_1\vec{v}_1 = -m_2\vec{v}_2$$

"Momentum-matched products"



Single photon VUV photoionization can give <u>quantitative cross section comparisons</u>, unlike REMPI

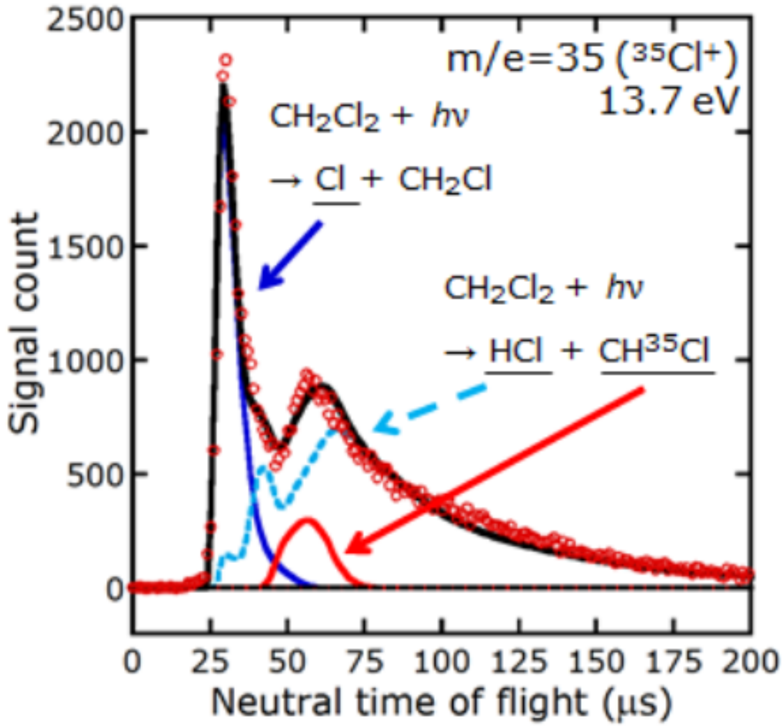
Determine the CH_2Cl  photoionization cross section by producing Cl and CH_2Cl in a 1:1 ratio

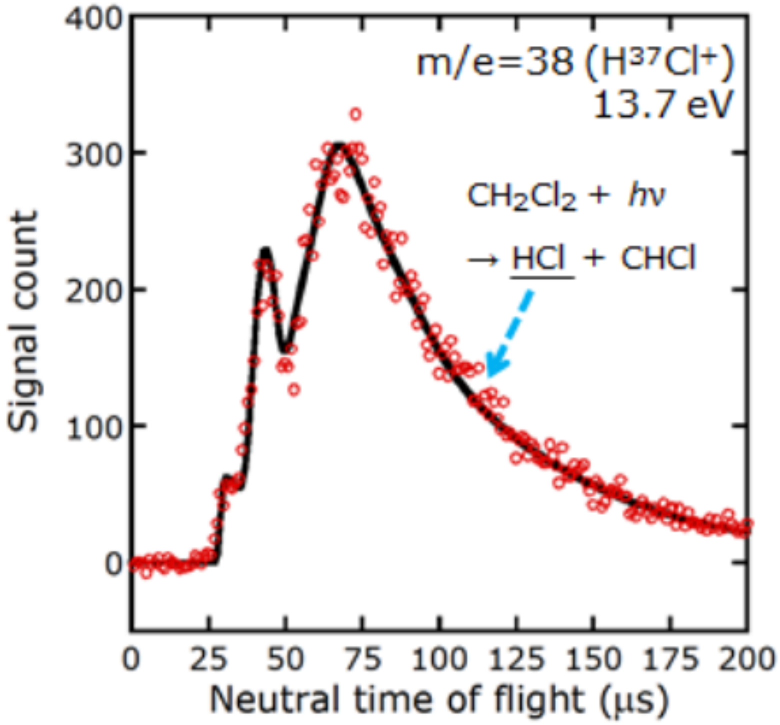


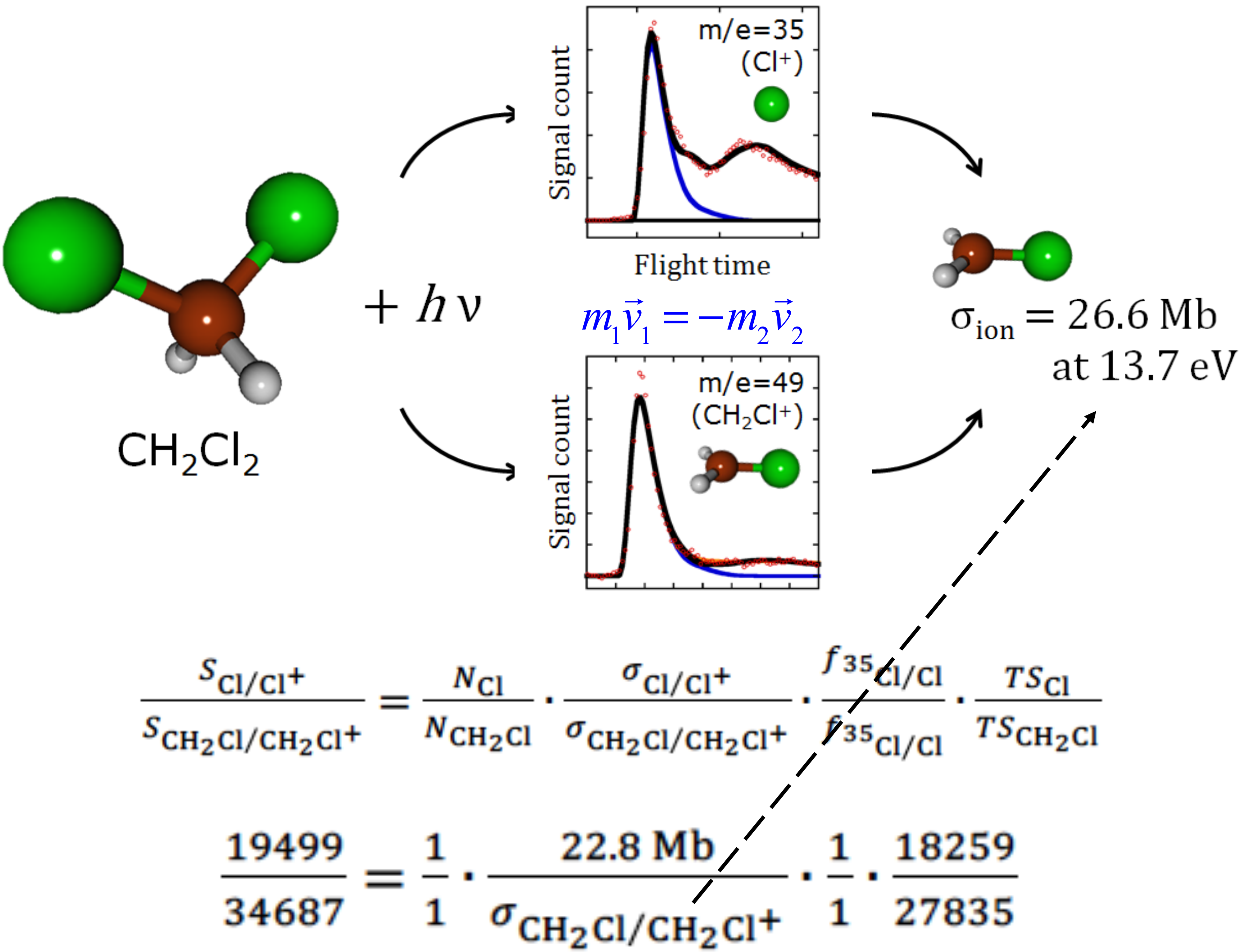
CH_2Cl_2 + hv (157 nm) ⟶ Cl + CH_2Cl

But also signal at Cl^+ from HCl elimination

Use velocity measurement to identify the Cl atom signal from C-Cl photofission



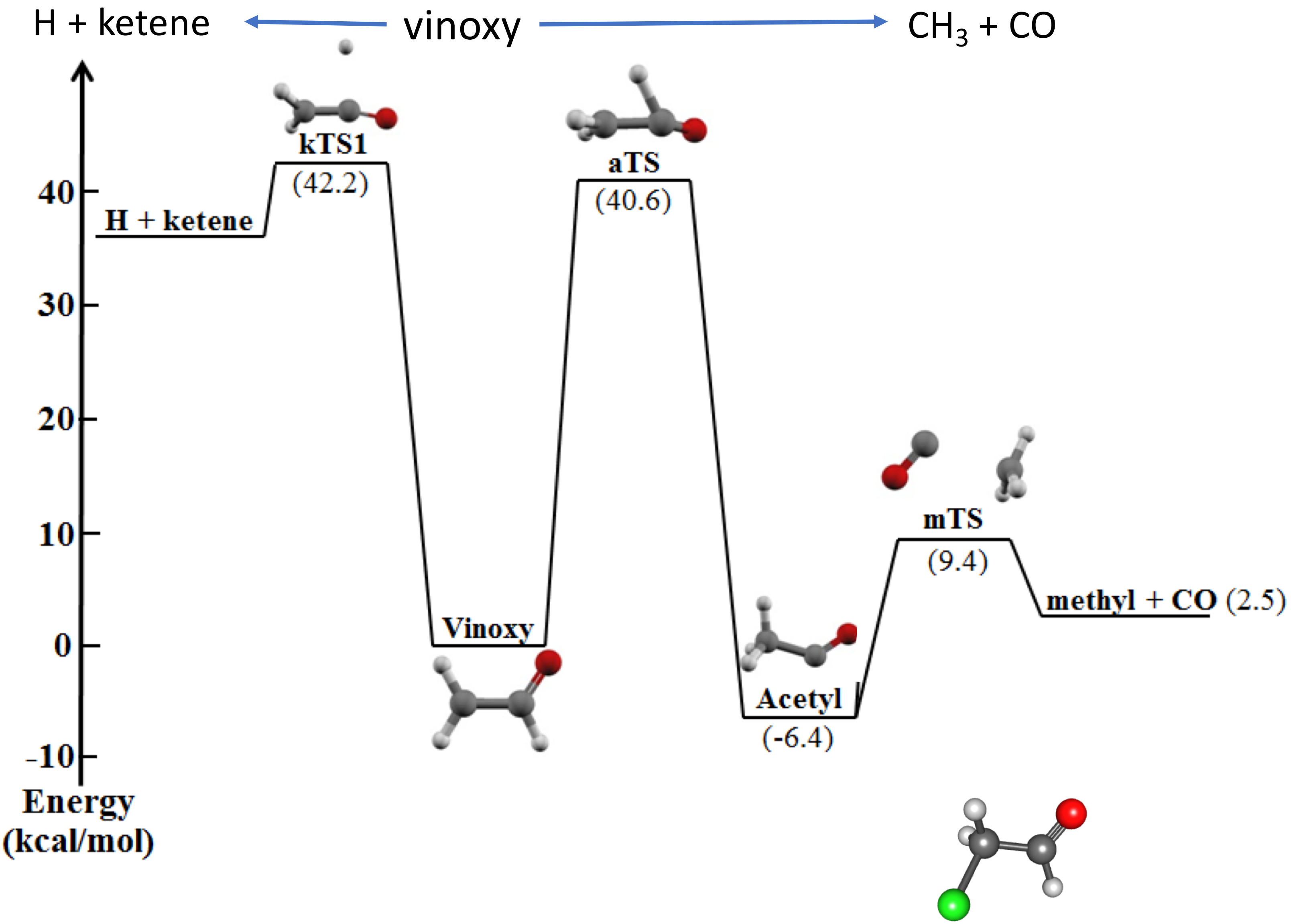




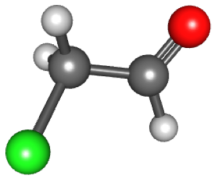
$$\frac{S_{Cl/Cl^+}}{S_{CH_2Cl/CH_2Cl^+}} = \frac{N_{Cl}}{N_{CH_2Cl}} \cdot \frac{\sigma_{Cl/Cl^+}}{\sigma_{CH_2Cl/CH_2Cl^+}} \cdot \frac{f35_{Cl/Cl}}{f35_{Cl/Cl}} \cdot \frac{TS_{Cl}}{TS_{CH_2Cl}}$$

$$\frac{19499}{34687} = \frac{1}{1} \cdot \frac{22.8\ \text{Mb}}{\sigma_{CH_2Cl/CH_2Cl^+}} \cdot \frac{1}{1} \cdot \frac{18259}{27835}$$

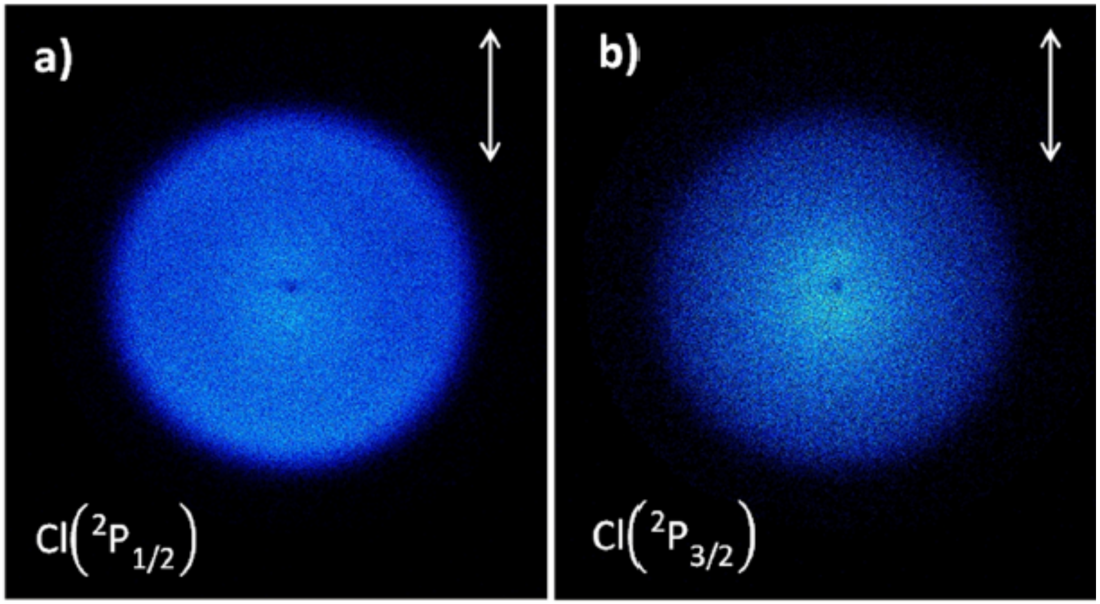
In our 2016 report we resolved the energetic barrier for the vinoxy radical intermediate to dissociate to H + ketene. It motivated us to study the radical's photolytic precursor

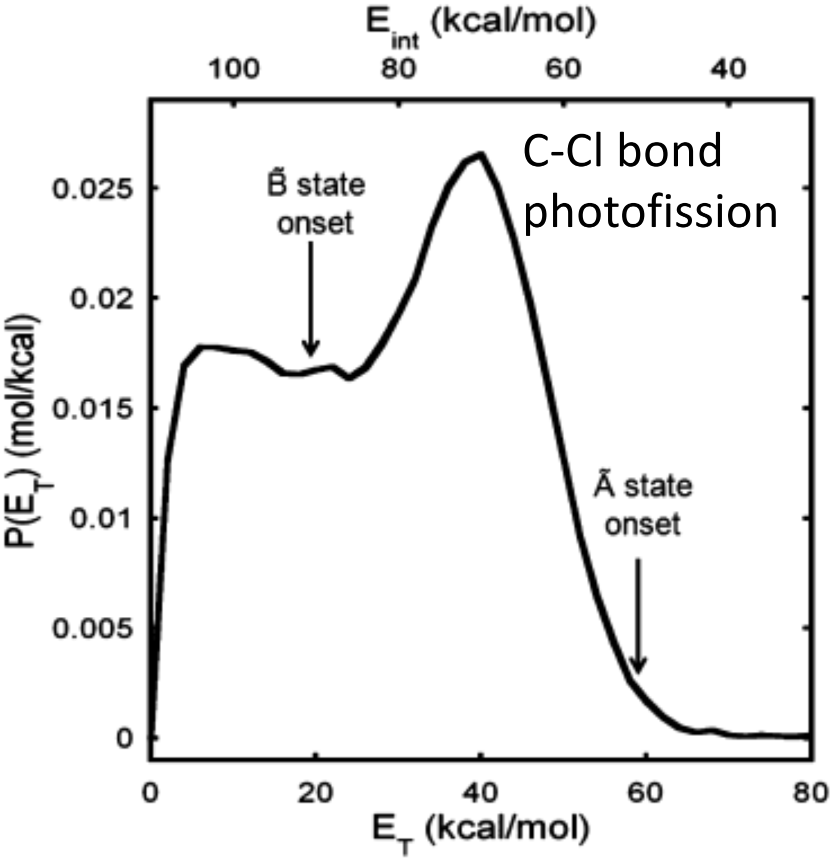

H + ketene ← vinoxy → CH_3 + CO

Determining the vibrational energy in the vinoxy radical as a function of the recoil kinetic energy E_T in C-Cl bond photofission at 157 nm



+ hv (157 nm) ⟶ ● + vinoxy





$$E_{vib} = h\nu + E_{int}(\text{precursor}) - D_o(C-X) - E_{int}(X) - E_T - E_{rot}$$

But E_{rot} is larger at higher E_T

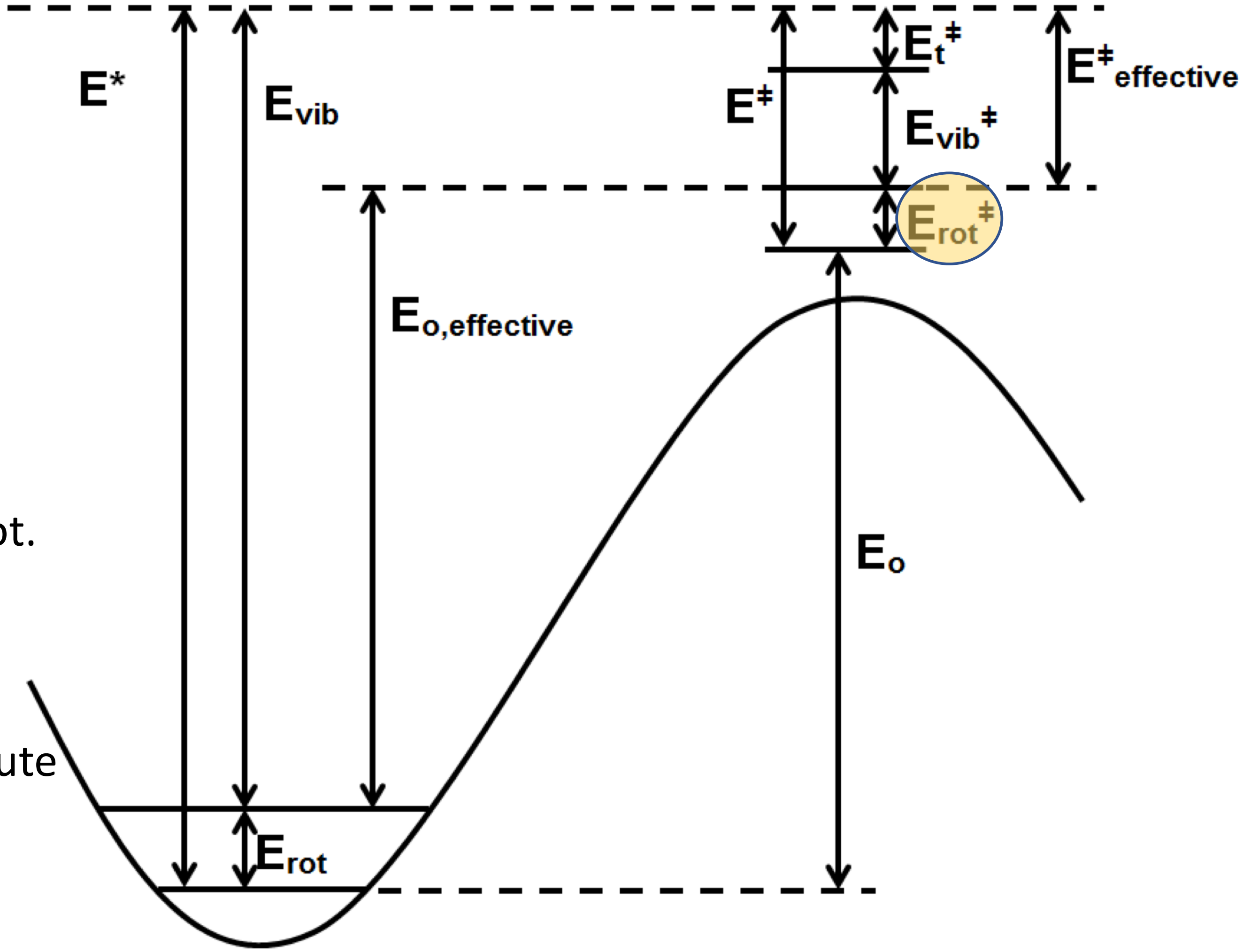
$$E_{vib} = h\nu + E_{int}(\text{precursor}) - D_o(C-X) - E_{int}(X) - \left[1 + \left(\frac{E_{rot}}{E_T}\right)_{\text{radical}}\right] E_T$$

vinoxy

Calculating the RRKM microcanonical rates for vinoxy to dissociate to H + ketene vs CH_3 + CO with the correct sum of states in the numerator, accounting for E_{rot}

Calculate $\vec{J}_{rot}$ at each measured E_T for Cl + vinoxy

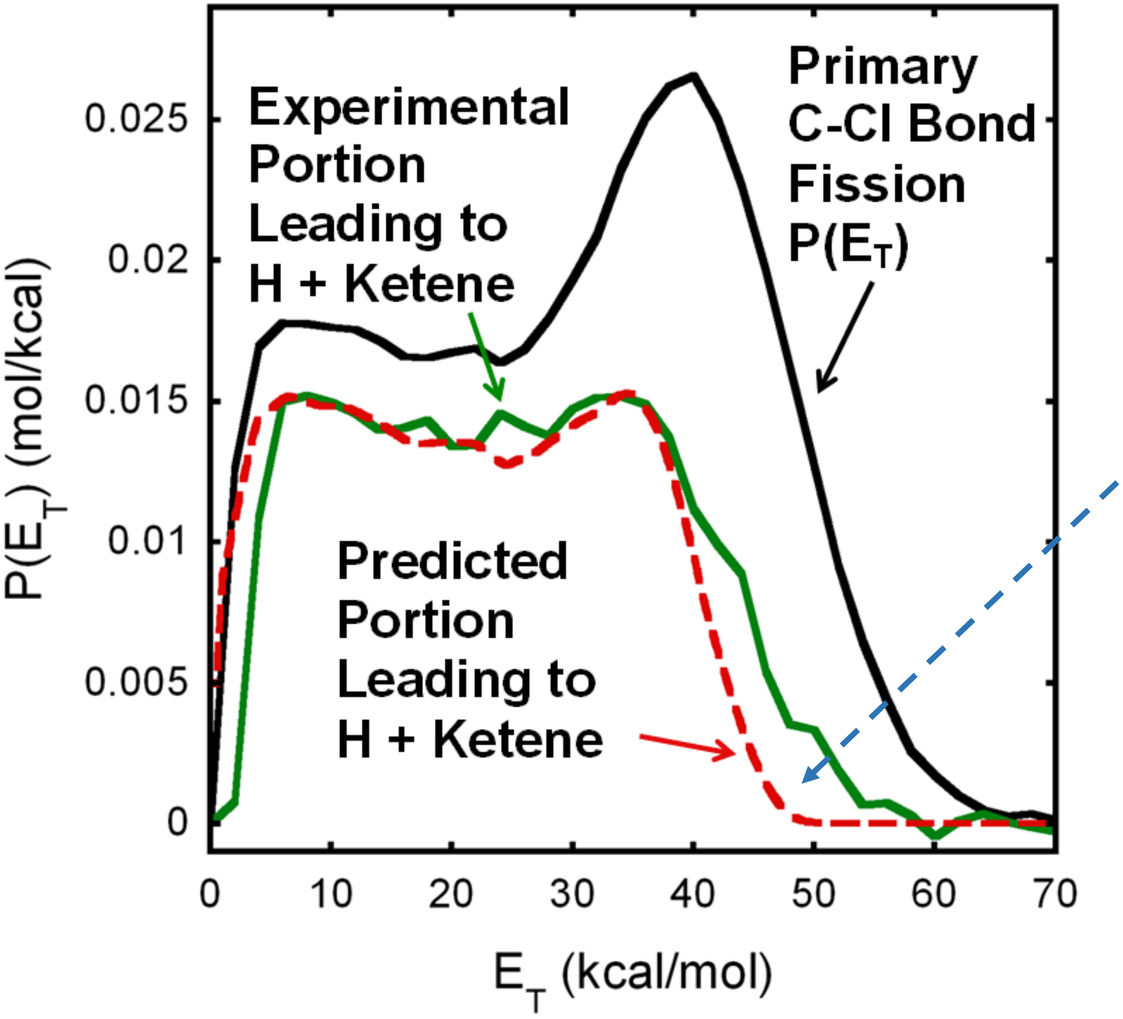
$$-\vec{J}_{rot} = \vec{J}_{orb} = \vec{r} \times \mu \vec{v}_{rel}$$



While $\vec{J}_{rot}$ is conserved, E_{rot} is not. Use the changing inertia tensor to calculate the E_{rot} at transition states for H + ketene and for the isomerization en route to CH_3 + CO

$$E_{rot} = \frac{1}{2} \vec{J}_{rot}^{\,T} I^{-1} \vec{J}_{rot}$$

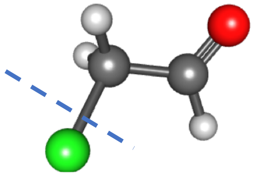
Raising the barrier for the vinoxy radical ⟶ H + ketene to 4 kcal/mol higher than the isomerization barrier en route to CH_3 + CO gives the best fit to the data



Speculated that
HCl photoelimination
in precursor with
E_T from 40 to 50
kcal/mol gave extra
ketene signal.
NSRRC expts in 2016-7
sought to confirm this.

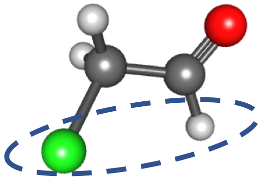
Determining the Primary Photodissociation Channels of Chloroacetaldehyde at 157 nm

C-Cl bond fission



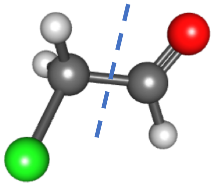
$\xrightarrow{157\text{ nm}}$ Cl + vinoxy

And, as suspected, HCl elim.



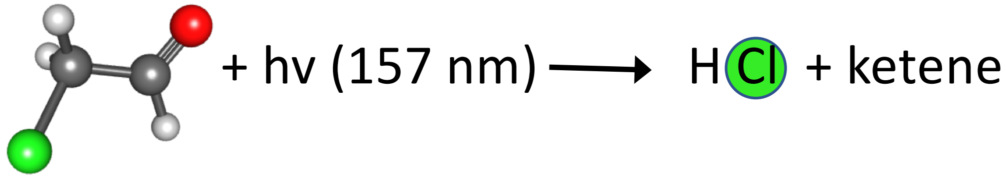
$\xrightarrow{157\text{ nm}}$ $HCl + CH_2CO$

New: C-C bond fission

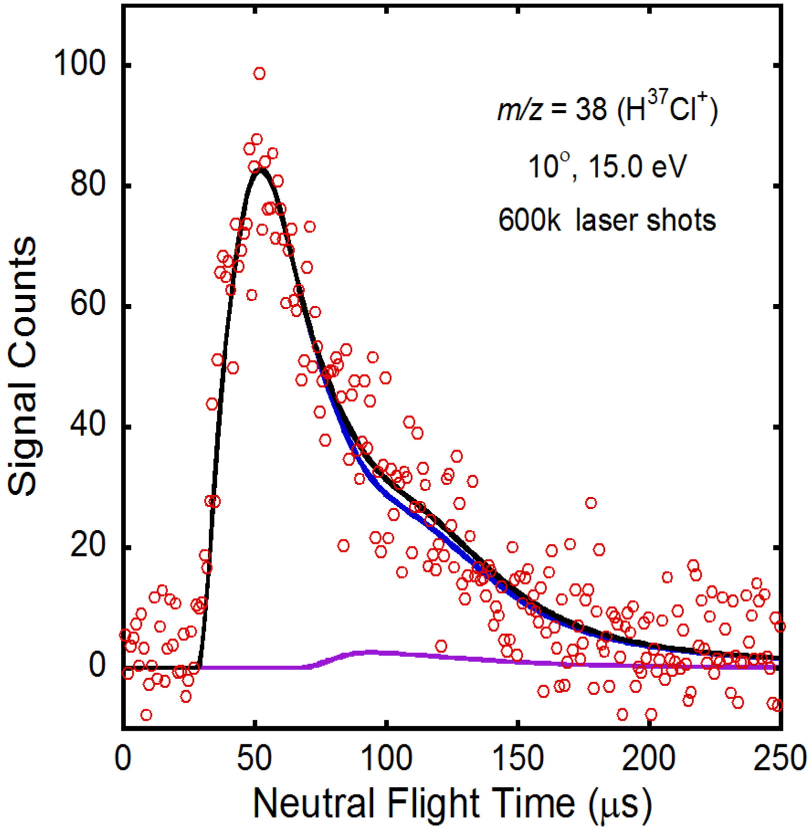


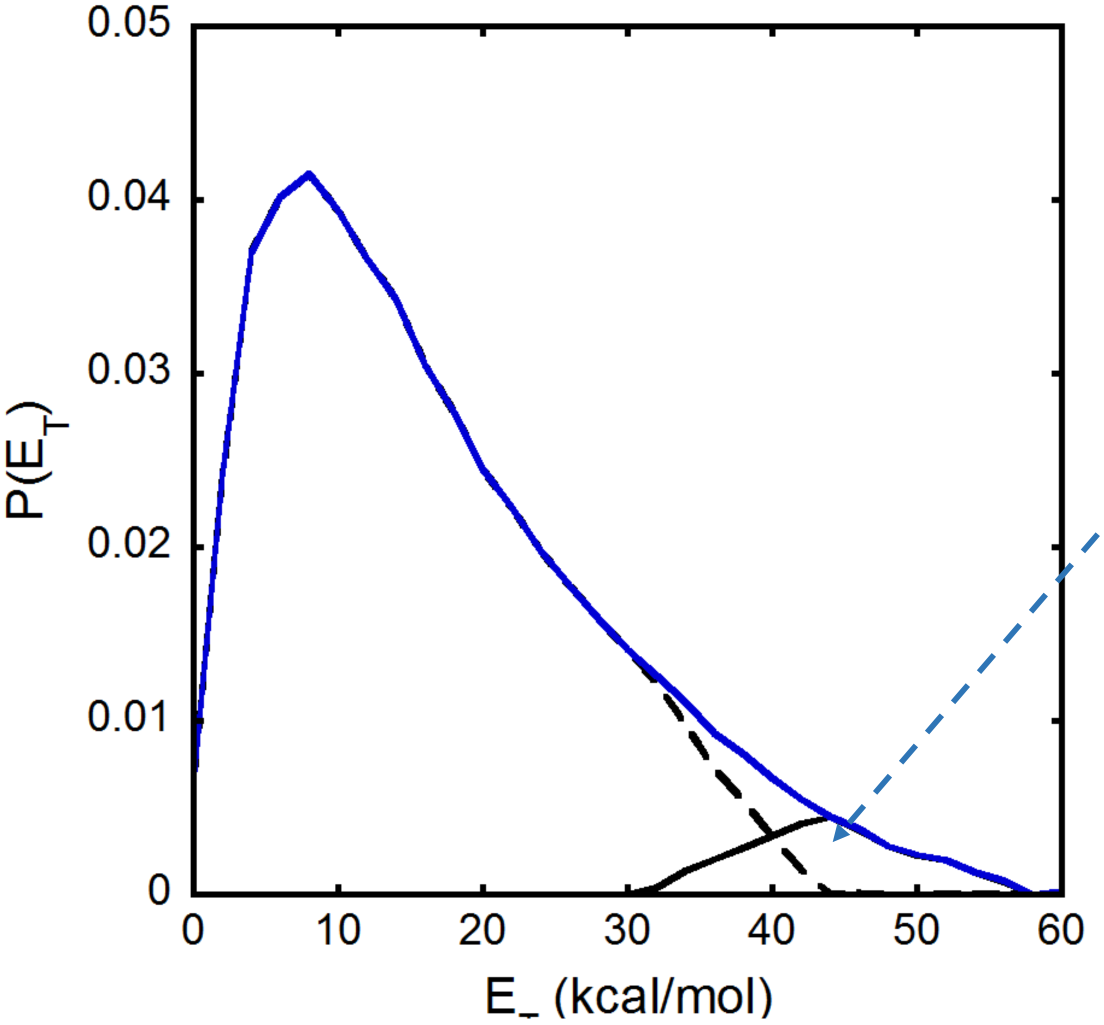
$\xrightarrow{157\text{ nm}}$ $CH_2Cl + HCO$

Quantified the product branching. Literature photoionization cross sections for Cl and HCl, and our measured photoionization cross section for CH_2Cl



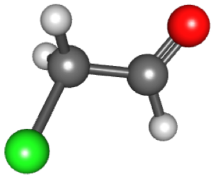
+ hv (157 nm) ⟶ HCl + ketene



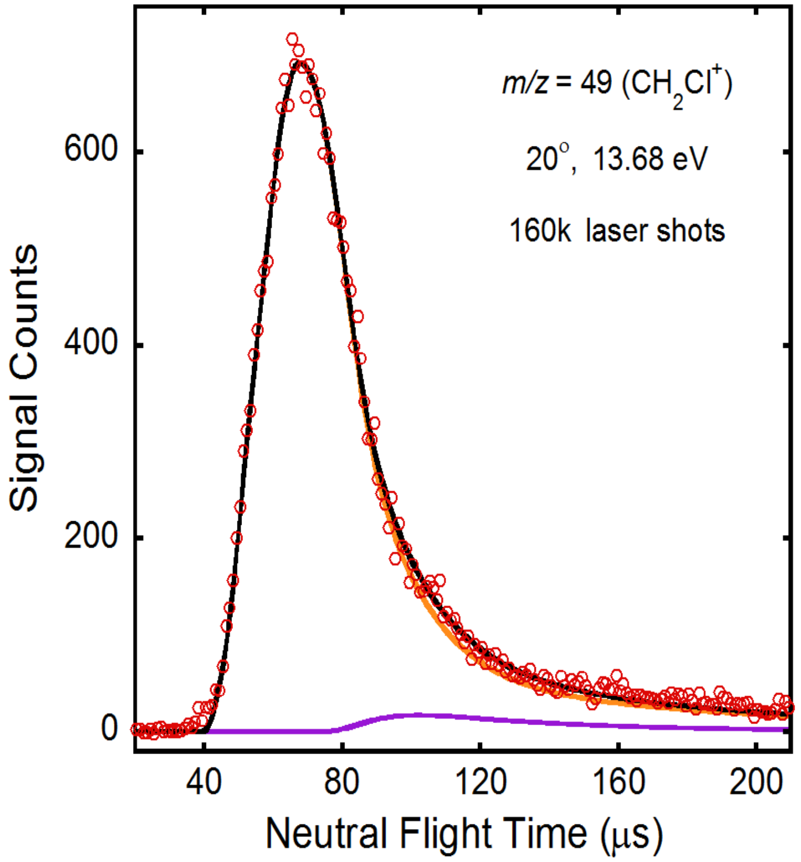


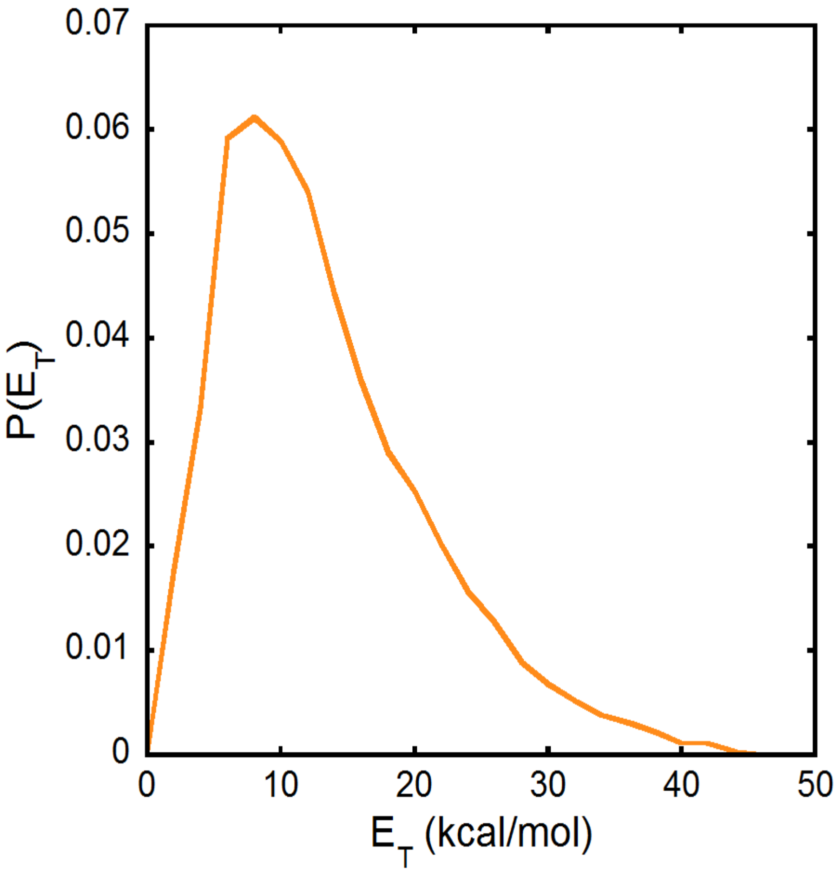
As suspected, HCl photoelimination in chloroacetaldehyde with E_T from ~40 to ~50 kcal/mol gave stable ketene, so accounts for the extra ketene signal in the imaging expts.

The new C-C bond photofission channel



+ hv (157 nm) ⟶ CH_2Cl + HCO





$$\frac{\Phi_{C-Cl}}{\Phi_{HCl}} = \text{obs}\left(\frac{{}^{35}\mathrm{Cl}^+}{\mathrm{H}^{35}\mathrm{Cl}^+}\right) \times \mathrm{TS}\left(\frac{\mathrm{H}^{35}\mathrm{Cl}}{{}^{35}\mathrm{Cl}}\right) \times \left(\frac{\sigma_{\mathrm{HCl/HCl}^+}}{\sigma_{\mathrm{Cl/Cl}^+}}\right)$$

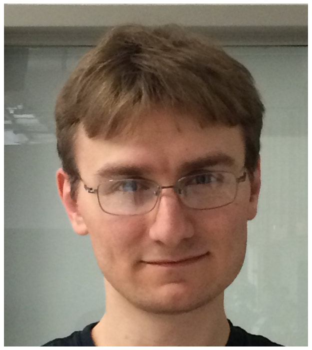
$$= \left(\frac{75328}{13813}\right) \times \left(\frac{143732}{62697}\right) \times \left(\frac{16\ \mathrm{Mb}}{22.8\ \mathrm{Mb}}\right) = 8.8,$$

$$\frac{\Phi_{C-Cl}}{\Phi_{C-C}} = \text{obs}\left(\frac{{}^{35}\mathrm{Cl}^+}{\mathrm{CH_2Cl}^+}\right) \times \mathrm{TS}\left(\frac{\mathrm{CH_2Cl}}{{}^{35}\mathrm{Cl}}\right) \times \left(\frac{\sigma_{\mathrm{CH_2Cl/CH_2Cl}^+}}{\sigma_{\mathrm{Cl/Cl}^+}}\right)$$

$$= \left(\frac{19001}{30371}\right) \times \left(\frac{34137}{10780}\right) \times \left(\frac{26.6}{22.8}\right) = 2.3$$

Photoproduct Branching Fractions are thus:

C−Cl fission	:	HCl elimination	:	C−C fission
0.65	:	0.07	:	0.28



“A Measurement of the Photoionization Cross Section of CH_2Cl via Photofragment Translational Spectroscopy of Dichloromethane”, **Preston G. Scrape**, Rosalind J. Xu, Jonathan D. Adams, Shih-Huang Lee and Laurie J. Butler, submitted to Phys. Chem. Lett. (2017).

“Primary Product Branching in the Photodissociation of Chloroacetaldehyde at 157 nm”, **Jonathan D. Adams**, Preston G. Scrape, Shenshen Li, Shih-Huang Lee and Laurie J. Butler, submitted to J. Phys. Chem. (2017).

Scientific and Technological Transitions

My former Ph.D. student Ryan Booth, at Kirtland AFB, applies molecular beam methods he learned in my group to ionic liquids.

Identification of multiple conformers of the ionic liquid [emim][tf2n] in the gas phase using IR/UV action spectroscopy

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In this study we investigate the effect of deuteration and molecular beam temperature on the hydrogen bond in the ionic liquid [emim][tf2n]. Using IR/UV double resonance spectroscopy, we probe the microscopic structure of the [emim][tf2n] ion pair and its mono-deuterated, [emim-d_1][tf2n], analog. Comparisons of the infrared absorption frequencies between these two species show that there are multiple conformers of the ion pair present in the gas phase and trapped through the molecular beam cooling process. Furthermore, each conformer has a characteristic red shift in the frequency of its C2–H group that reveals the variation in strength of a hydrogen bond between the cation and anion.

Interactions with other Groups and Organizations

Experimental Collaborators

Shih-Huang Lee of Taiwan's National Synchrotron Radiation Research Center co-authored three of the five publications acknowledging our ARO support.

Theory Collaborations

Ongoing with D. Mazziotti group, The University of Chicago

Ongoing with J. Subotnik group, Univ. of Pennsylvania, but first results on chloroacetaldehyde product branching was discouraging.

Ongoing with J. Bowman, but not yet on ARO systems.

Synthesis of Photolytic Precursors for FOX-7 intermediate

Worth pursuing (by Szpunar): Reddy Damavarapu, in the group of Wendy Balas at ARDEC, Pickatinny, was willing to pursue the synthesis of a photolytic precursor needed for the FOX-7 intermediate. The best target for the experiments is 1,1-diamino,2-nitro,2-iodoethene, but any halogenated precursor would do. Reddy trained with my UChicago colleague Prof. Phil Eaton (of octanitrocubane fame)

Publications Acknowledging WN911NF-14-1-0244

"Further Studies into the Photodissociation Pathways of 2-Bromo-2-Nitropropane and the Dissociation Channels of the 2-Nitro-2-Propyl Radical Intermediate", R. S. Booth, M. D. Brynteson, S.-H. Lee, J. J. Lin, and L. J. Butler, J. Phys. Chem. A 118, 4707-4722 (2014).

"Thermal decomposition pathways for 1,1-diamino-2,2-dinitroethene (FOX-7)", R. S. Booth and L. J. Butler, J. Chem. Phys. 141, 134315 (2014).

"The Onset of H + Ketene Products from Vinoxy Radicals Prepared by Photodissociation of Chloroacetaldehyde at 157 nm", Chow-Shing Lam, Jonathan D. Adams, and Laurie J. Butler, J. Phys. Chem. A, 10.1021/acs.jpca.6b01256 (2016).

"A Measurement of the Photoionization Cross Section of CH_2Cl via Photofragment Translational Spectroscopy of Dichloromethane", Preston G. Scrape, Rosalind J. Xu, Jonathan D. Adams, Shih-Huang Lee and Laurie J. Butler, Chem. Phys. Lett. 687 284-289 (2017).

"Primary Product Branching in the Photodissociation of Chloroacetaldehyde at 157 nm", Jonathan D. Adams, Preston G. Scrape, Shenshen Li, Shih-Huang Lee and Laurie J. Butler, J. Phys. Chem. A, 10.1021/acs.jpca.7b05318 (2017).