SAND2019-5118PE

GAS PHASE CHEMICAL PHYSICS

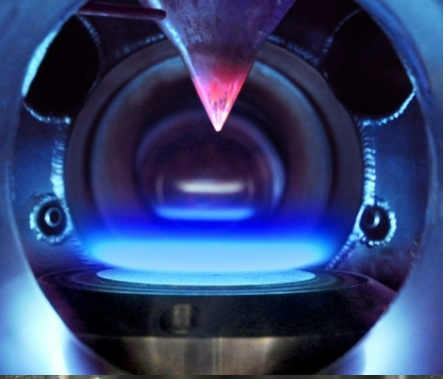
Isomer-Resolved Probing of Complex Systems of Reactions

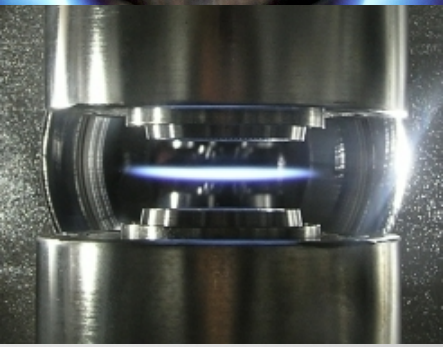
Nils Hansen

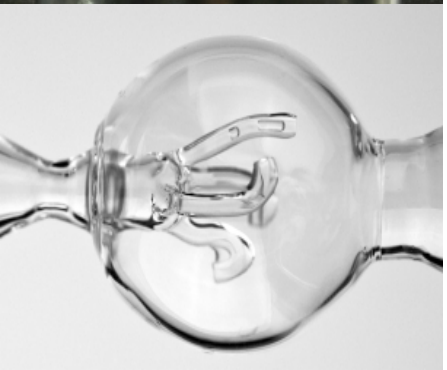
Sandia National Laboratories

COMBUSTION RESEARCH FACILITY
CRF
SANDIA NATIONAL LABORATORIES / CALIFORNIA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.







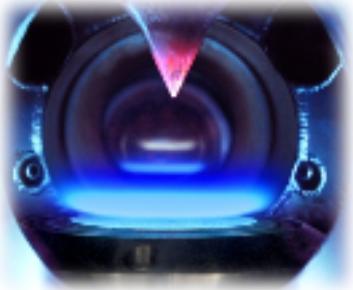
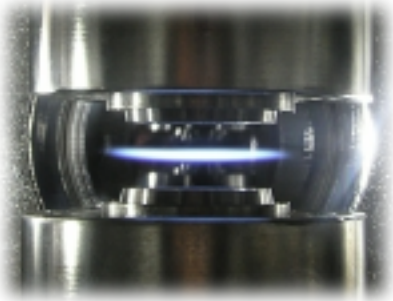
- ✓ Introduction
- ✓ Experimental Procedures
- ✓ Formation of Aromatic Species in Flames
  - ➢ Identification of aliphatically bridged multi-core PAHs
- ✓ Low-Temperature Oxidation Studies
  - ➢ Identification and quantification of peroxides
- ✓ Ozone-Assisted Combustion
  - ➢ Identification of the Criegee Intermediate reaction network
- ✓ Rotational (Microwave) Spectroscopy
- ✓ Summary and Outlook

GAS PHASE CHEMICAL PHYSICS

Complex Systems of Reactions and Combustion Mechanism Development

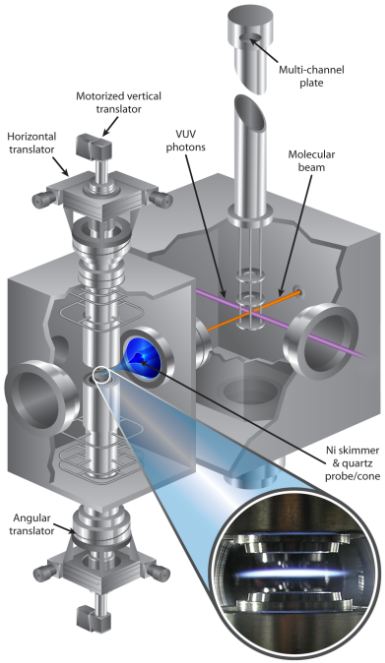
- ✓ Studying the chemistry of complex systems of reaction networks
- ✓ Gaining insights into the *scientifically relevant aspects* (key intermediates and chemical pathways) by addressing the "right" level of detail for
  - ➢ *formation of polycyclic aromatic hydrocarbons (PAHs)*
  - ➢ *low-temperature oxidation and ignition chemistry (detection, identification, and quantification of KHPs)*

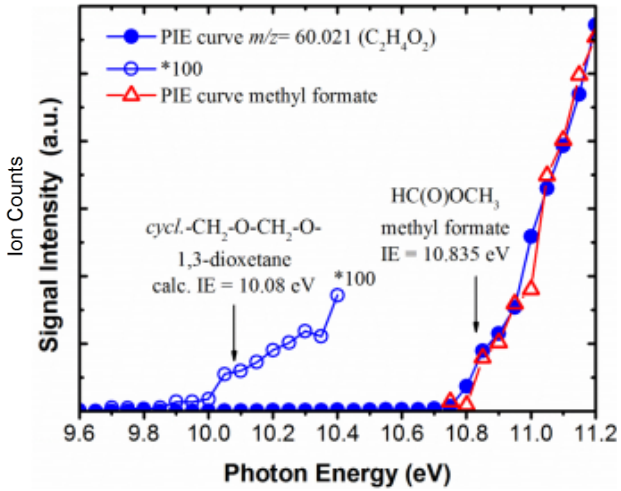
- ✓ experiments and analysis procedures, theory, and new experiments

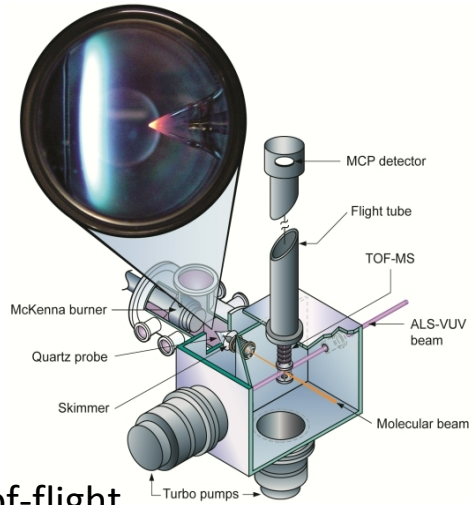





GAS PHASE CHEMICAL PHYSICS

Gaining Experimental Insights Into Complex Systems of Reactions Under Idealized Conditions





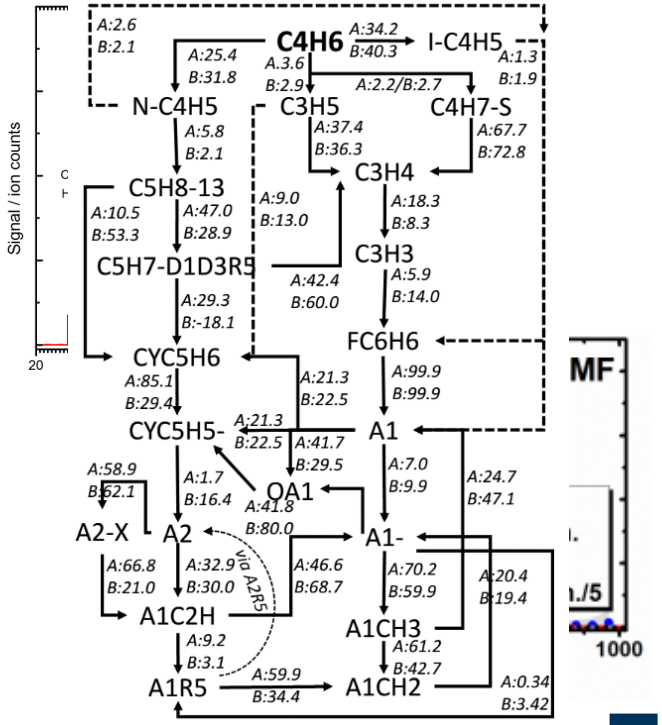


- ✓ Orthogonal extraction reflectron time-of-flight
- ✓ Detection limit: ~0.5 ppm
- ✓ Mass resolution $m/\Delta m$ ~ 4000
- ✓ Electron and photon ionization (at the Advanced Light Source)
- ✓ Continuous ionization, rapid (35 kHz) ion extraction

GAS PHASE CHEMICAL PHYSICS

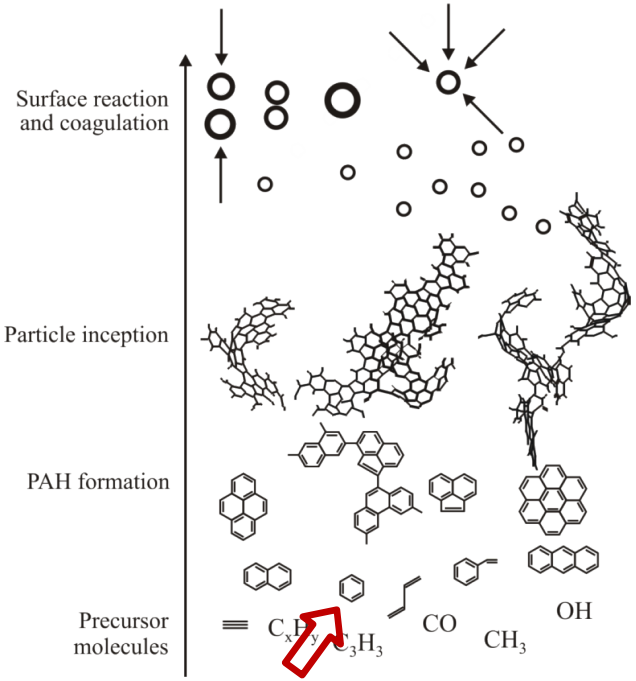
Gaining Experimental Insights Into Complex Systems of Reactions Under Idealized Conditions

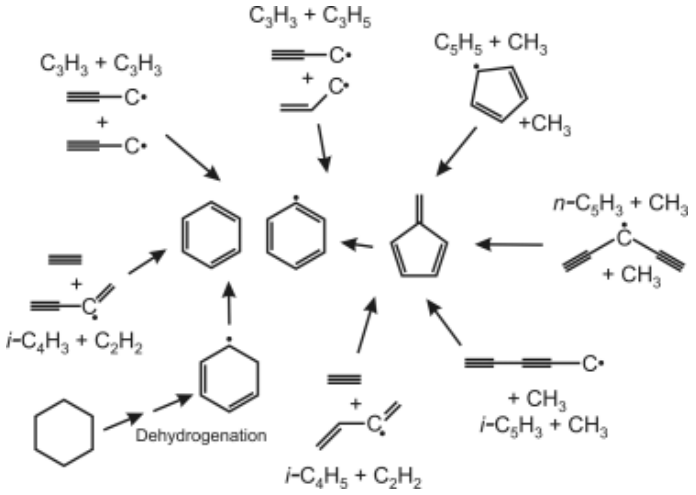
1. **Sample from Complex Systems and record Mass Spectra**
   at various positions from and temperatures in the reactors
2. **Identify Components**
   based on m/z ratios, ionization thresholds, fragmentation patterns, PIE curves
3. **Determine the Quantitative Composition of the Reactors**
   calibrate the system (mass discrimination factors), measure (or calculate) photo- and electron ionization cross sections
4. **Identify Relevant Reaction Pathways**
   from species' identities and their mole fraction data
   combine measurements of mole fractions with kinetic modeling results
5. **Gaining Insights into Relevant Chemical Aspects**
   for low-temperature oxidation and PAH formation

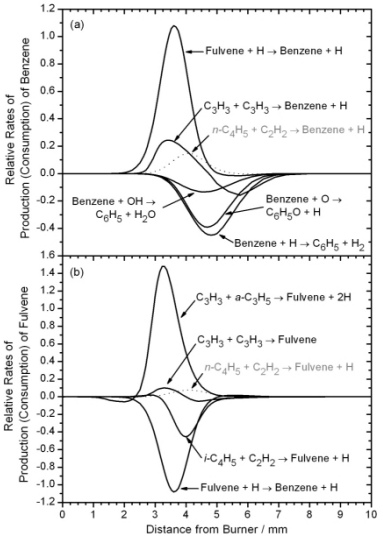


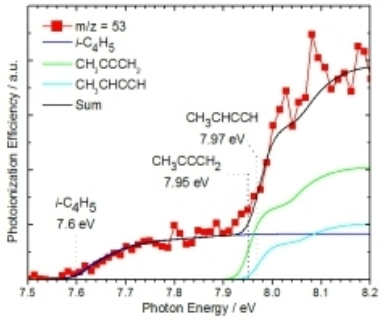
GAS PHASE CHEMICAL PHYSICS

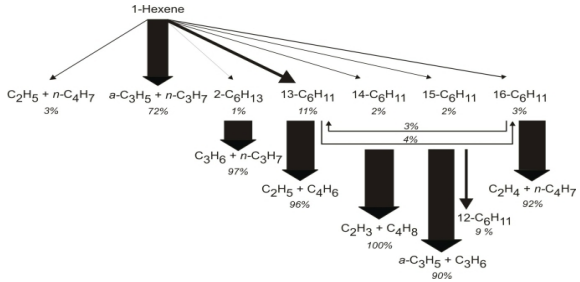
Formation of Benzene







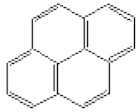




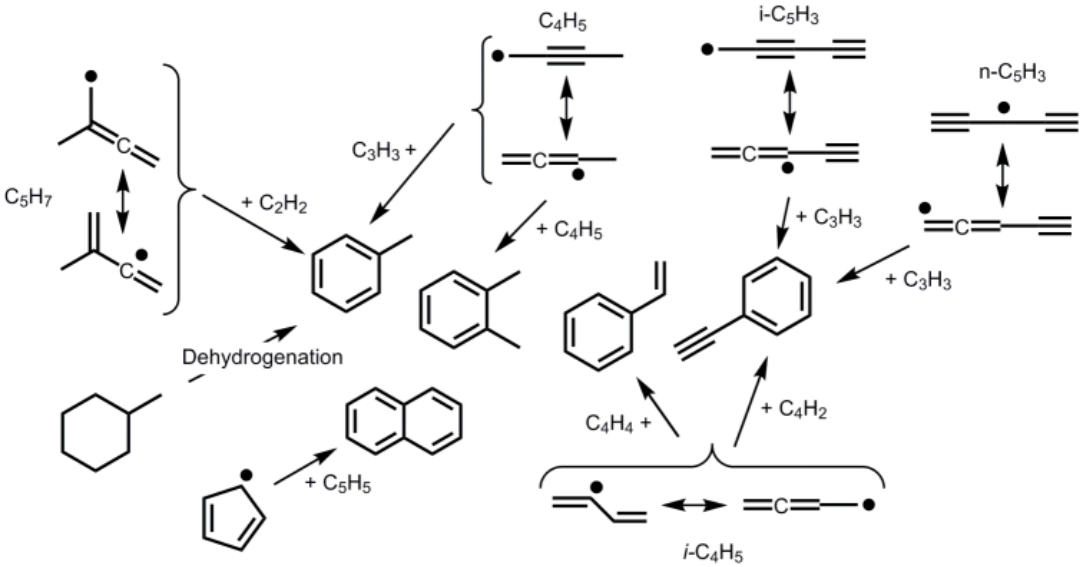
GAS PHASE CHEMICAL PHYSICS

N. Hansen *et al., Combust. Expl. Shock Waves,* **2012,** 48, 508-515

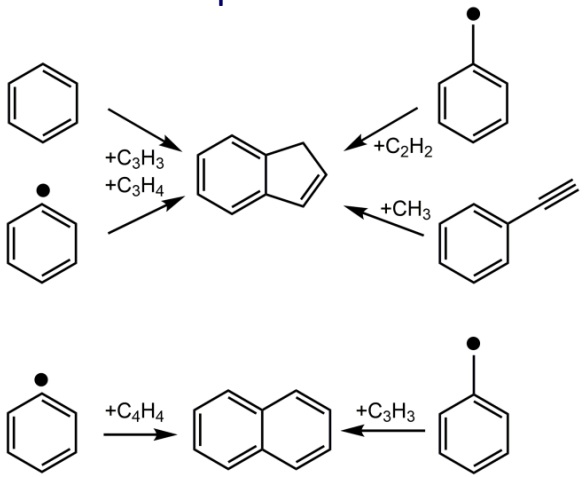
Molecular-Growth From The First Aromatic Ring to Pyrene



✓ What are the first aromatic species and how are they formed?

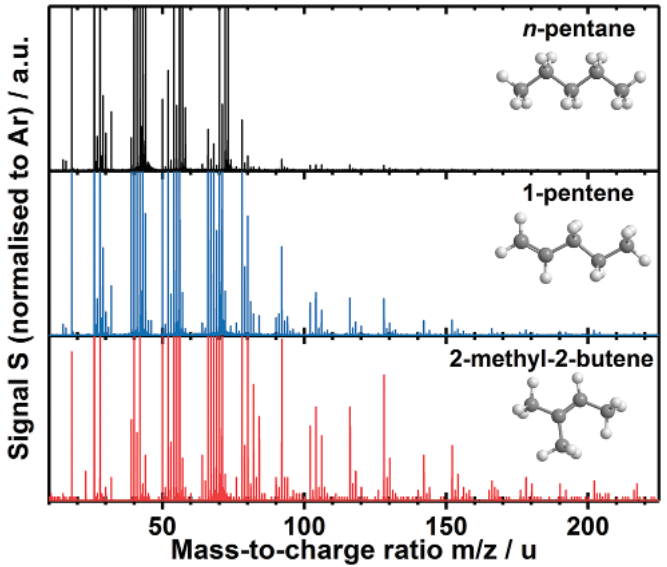


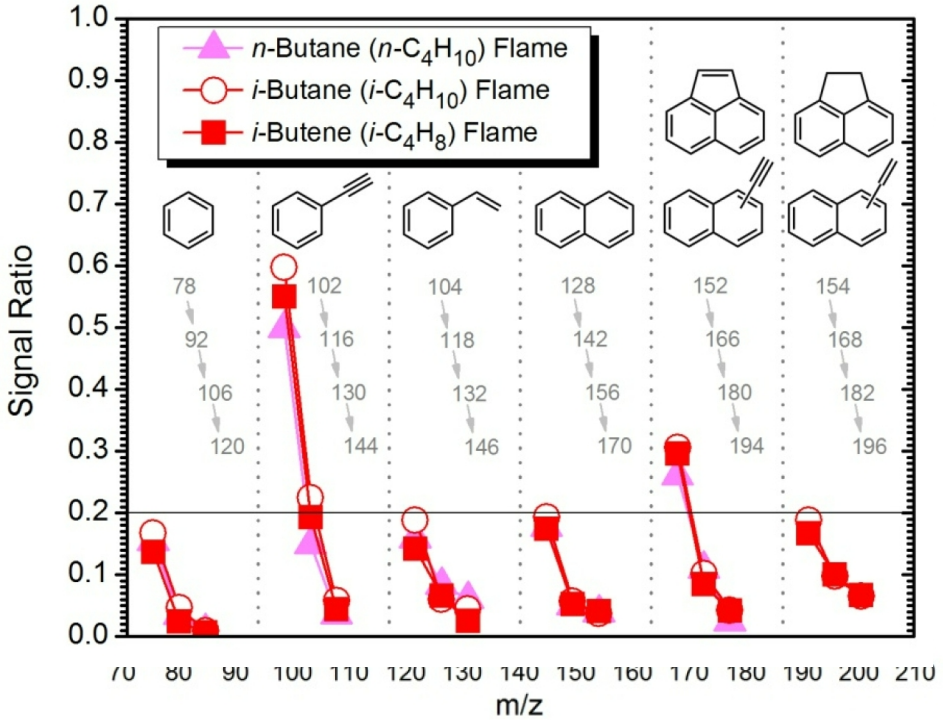
✓ Formation of Indene and Naphthalene



S. A. Skeen *et al., Energy Fuels,* **2011,** 25(12), 5611-5625
L. Ruwe *et al., Combust. Flame,* **2017,** 175, 34-46 and *Phys. Chem. Chem. Phys.,* **2018,** 20, 10780-10795

Molecular-Growth From The First Aromatic Ring to Pyrene



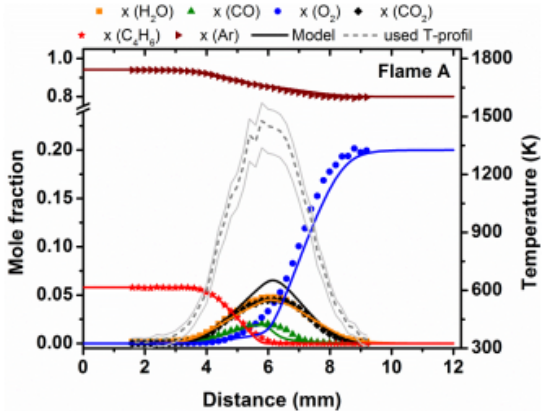


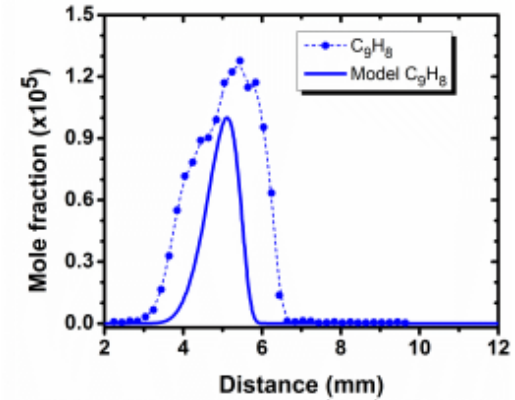
N. Hansen *et al., Combust. Flame,* **2017,** 180, 250-261

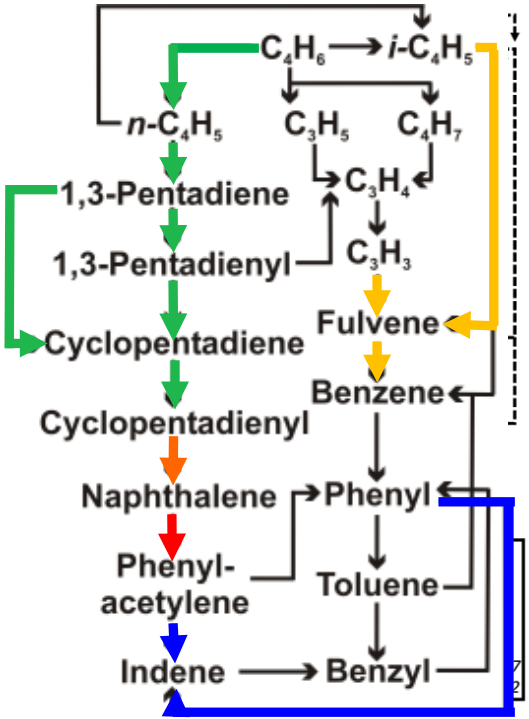
L. Ruwe *et al., Combust. Flame,* **2017,** 175, 34-46 and *Phys. Chem. Chem. Phys.,* **2018,** 20, 10780-10795

GAS PHASE CHEMICAL PHYSICS

Molecular-Growth From The First Aromatic Ring to Pyrene







- ✓ indene (A1R5) is formed via $C_6H_5 + C_3H_3$ and CH_3 + phenylacetylene (A1C2H) reactions
- ✓ with A1C2H being formed through naphthalene oxidation

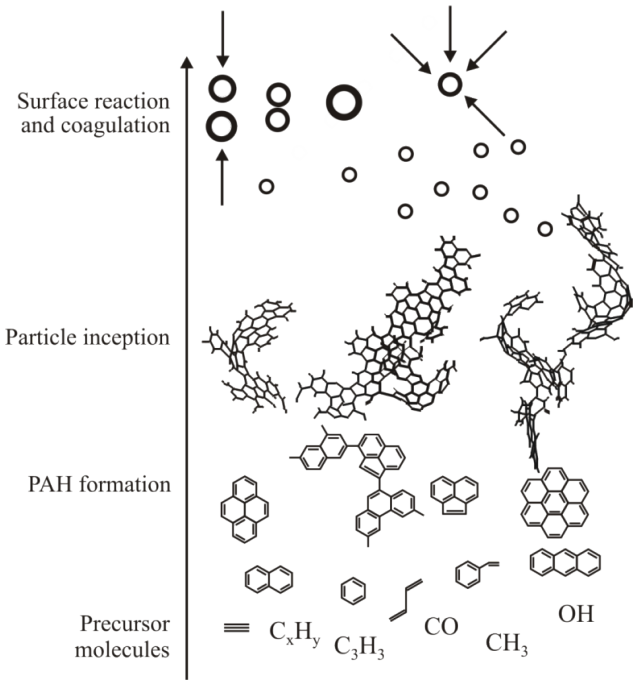
providing evidence for non-sequential growth

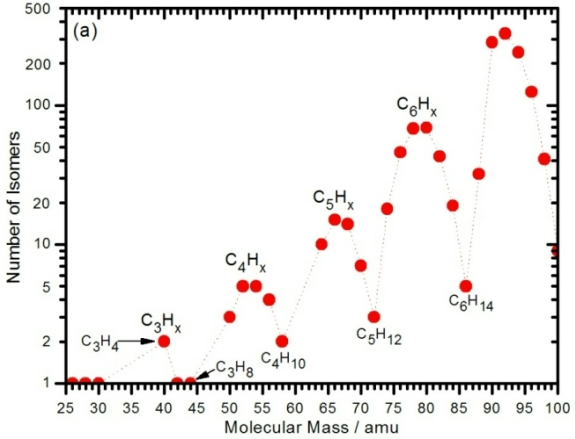
- ➢ highlights the need to better understand the 2nd ring formation

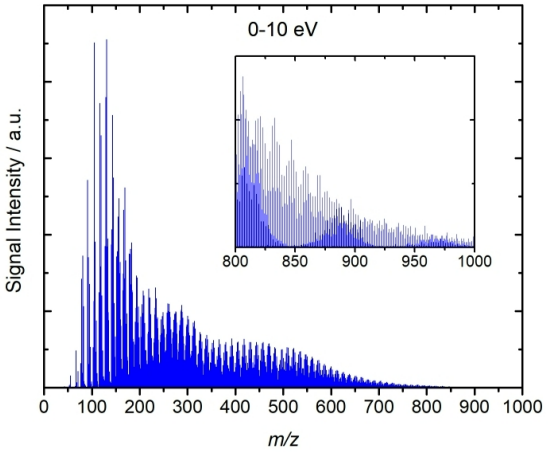
GAS PHASE CHEMICAL PHYSICS

K. Moshammer *et al., Proc. Combust. Inst.*, **2017,** 36(1), 947-955

PAH and Soot Formation Chemistry







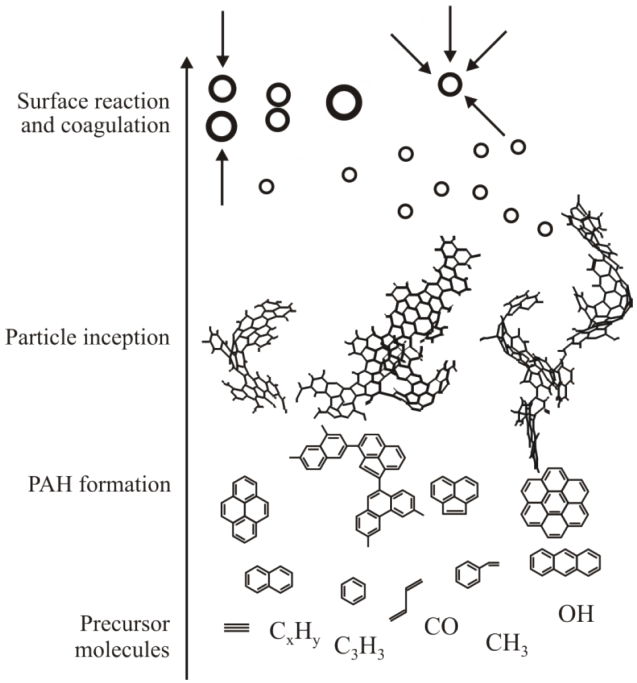
Challenges:

- Already the formation of the „first“ aromatic ring is governed by many different reactions involving many different reactants
- Number of possible isomers increases with molecular size
- The isomer-selective approach will break down

What is the right level of detail?

GAS PHASE CHEMICAL PHYSICS

PAH and Soot Formation Chemistry



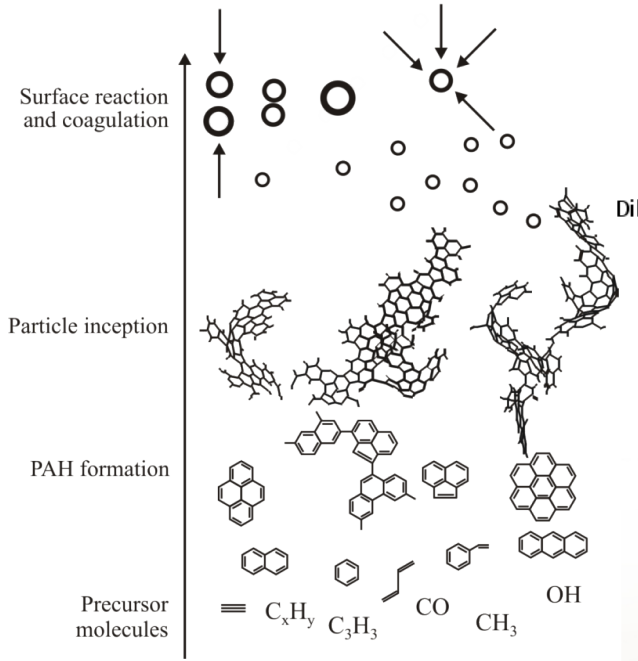
- ✓ PAH formation is governed by basic gas-phase organic chemistry, *i.e.* radical-radical and radical-molecule reactions
- ✓ we know how PAH radicals react, or more generally we know the outcome of A + B ⇄ C

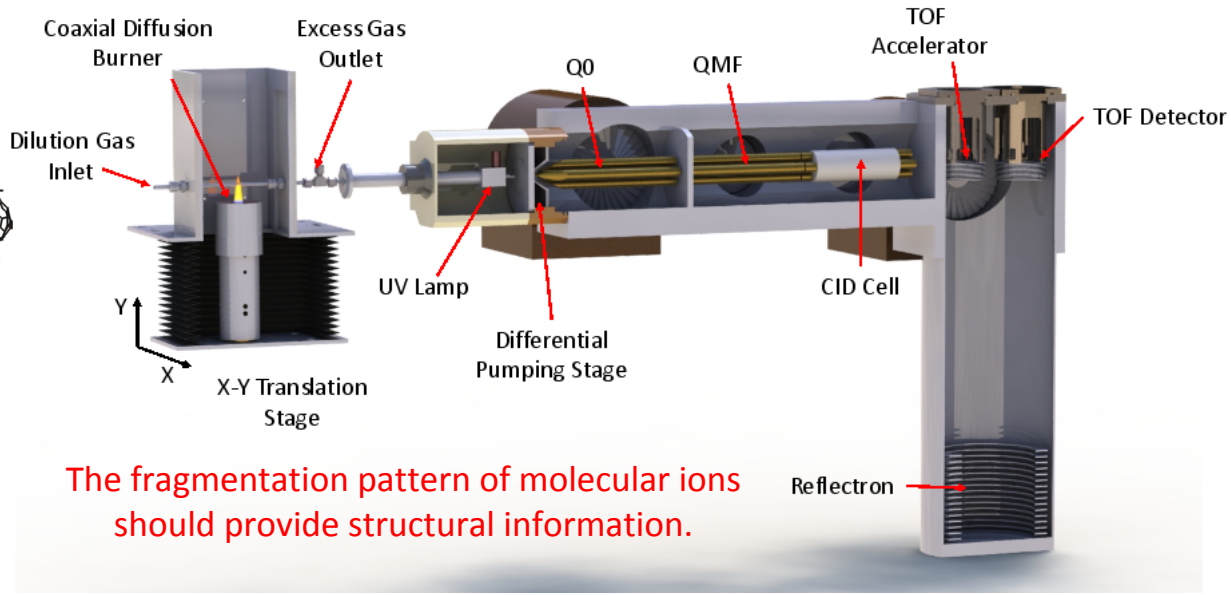
  ⇒ wherever five- and six-membered rings can form, they do
- ✓ the goal is not to identify all possible isomeric structures
- ✓ the goal is to identify the important intermediates at the right level of detail

  ⇒ re-occurring reactive structural features
- ✓ The diagnostic technique should be able to:
  - ➢ identify five-membered ring structures
  - ➢ aliphatically bridged PAHs
  - ➢ reactive side chains
  - ➢ functional groups, etc.

GAS PHASE CHEMICAL PHYSICS

Addressing the Complexity of Reaction Systems: Tandem Mass Spectrometry





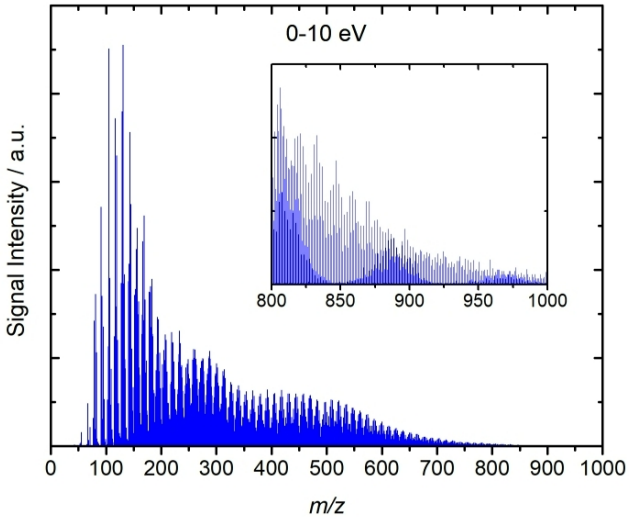
The fragmentation pattern of molecular ions should provide structural information.

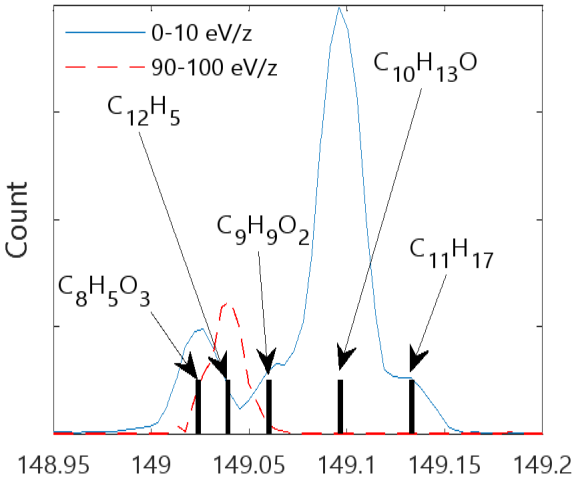
GAS PHASE CHEMICAL PHYSICS

B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(48), 9338-9349

Tandem Mass Spectrometry: General Performance of the Mass Spectrometer

- ✓ atmospheric pressure photoionization (APPI)
- ✓ two modes of operation:
  - ➢ time-of-flight mode
  - ➢ MS-MS mode (Δm ~1)
- ✓ Resolution: TOF ~8000
- ✓ collision gas: Ar
- ✓ sensitivity: tbd

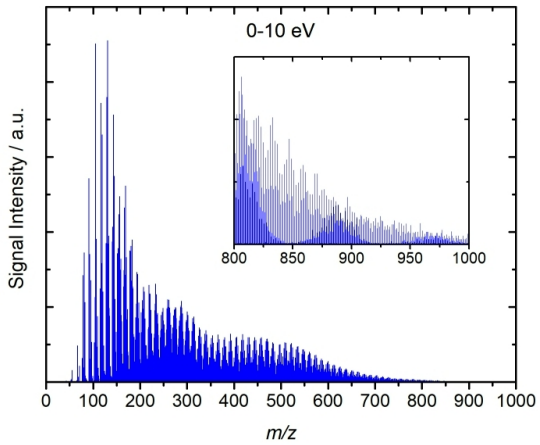




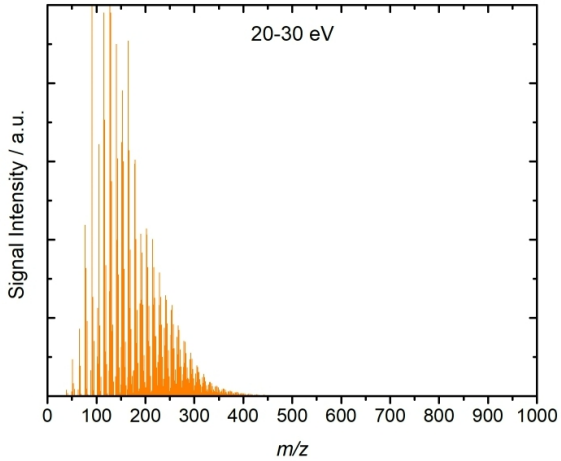
GAS PHASE CHEMICAL PHYSICS

B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(48), 9338-9349

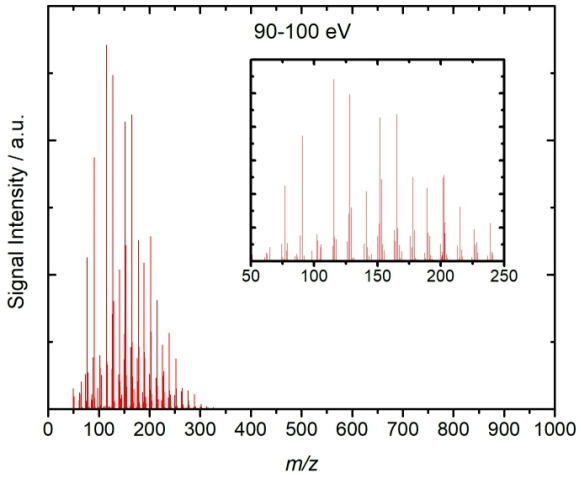
Tandem Mass Spectrometry
TOF-Mode: Identification of core-PAH Structures



Evidence for aliphatically bridged PAHs



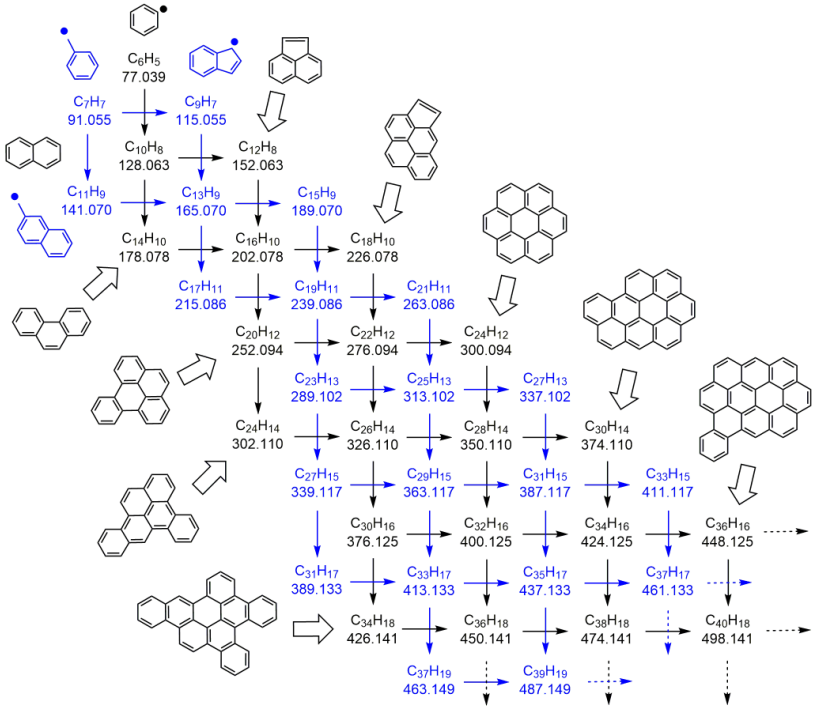
Identification of core-PAH structures



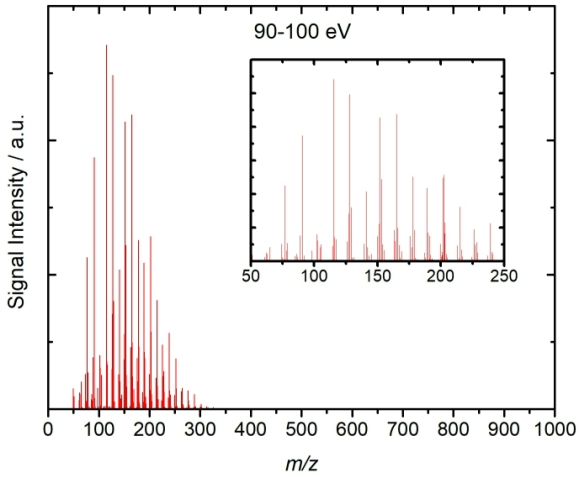
GAS PHASE CHEMICAL PHYSICS

B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(48), 9338-9349

Tandem Mass Spectrometry
TOF-Mode: Identification of core-PAH Structures



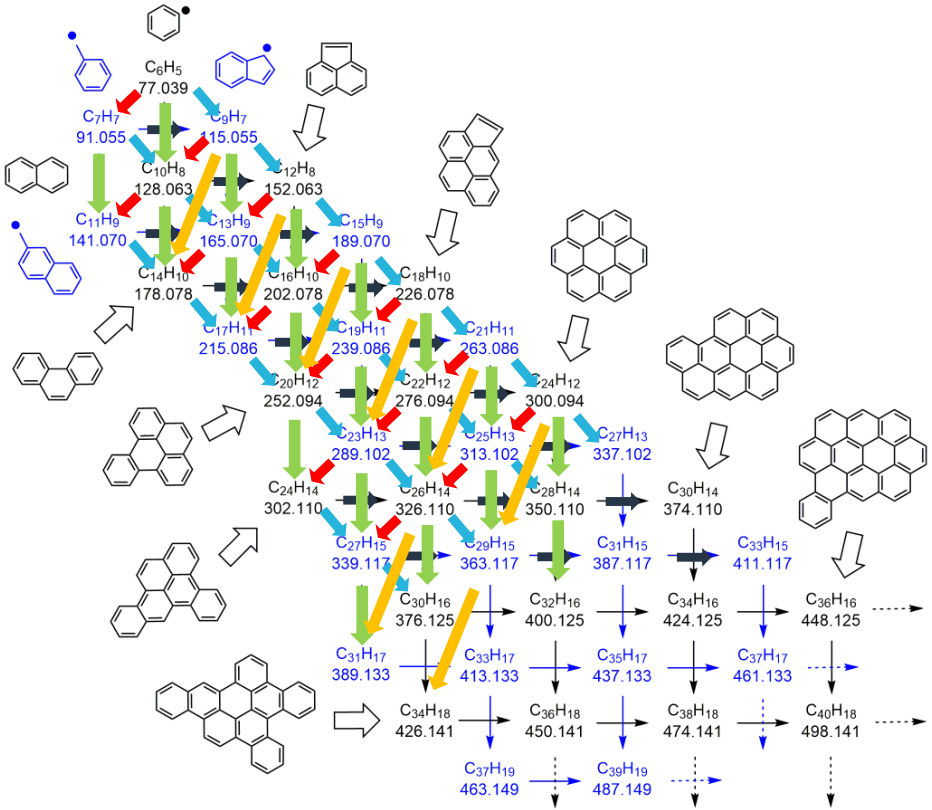
Identification of core-PAH structures



GAS PHASE CHEMICAL PHYSICS

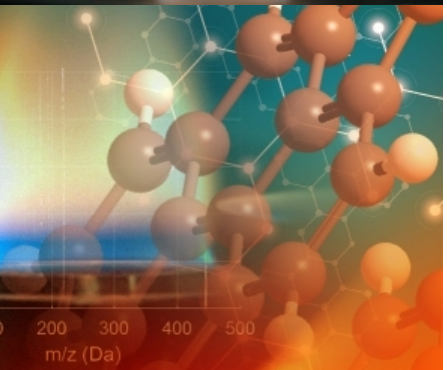
B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(48), 9338-9349

Identification of Main Reaction Pathways:



GAS PHASE CHEMICAL PHYSICS

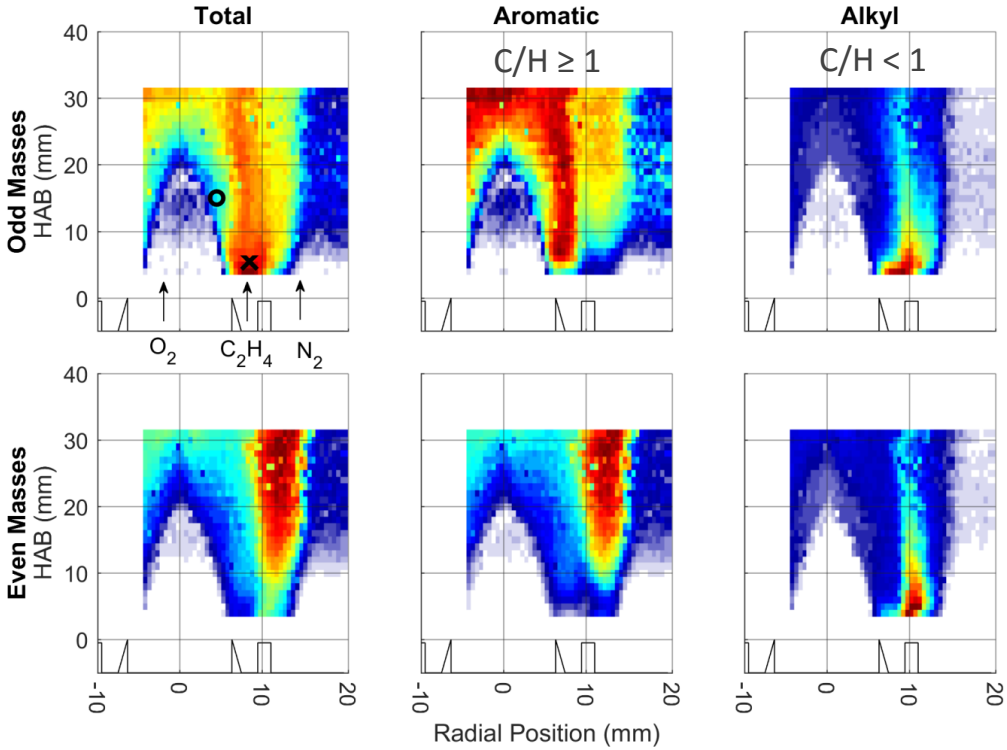
B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(48), 9338-9349



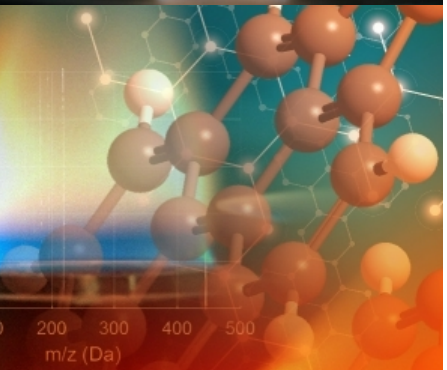
2D-Color Maps of PAHs in Co-Flow Diffusion Flames

radicals

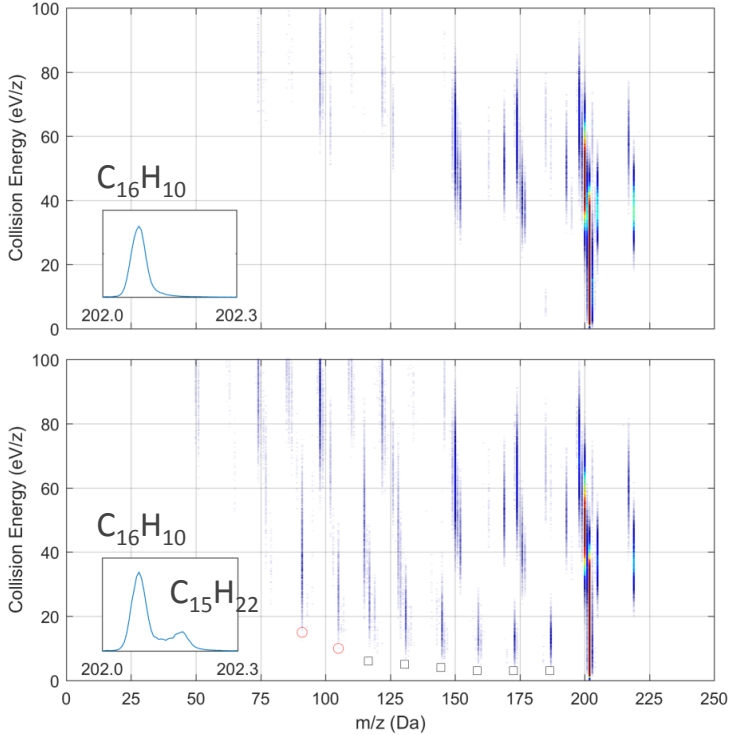
closed shell

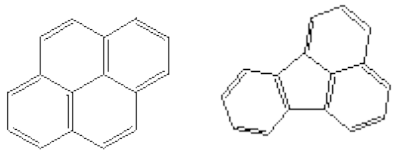


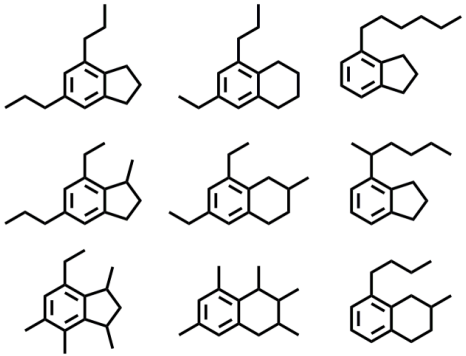
B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen,
J. Phys. Chem. A, **2018,** 122(48), 9338-9349



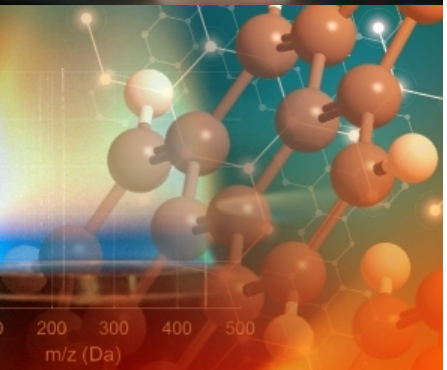
Tandem Mass Spectrometry (MS-MS Mode): Identification of aliphatically substituted PAHs



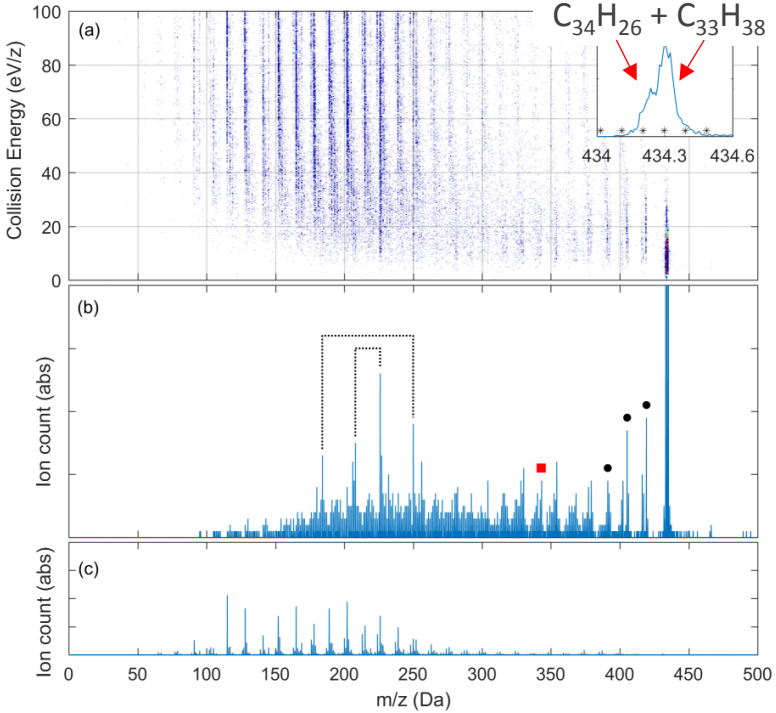


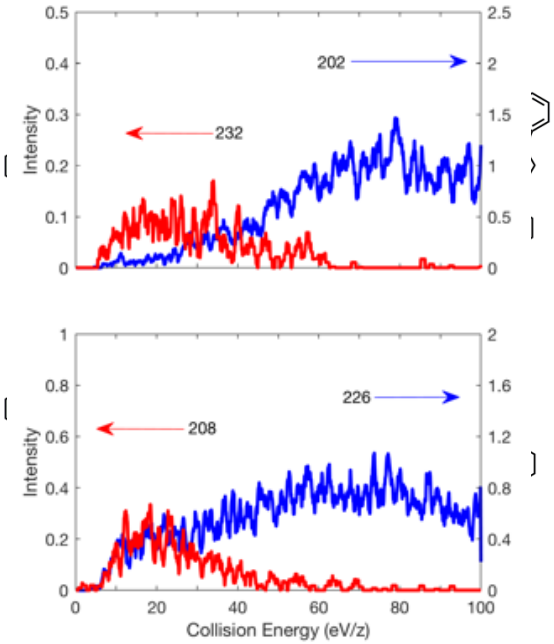


B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen,
J. Phys. Chem. A, **2018,** 122(48), 9338-9349

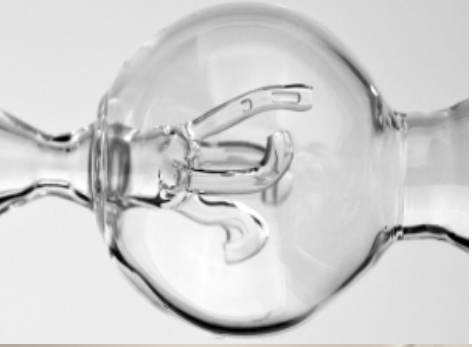


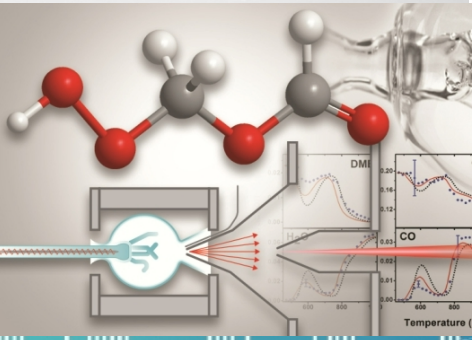
Tandem Mass Spectrometry (MS-MS Mode): Identification of aliphatically bridged PAHs

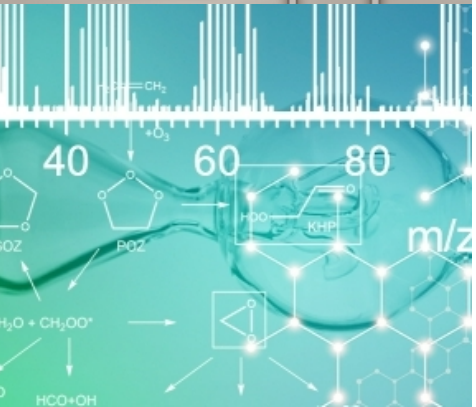




B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen,
J. Phys. Chem. A, **2018,** 122(48), 9338-9349



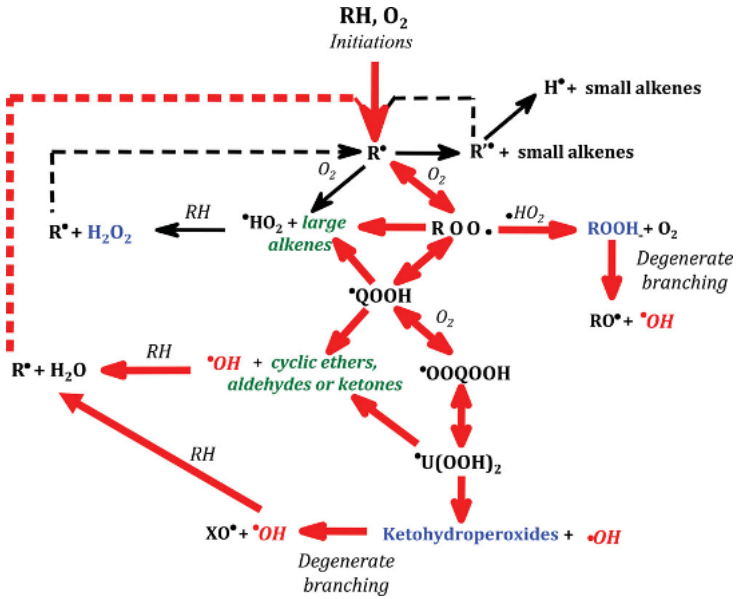




Introduction

Peroxy Radicals and Their Subsequent Reactions

- ❑ Low-Temperature Combustion
  - ✓ Temperature, pressure, and fuel structure determine whether these reactions are chain-terminating, propagating, or chain-branching
- ❑ Earth's Atmosphere
  - ✓ Oxidation of volatile organic compounds (VOCs)
  - ✓ Formation of Highly-Oxygenated Multi-functional (HOM) compounds

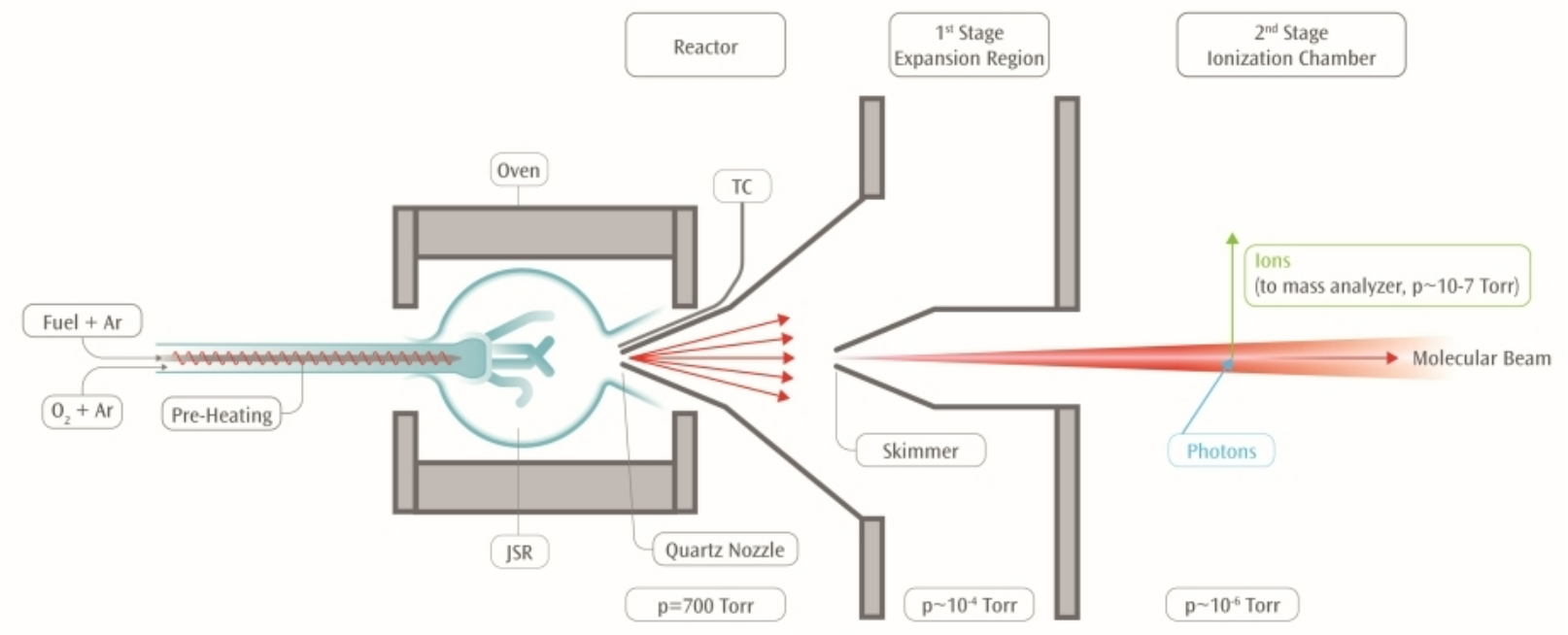


O. Herbinet, F. Battin-Leclerc, *Int. J. Chem. Kin.*, **2014,** 46(10), 619-639

GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation and Ignition Chemistry

Molecular-Beam Sampling Jet-Stirred Reactor

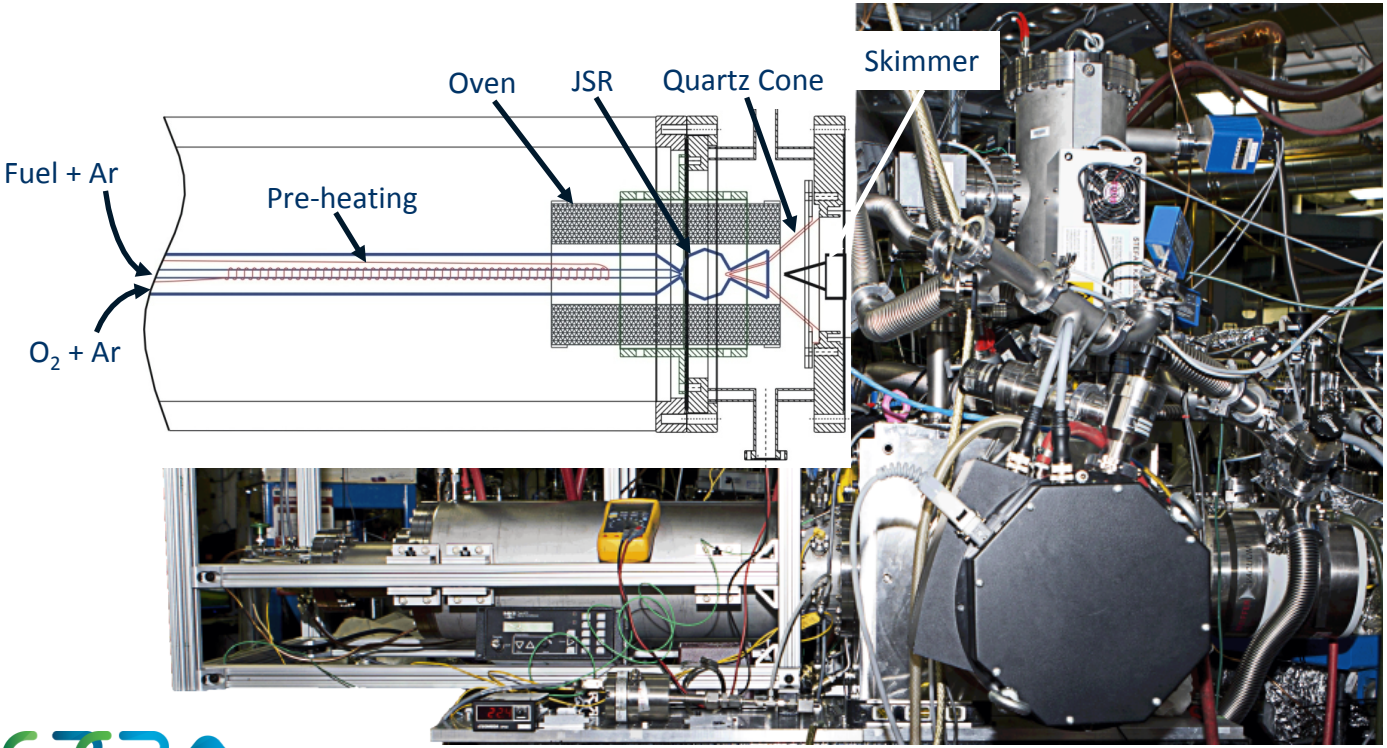


GAS PHASE CHEMICAL PHYSICS

K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

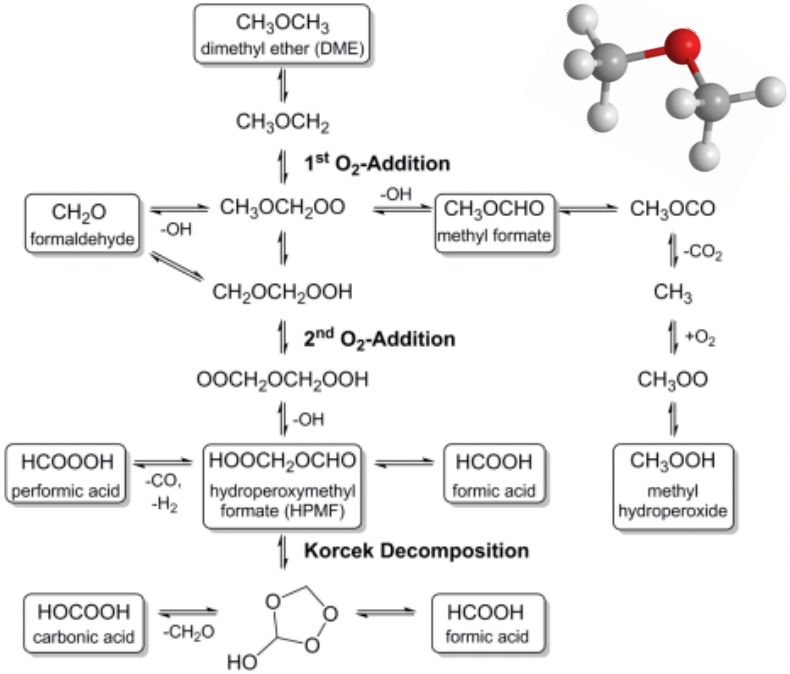
Low-Temperature Oxidation and Ignition Chemistry

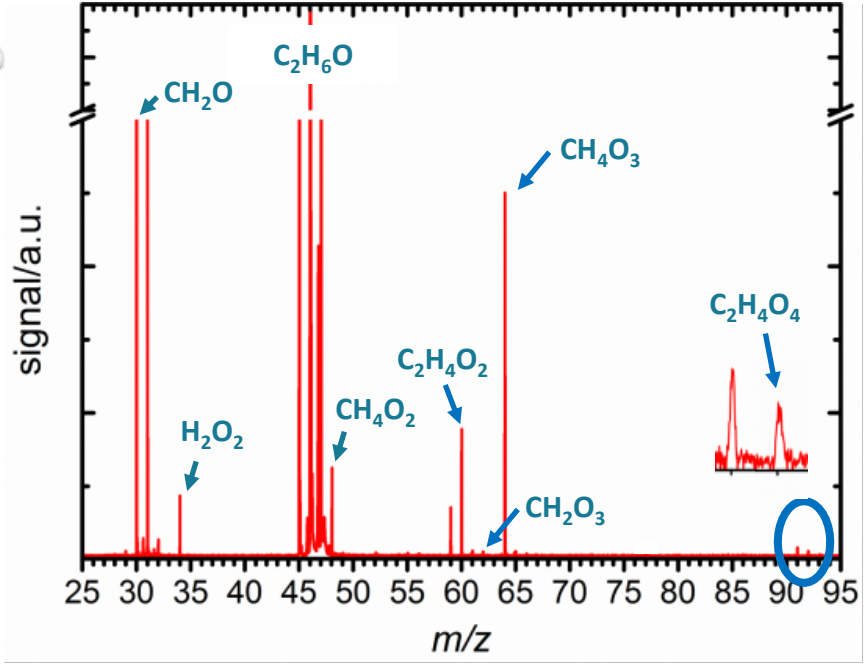
Molecular-Beam Sampling Jet-Stirred Reactor



GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation Chemistry of Dimethyl Ether (DME)





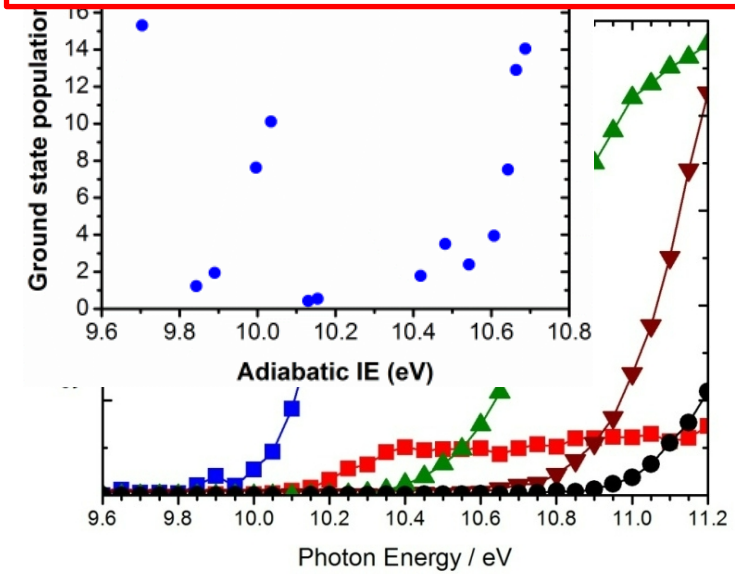
K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

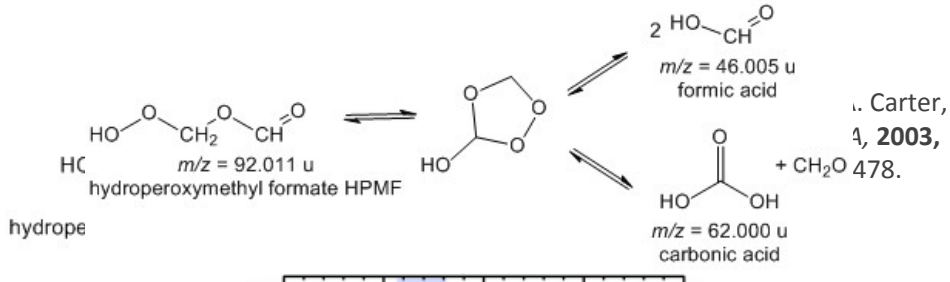
GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation of DME

Identification of the Ketohydroperoxide HPMF

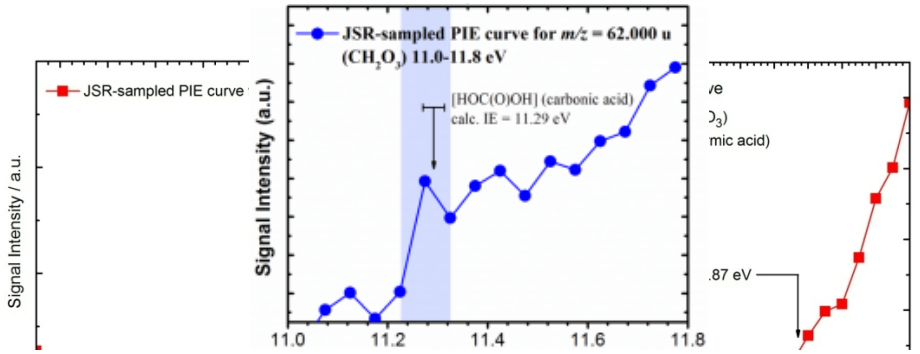
Fragment pattern gives additional evidence for the experimental detection of HPMF





. Carter,
4, **2003,**
478.

hydrope

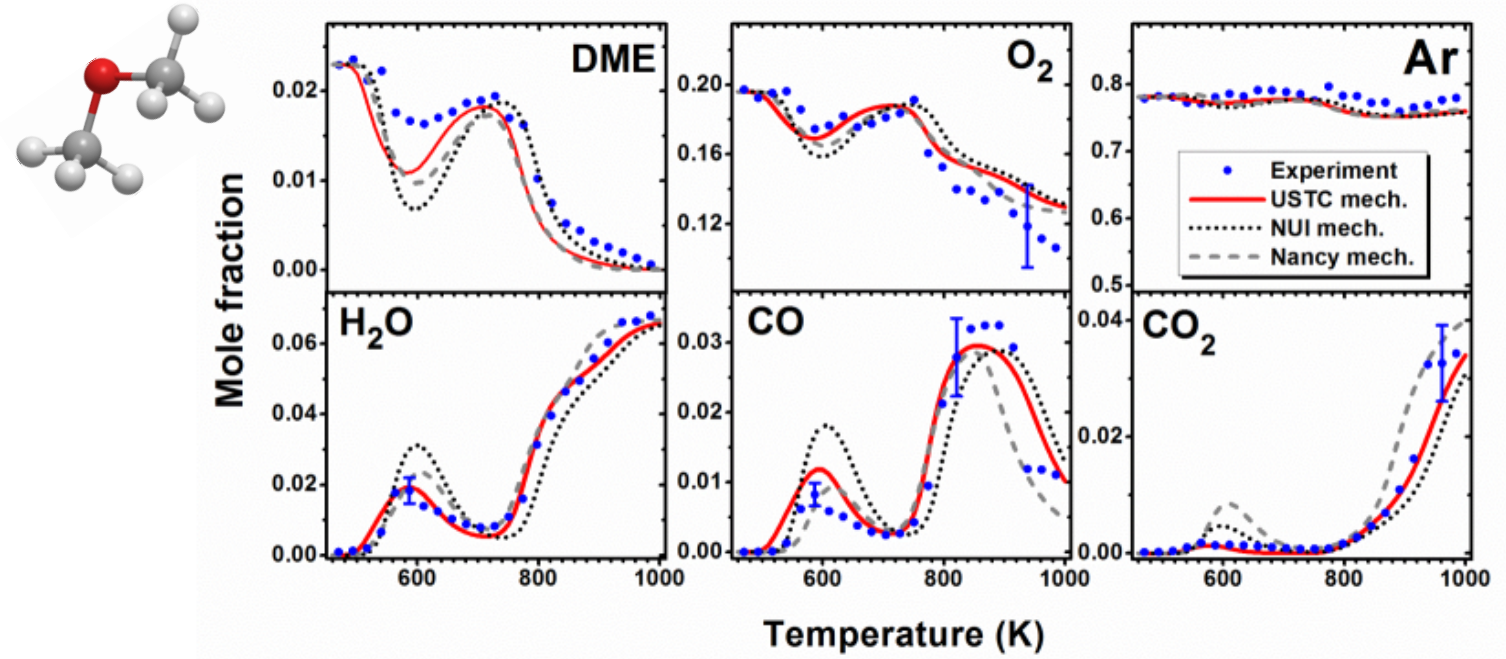


Detection of carbonic acid provides evidence for the Korcek decomposition mechanism!

K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

Low-Temperature Oxidation of DME

Quantification of the Main Species

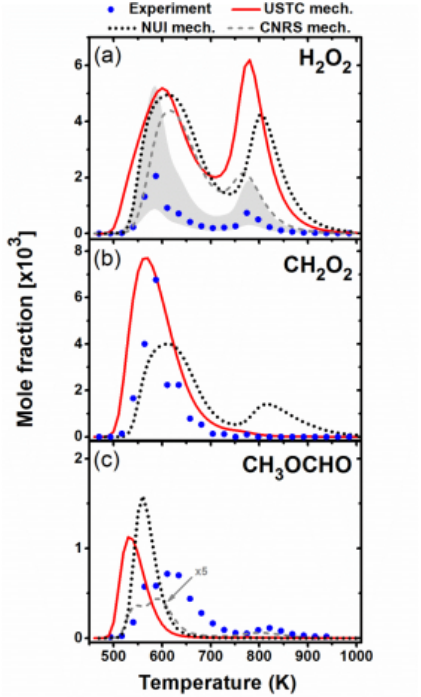


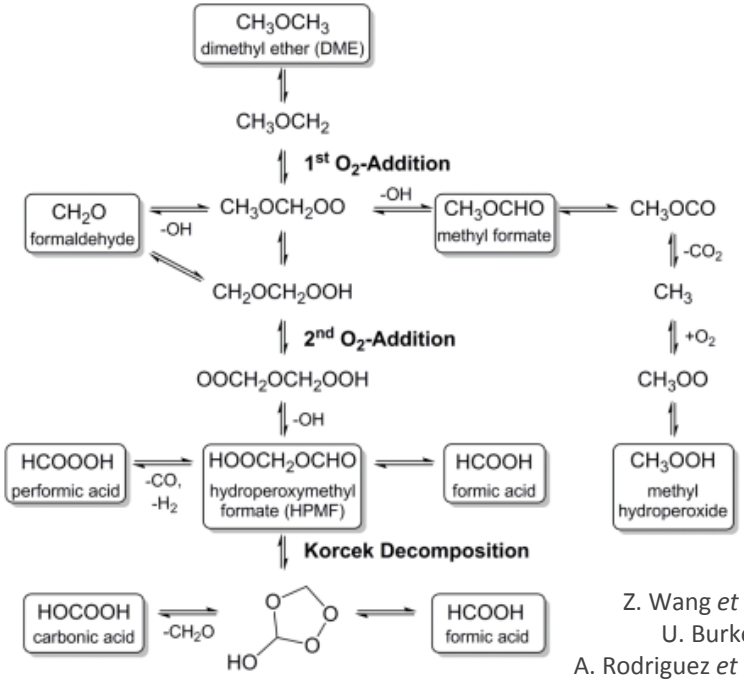
K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374

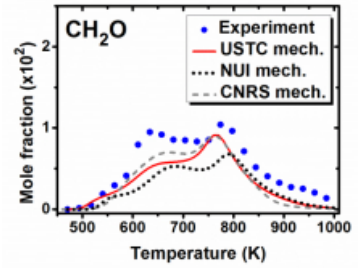
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

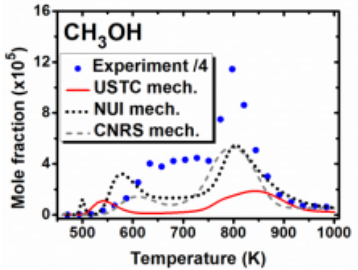
Low-Temperature Oxidation of DME

Quantification of Some Intermediates









Models:

Z. Wang *et al., Combust. Flame,* **2015,** 162, 1113-1125 (USTC)
U. Burke *et al., Combust. Flame,* **2015,** 162, 315-330 (NUI)
A. Rodriguez *et al., J. Phys. Chem. A,* **2015,** 119, 7905-2923 (CNRS)

K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation of DME

Quantification of CH_3OOH and the Ketohydroperoxide HPMF

- using calculated photoionization cross sections

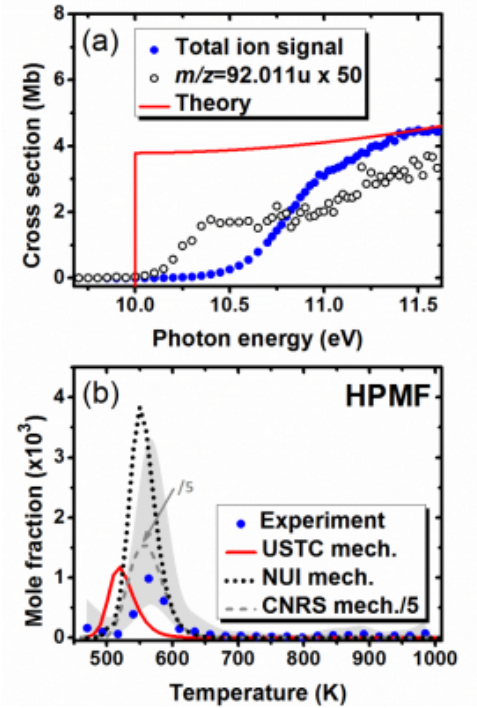
R. R. Lucchese, Texas A&M

ePolyScat (version E3)

F. A. Gianturco *et al., J. Chem. Phys.,* **1994,** 100, 6464-6471

A.P.P. Natalense *et al., J. Chem. Phys.,* **1999,** 111, 5344-5348

A. W. Jasper, Argonne



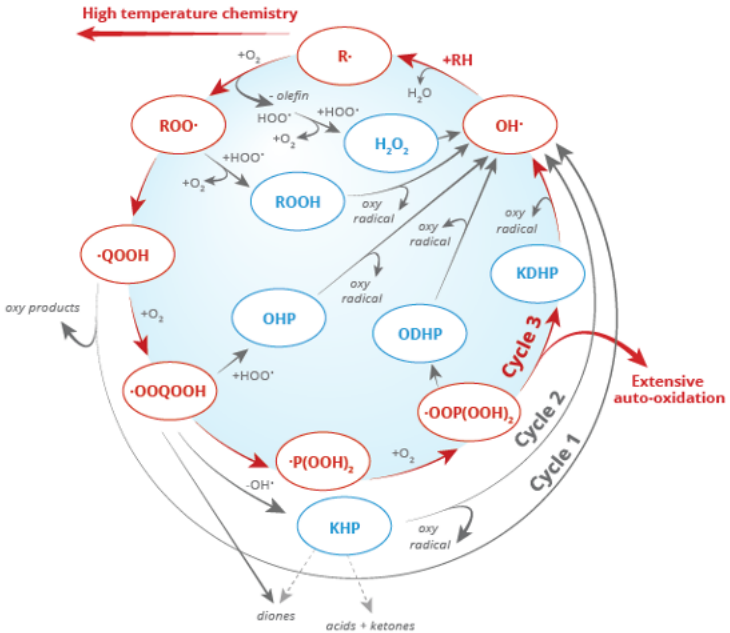
- tested against a variety of known species
  ⇒ uncertainty ≤ a factor of 2
- it calculates total cross sections
  ⇒ fragmentation pattern needs to be known
- it doesn't calculate Franck-Condon overlaps
  ⇒ scale to experimental photoionization efficieny curves

GAS PHASE CHEMICAL PHYSICS

K. Moshammer *et al., J. Phys. Chem. A,* **2015,** 119, 7361-7374
K. Moshammer *et al., J. Phys. Chem. A,* **2016,** 120, 7890-7901

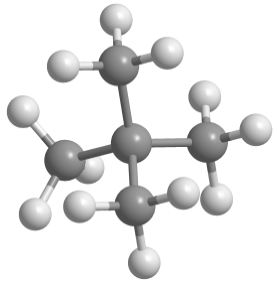
Low-Temperature Oxidation

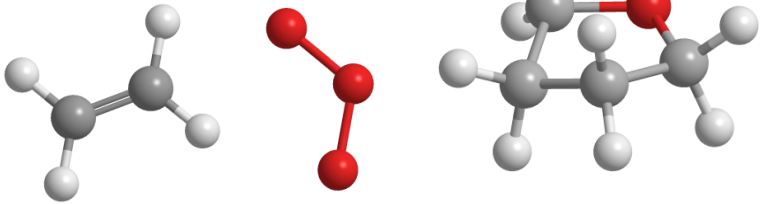
neo-Pentane and Tetrahydrofuran as Logical Extension



Z. Wang, O. Herbinet, N. Hansen, F. Battin-Leclerc, *Progr. Energy Combust. Sci.*, **2019,** 73, 132-181

- ❑ apply the insights gained from the DME project to study the low-temperature oxidation of a more complex molecular system:
  - ✓ *neo*-pentane
  - ✓ tetrahydrofuran (THF)
  - ✓ ethylene ozonolysis

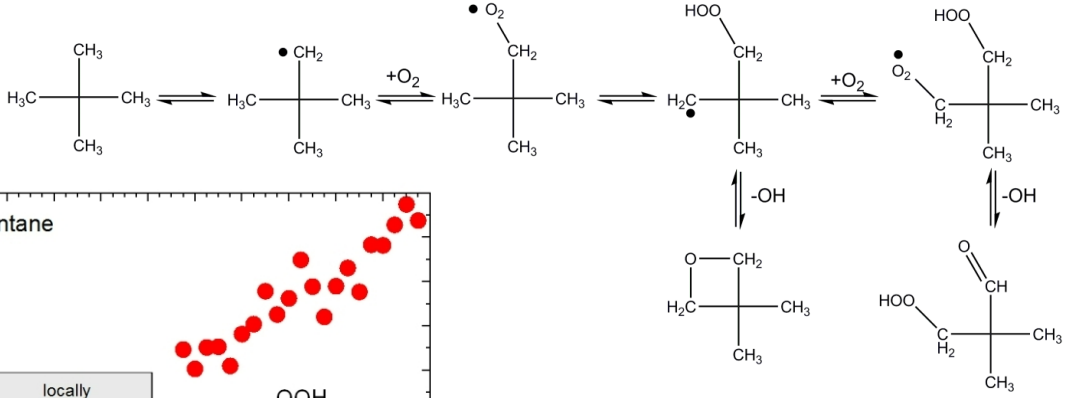


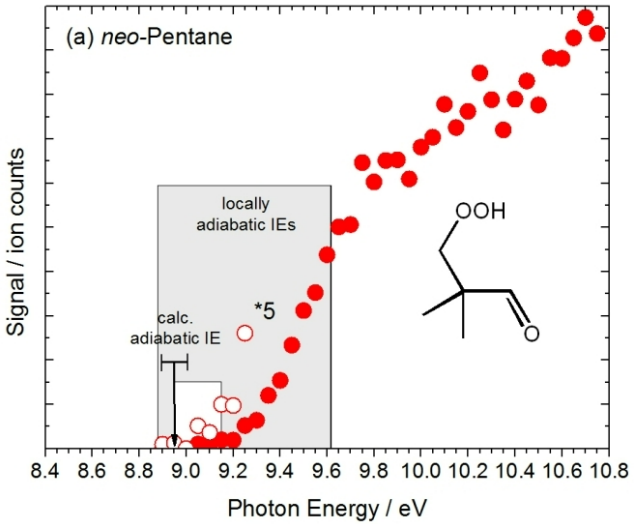


GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation of *neo*-Pentane

Detection and Identification of the KHP





Fragmentation Channel	Calculated AE, eV[a]	Experimentally observed AE, eV
HOO-CH_2-$C(CH_3)_2H^+$ ($C_4H_{10}O_2^+$) + CO	9.41	9.40
HOO-CH_2-$C(CH_3)_2CO^{\cdot+}$ ($C_5H_9O_3^+$) + H	10.18	10.1
HOO-CH_2-$C(CH_3)_2^{\cdot+}$ ($C_4H_9O_2^+$) + ·CHO	10.44	10.5
·$C(CH_3)_2CHO^+$ ($C_4H_7O^+$) + ·CH_2OOH	10.70	10.65

GAS PHASE CHEMICAL PHYSICS

N. Hansen *et al., Proc. Combust. Inst.,* **2019,** to be submitted

Low-Temperature Oxidation of Tetrahydrofuran

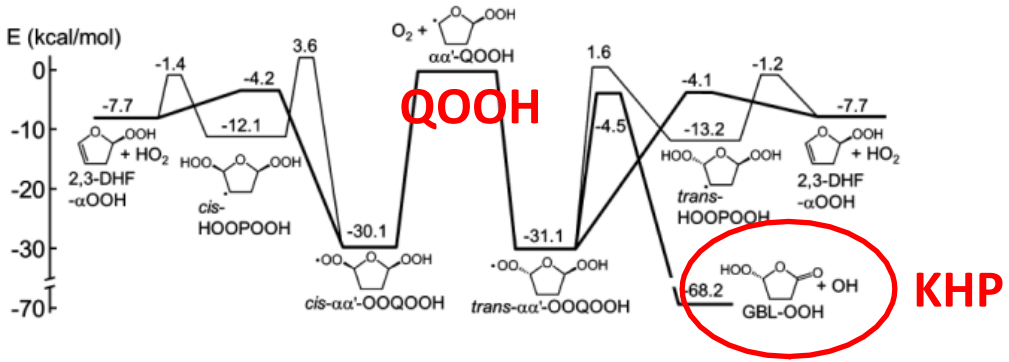
Isomer-resolved Identification and Quantification of the KHP

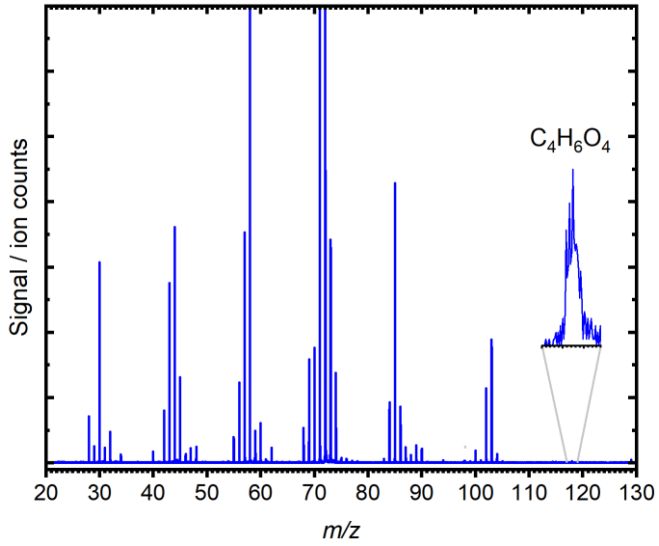
THE JOURNAL OF PHYSICAL CHEMISTRY A — Article — pubs.acs.org/JPCA

Pressure-Dependent Competition among Reaction Pathways from First- and Second-O_2 Additions in the Low-Temperature Oxidation of Tetrahydrofuran

Ivan O. Antonov, Judit Zádor, Brandon Rotavera, Ewa Papajak, David L. Osborn, Craig A. Taatjes, and Leonid Sheps*

Combustion Research Facility, Sandia National Laboratories, Livermore, California 94551, United States





Antonov *et al., J. Phys. Chem. A* **2016,** *120,* 6582−6595

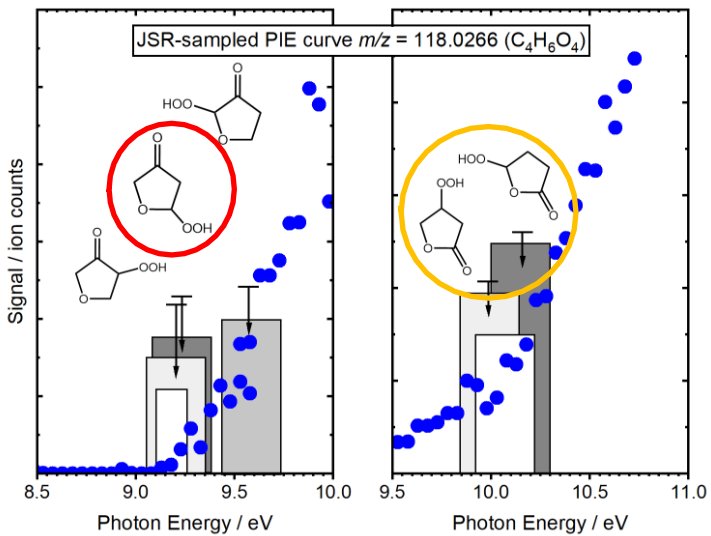
N. Hansen *et al., J. Phys. Chem. A,* **2019,** to be submitted

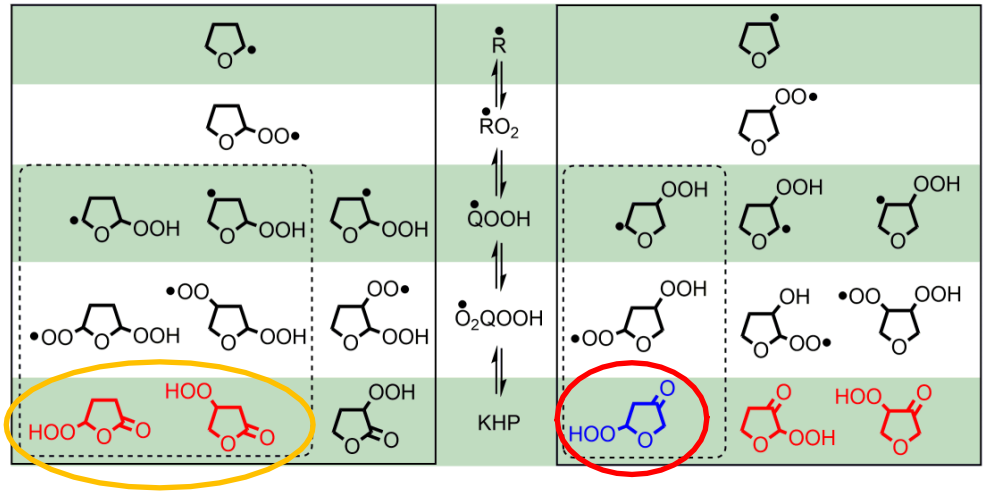
GAS PHASE CHEMICAL PHYSICS

Low-Temperature Oxidation of Tetrahydrofuran

Isomer-resolved Identification of the KHP

"…energies were calculated using M06-2X/cc-pVTZ geometries and frequencies and a high level energy correction that approximates the CCSD(T)/CBS result, where ~CCSD(T)/CBS = CCSD(T)/cc-pVTZ + MP2/CBS – MP2/cc-pVTZ and the CBS limit was approximated using a two point formula and the cc-pVTZ and cc-pVQZ basis sets." – Ahren Jasper (Argonne)





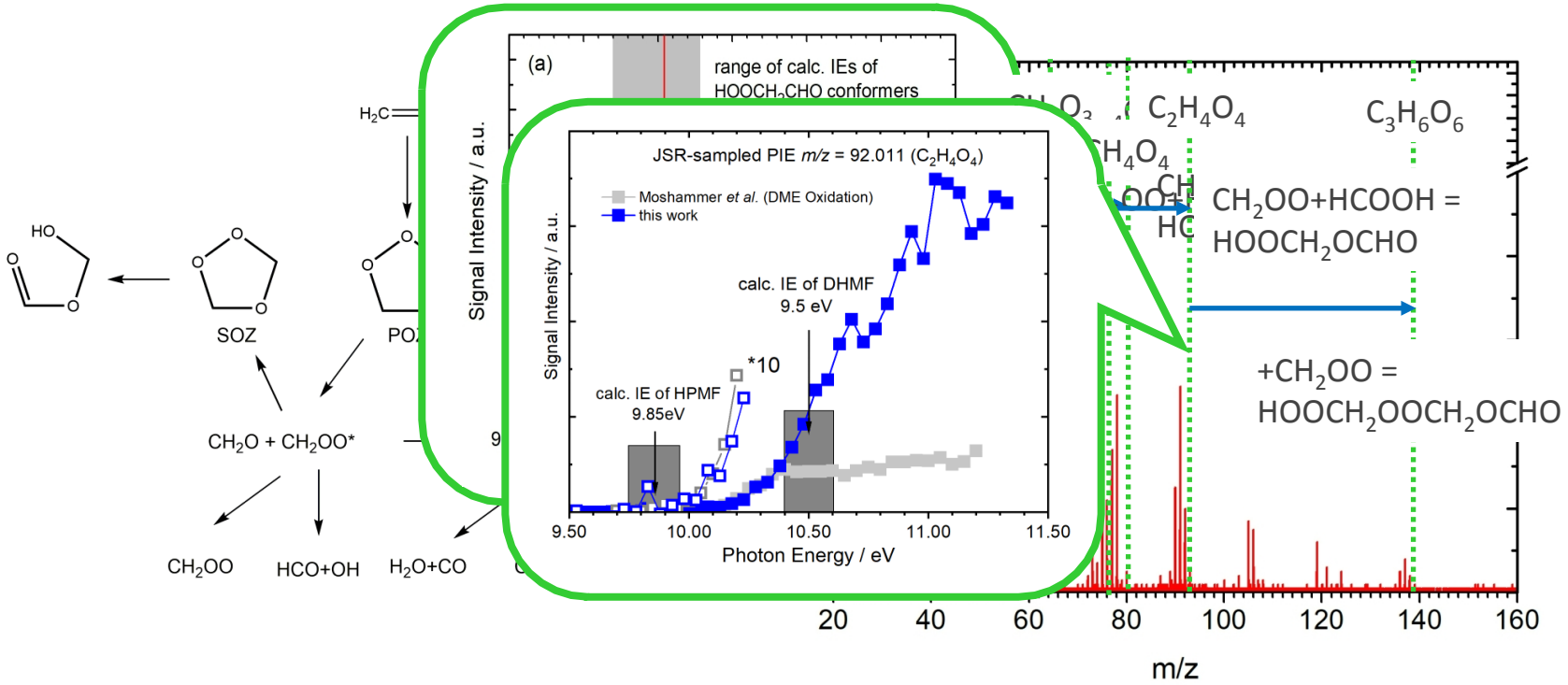
✓ successfully identified at least two different isomeric forms of the KHP

N. Hansen *et al., J. Phys. Chem. A,* **2019,** to be submitted

GAS PHASE CHEMICAL PHYSICS

Ozonolysis of Ethylene

Ketohydroperoxide and Criegee Intermediate Reactions

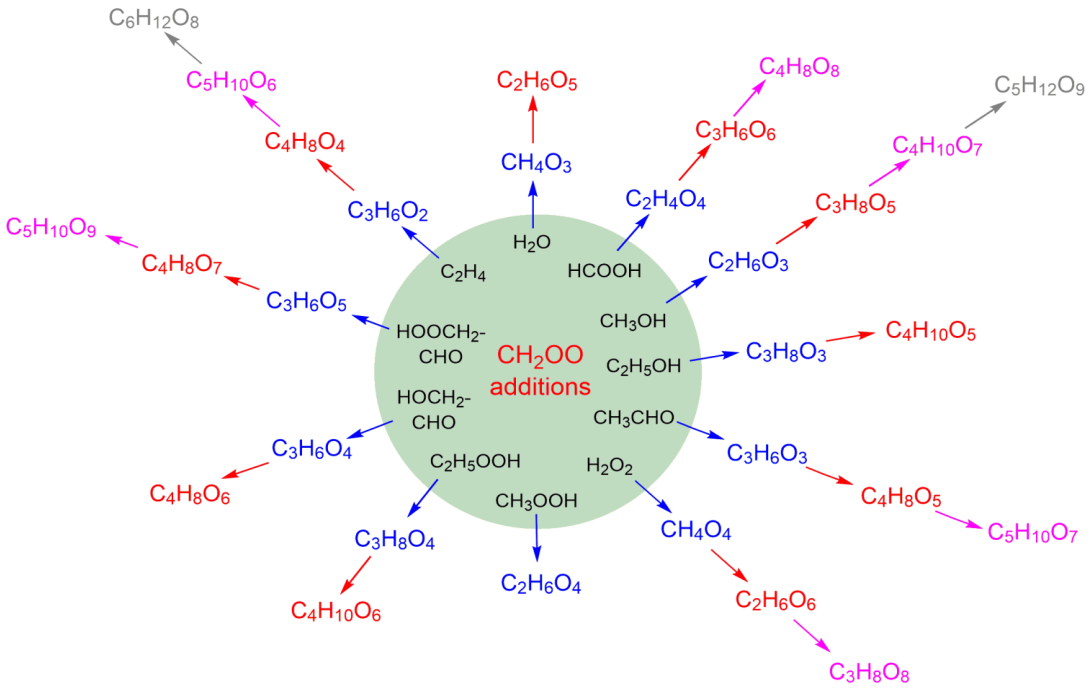


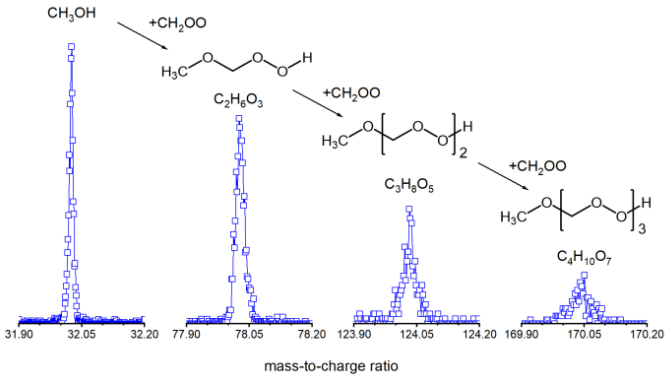
GAS PHASE CHEMICAL PHYSICS

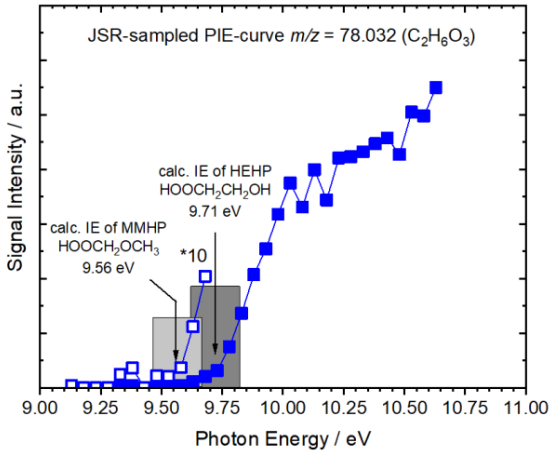
A. C. Rousso, A. W. Jasper, Y. Ju, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(43), 8674-8685 and *Phys. Chem. Chem. Phys.,* **2019,** 21, 7341-7357

Ozonolysis of Ethylene

Network of Criegee Intermediate Reactions



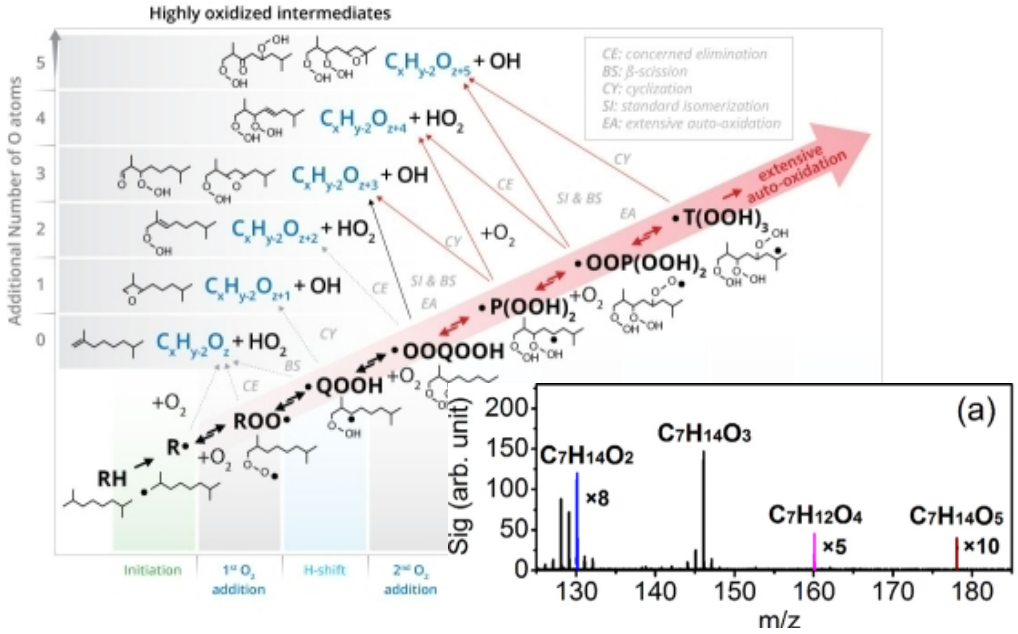




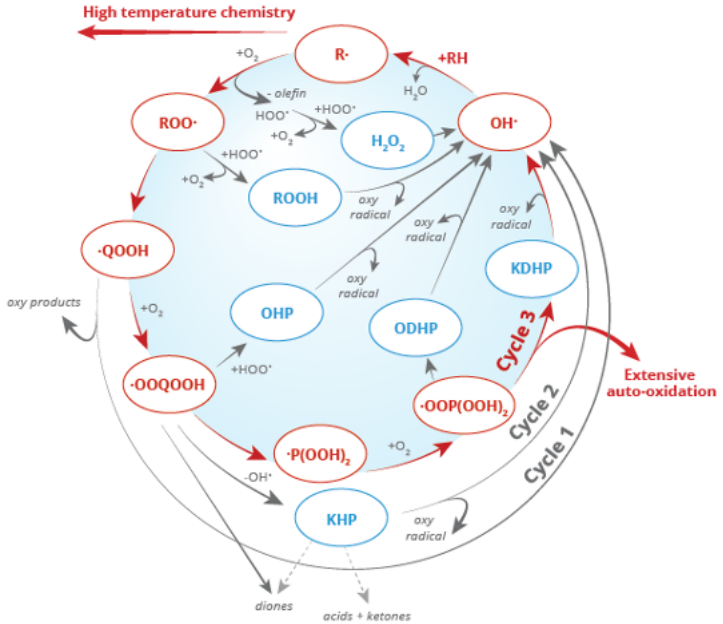
GAS PHASE CHEMICAL PHYSICS

A. C. Rousso, A. W. Jasper, Y. Ju, N. Hansen, *J. Phys. Chem. A,* **2018,** 122(43), 8674-8685 and *Phys. Chem. Chem. Phys.,* **2019,** 21, 7341-7357

Highly Oxygenated Molecules in Ignition Chemistry
3rd O_2 Addition



Z. Wang *et al., Combust. Flame,* **2016,** 280, 386-396, *Proc. Combust. Inst.,* **2017,** 36, 373–382, and *Proc. Nat. Acad. Sci.,* **2017,** 114(50), 13102-13107



Z. Wang, O. Herbinet, N. Hansen, F. Battin-Leclerc, *Progr. Energy Combust. Sci.,* **2019,** 73, 132-181

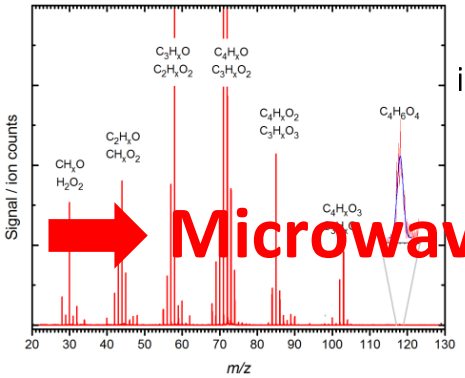
GAS PHASE CHEMICAL PHYSICS

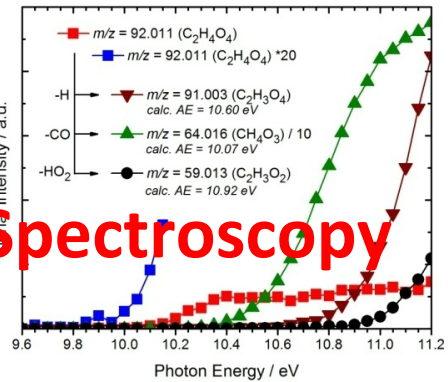
Addressing the Complexity of Reaction Systems: Rotational Spectroscopy

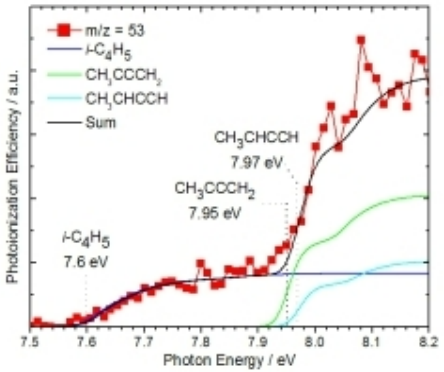
- dissociative ionization might preclude a complete qualitative and quantitative interpretation of the sampled mass spectra
- similar ionization energies and photoionization efficiency curves may prevent isomer-specific assignments
- small Franck-Condon overlaps might hamper an adequate formation and sensitive detection of the corresponding ion
- access to synchrotron facilities for photoionization measurements might be very competitive and limited

G

➢ iates urren







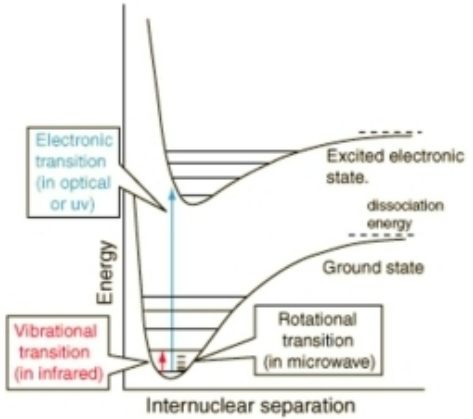
Microwave Spectroscopy

GAS PHASE CHEMICAL PHYSICS

Microwave Spectroscopy as a Diagnostic Tool

MW spectroscopy is the most accurate way to determine molecular structures

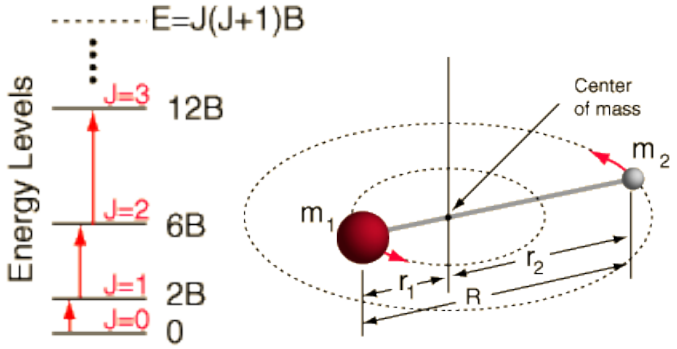
- ✓ rotational transitions are uniquely dependent on the molecular structure
- ✓ characteristic fingerprints due to *fine* and *hyperfine structures,* and *internal rotation effects*
- ✓ superior resolution ($E/\Delta E \sim 10^6$)



Challenges:

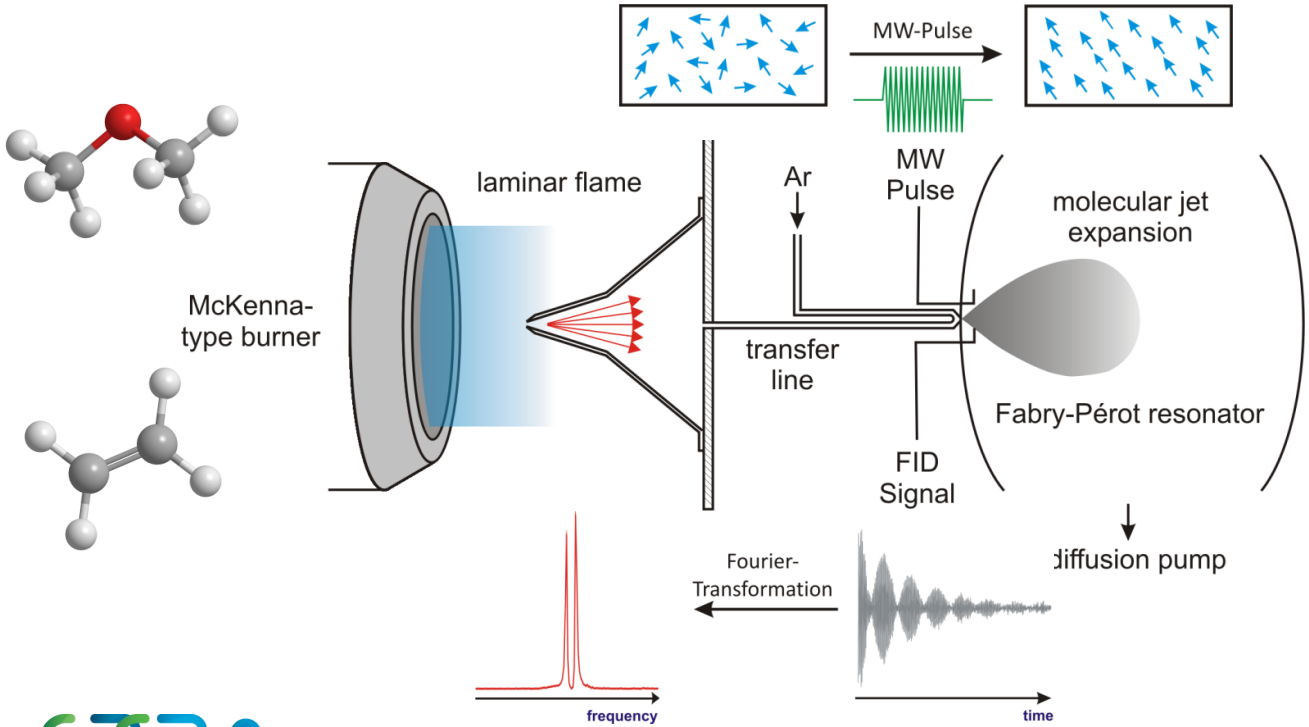
the rotational temperature of the targeted species must be:

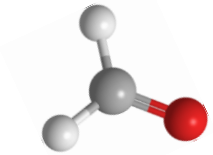
- ➢ sufficiently cooled after sampling from the hot (up to ~2300 K) environment of the reactors
- ➢ independent of the varying temperatures at different sampling positions



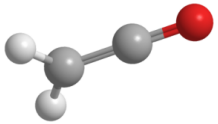
GAS PHASE CHEMICAL PHYSICS

Addressing the Complexity of Reaction Systems: Rotational Spectroscopy

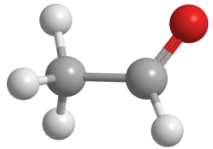




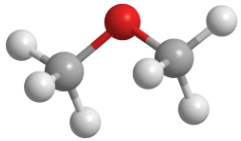
$2_{1,1}$-$2_{1,2}$ (14488.479 MHz)



$1_{0,1}$-$0_{0,0}$ (20209.201 MHz)



$1_{0,1}$-$0_{0,0}$ (19262.140 MHz)

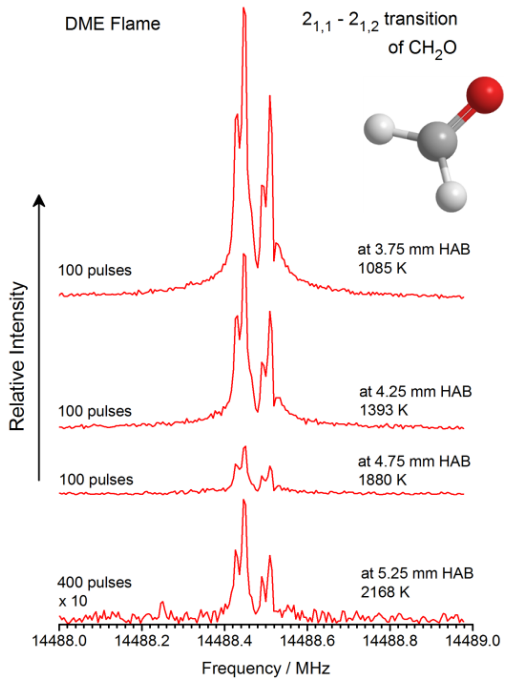


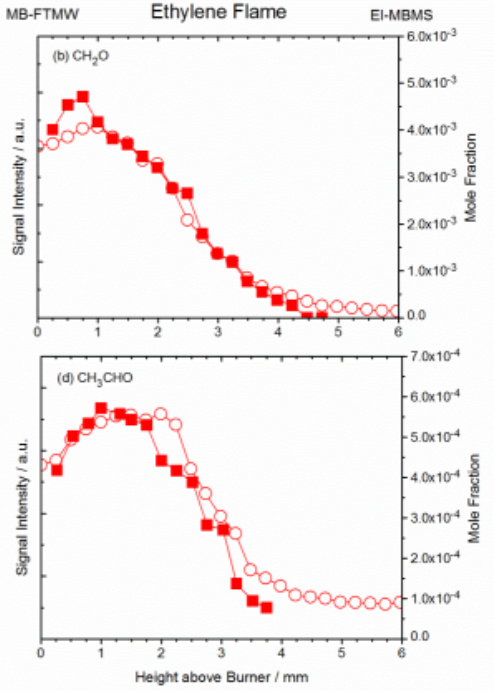
$2_{0,2}$-$1_{1,1}$ (9118.816 MHz)

N. Hansen *et al., RSC Advances,* **2017,** 7(60), 37867-37872

GAS PHASE CHEMICAL PHYSICS

Addressing the Complexity of Reaction Systems: Rotational Spectroscopy



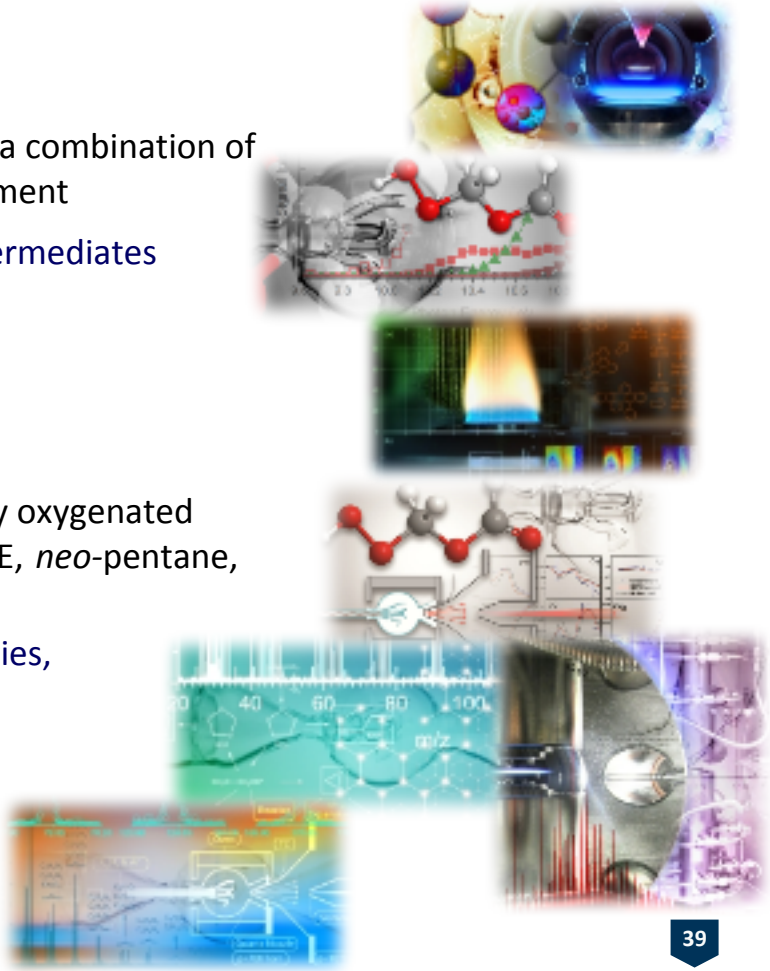


N. Hansen *et al., RSC Advances,* **2017,** 7(60), 37867-37872

GAS PHASE CHEMICAL PHYSICS

Summary

- address the complexity of chemical reaction networks with a combination of experiments, data analysis procedures, and model development
  - ✓ identify reaction pathways, detect and quantify key intermediates
- molecular-weight growth reactions and formation of PAHs
  - ✓ identification of the foundational PAHs
  - ✓ detection of aliphatically bridged multi-core PAHs
- detection, identification, and quantification of elusive highly oxygenated intermediates during the low-temperature oxidation of DME, *neo*-pentane, and THF
  - ✓ conformer-dependent ionization and appearance energies, photoionization cross sections
- identification of Criegee-Intermediate reaction network
- rotational spectroscopy as analytical tool



GAS PHASE CHEMICAL PHYSICS

Acknowledgments

Experiments:

- P. Dagaut (CNRS Orleans, France)
- K. Kohse-Höinghaus (Universität Bielefeld, Germany)
- D. Popolan-Vaida (University of Florida)
- S. M. Sarathy (KAUST, Saudi Arabia)
- B. Yang (Tsinghua University, Beijing, China)
- S. A. Skeen (Sandia National Laboratories)
- J.-U. Grabow (Universität Hannover, Germany)
- Y. Ju (Princeton University)
- P. G. Fugazzi (Sandia National Laboratories)

Modeling and Theoretical Support:

- A. W. Jasper (Argonne National Laboratory)
- S. J. Klippenstein (Argonne National Laboratory)
- F. Mauss (Cottbus, Germany)

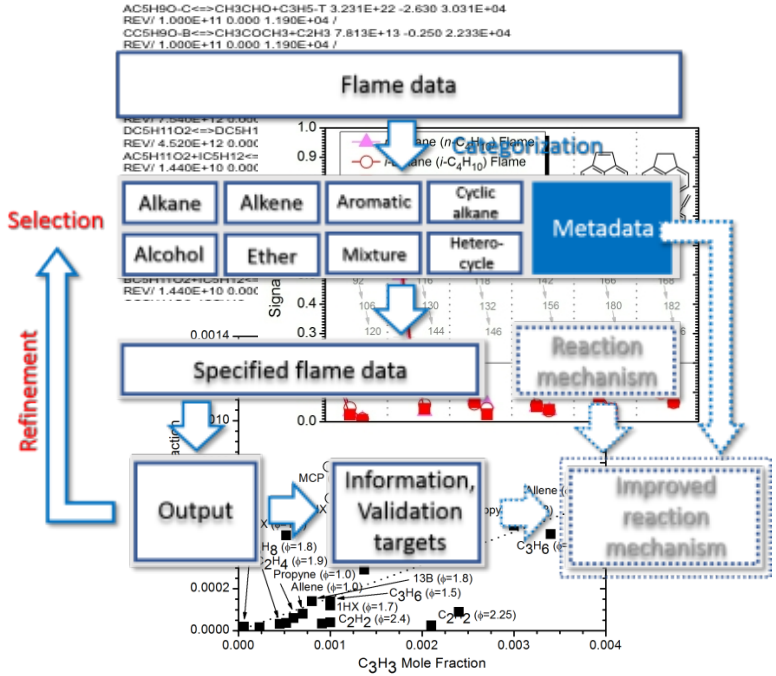
Postdocs and Students:

- K. Moshammer, A. Rousso, J. Wullenkord, L. Ruwe, B. Adamson

Funding: Basic Energy Sciences, US Department of Energy
Sandia's LDRD program

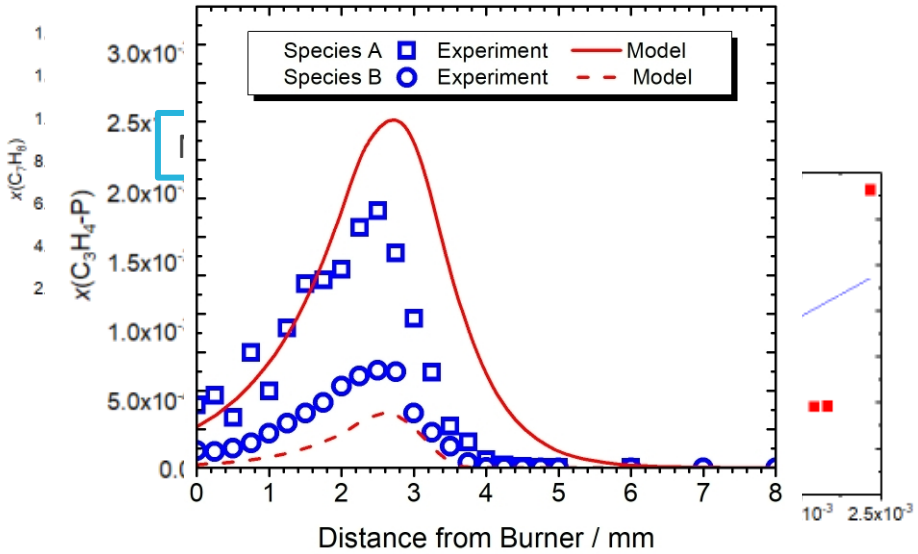
GAS PHASE CHEMICAL PHYSICS

Addressing the Complexity of Reaction Systems: New Validation Targets



Development of a Low-Pressure Flame Database

more than 50 flames from five different labs



N. Hansen *et al., Proc. Combust. Inst.*, **2011,** 33, 585-592

N. Hansen *et al., Combust. Flame,* **2017,** 180, 250-261

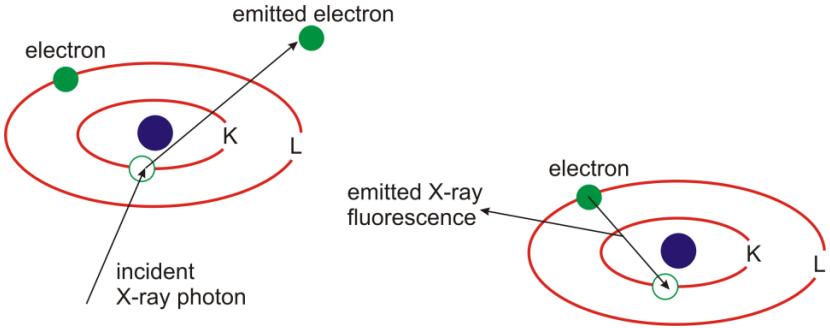
N. Hansen *et al., Proc. Combust. Inst.*, **2019,** 37(1), 743-750 (distinguished paper award)

GAS PHASE CHEMICAL PHYSICS

Measuring 2D Temperature Fields with Kr X-Ray Fluorescence

Beamline 7BM at the Advanced Photon Source (APS) of the Argonne National Laboratory

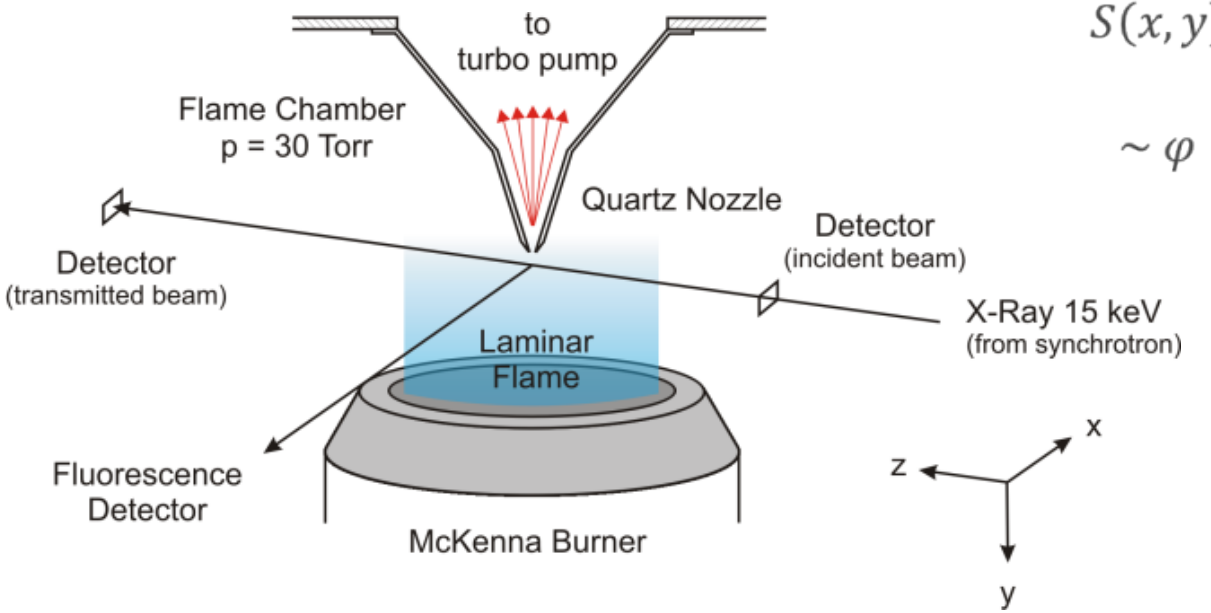
- X-ray fluorescence beamline
- Synchrotron-generated 5.1-22 keV
- High photon flux (2 x 10^{11} photons/s)
- Size of focal point: 5 x 7 µm
- Kr excitation at 15 keV and fluorescence detection at 12.6 keV (Kr Kα)



GAS PHASE CHEMICAL PHYSICS

N. Hansen *et al., Combust. Flame,* **2017,** 181, 214-224

Measuring 2D Temperature Fields with Kr X-Ray Fluorescence



$$S(x,y) \sim \varphi \times x_{Kr}(x,y) \times \frac{n}{V}$$

$$\sim \varphi \times x_{Kr}(x,y) \times \frac{p}{T(x,y)}$$

$S(x,y)$: fluorescence signal

φ: photon flux incident X-ray beam

$x_{Kr}(x,y)$: Kr mole fraction

n: number density

p: pressure

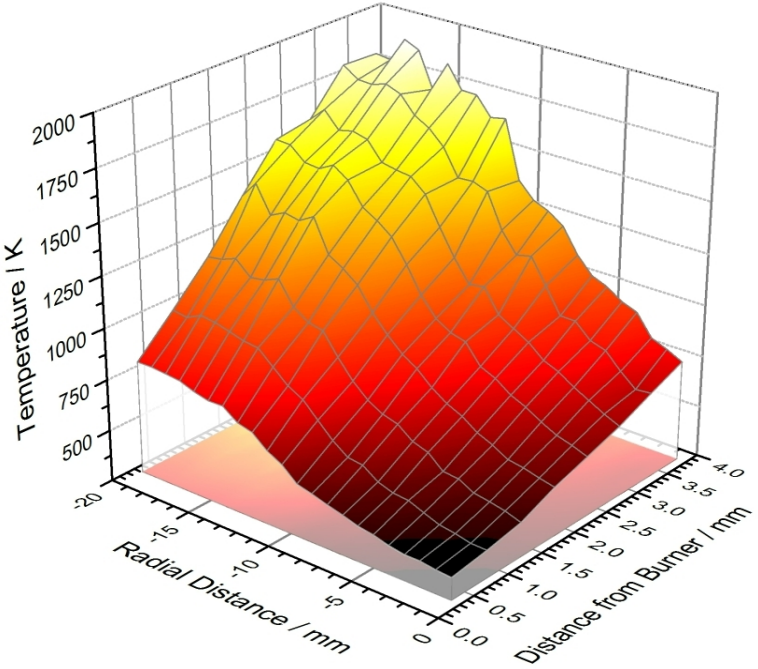
$T(x,y)$: local temperature

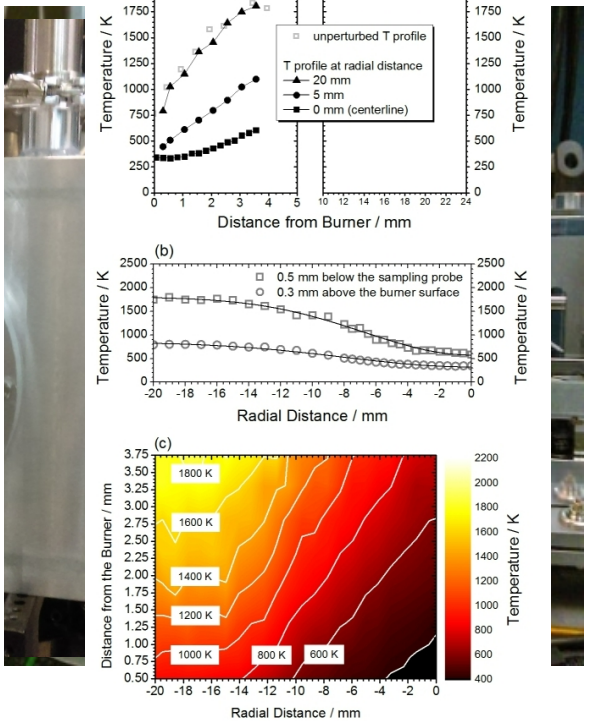
Flame conditions: 14.5% C_2H_4, 25.5% O_2, 55% Ar, 5% Kr, Φ=1.7, 30 Torr, 0.00404 g/cm^2/sec

GAS PHASE CHEMICAL PHYSICS

N. Hansen *et al., Combust. Flame,* **2017,** 181, 214-224

Measuring 2D Temperature Fields with Kr X-Ray Fluorescence

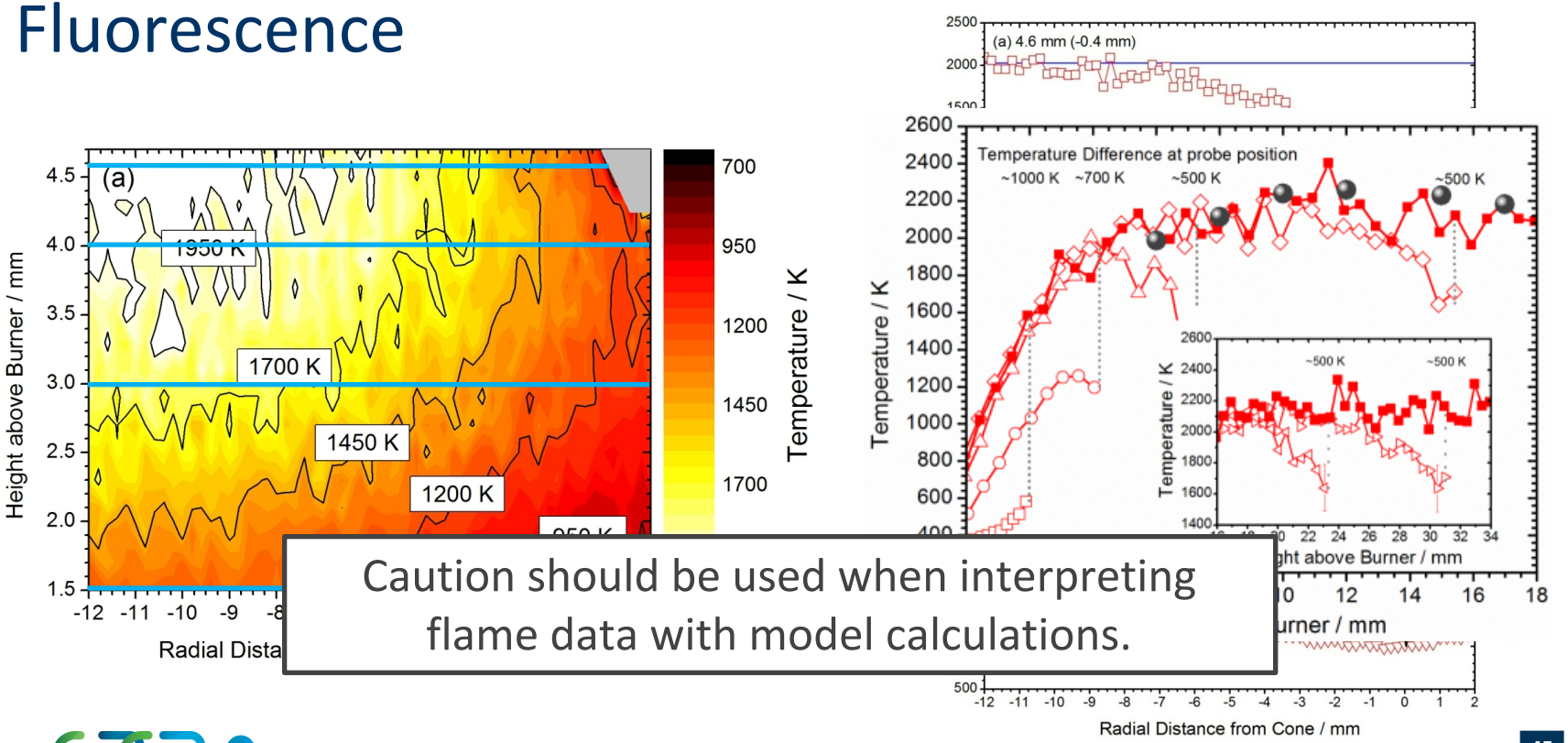




N. Hansen *et al., Combust. Flame,* **2017,** 181, 214-224

GAS PHASE CHEMICAL PHYSICS

Measuring 2D Temperature Fields with Kr X-Ray Fluorescence



Caution should be used when interpreting flame data with model calculations.

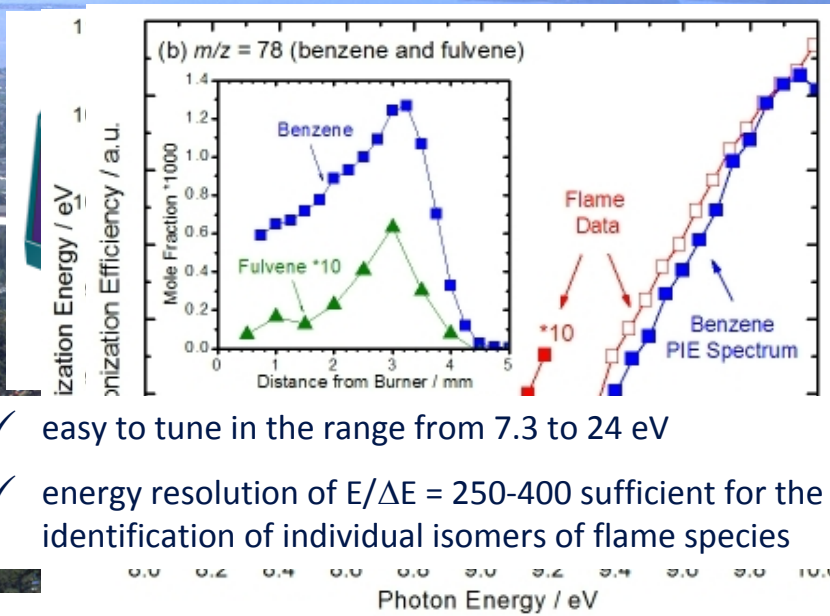
N. Hansen *et al., Combust. Flame,* **2017,** 181, 214-224

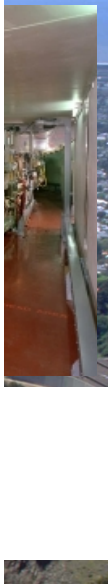
GAS PHASE CHEMICAL PHYSICS

Advanced Light Source

Synchrotron Radiation at the Lawrence Berkeley National Laboratory

- ✓ 3rd Generation light source for vacuum ultraviolet (VUV) and soft X-rays
- ✓ Photons are generated by the acceleration of ultarelativistic electrons through magnetic fields





- ✓ easy to tune in the range from 7.3 to 24 eV
- ✓ energy resolution of $E/\Delta E$ = 250-400 sufficient for the identification of individual isomers of flame species

GAS PHASE CHEMICAL PHYSICS