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Extreme Gradients

1:30 PM, Wednesday
August 31, 2011

Ken Brezinsky

Workshop for Techniques for High-Pressure Combustion
Argonne National Laboratory

High Pressure Shock Tube

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High Pressure Shock Tube Laboratory at University of Illinois at Chicago

HPST Operating Conditions
Temperatures: 800-2500 K
Pressures: 20-1000 atm
Reaction Times: 0.5-3.0 ms

Species Measurement

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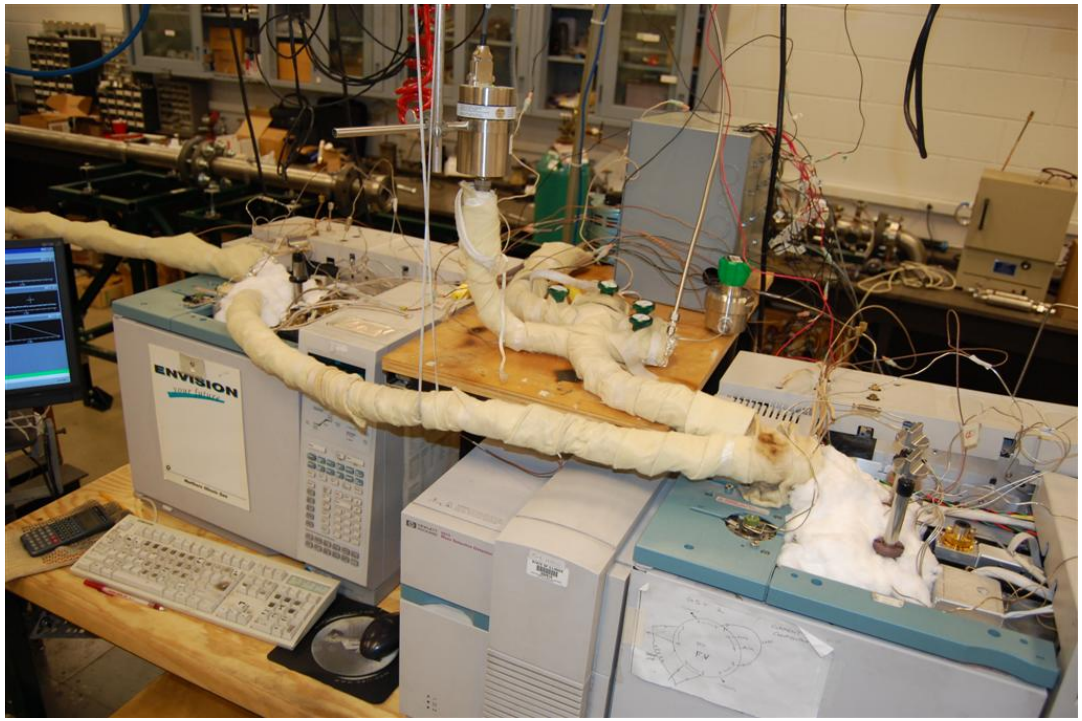
Direct Connection between High Pressure Shock Tube and GC-MS Analytical System



Species Measurement

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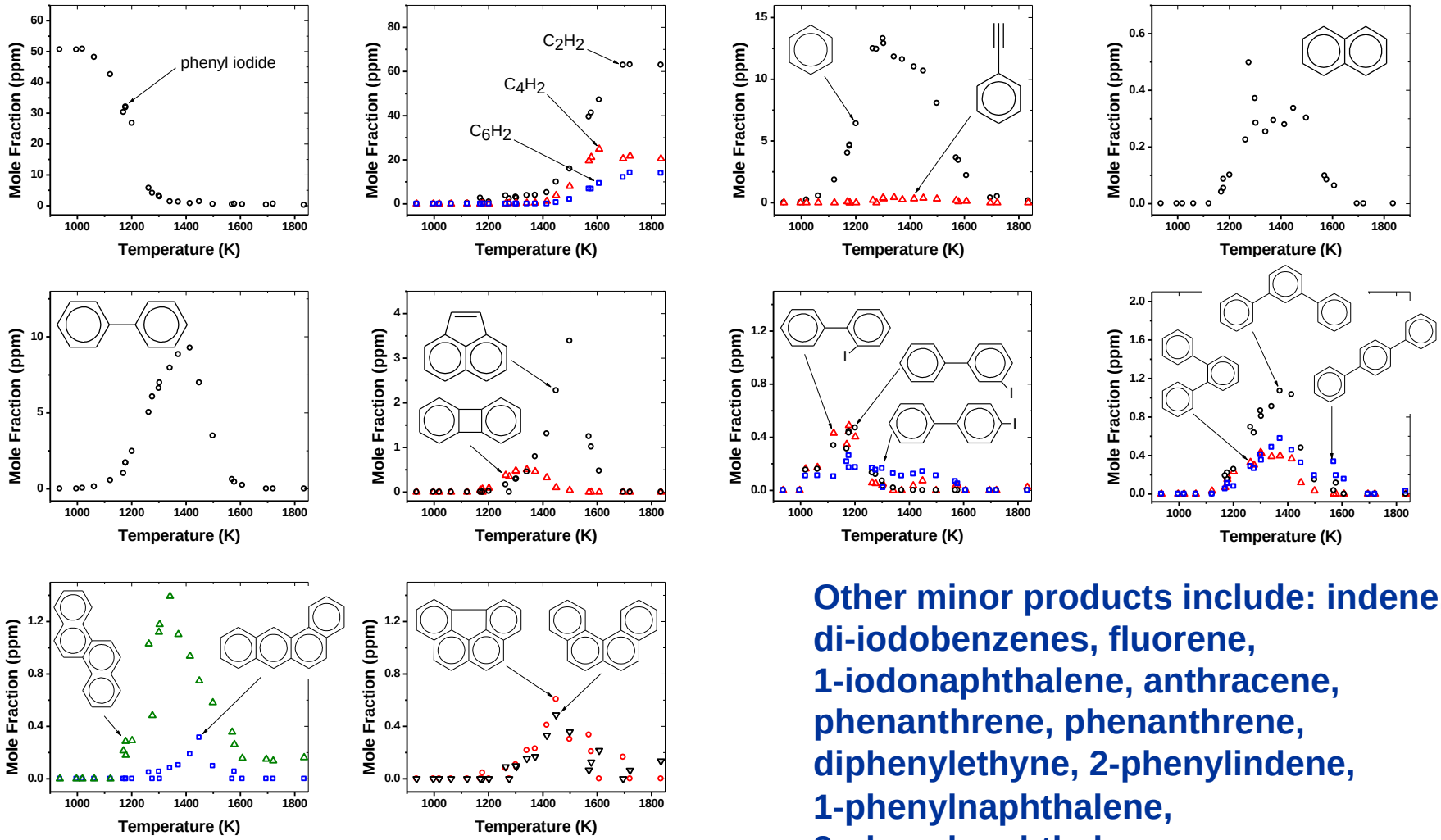
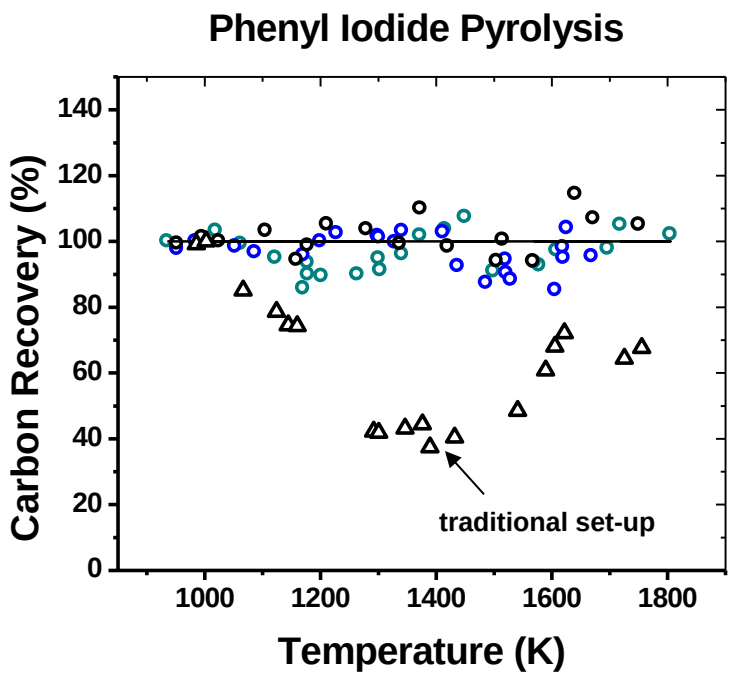
Phenyl Iodide Decomposition

$P_{nominal}$ = 50 atm, $[C_6H_5I]_0$ = 50.6 ppm, Reaction Time = 1.24 – 1.99 ms



Other minor products include: indene, di-iodobenzenes, fluorene, 1-iodonaphthalene, anthracene, phenanthrene, phenanthrene, diphenylethyne, 2-phenylindene, 1-phenylnaphthalene, 2-phenylnaphthalene, pyrene

Carbon Recovery



Δ : $P_{nominal}$ = 50 atm, $[C_6H_5I]_0$ = 46.6 ppm, Reaction Time = 1.25 – 1.87 ms

o : $P_{nominal}$ = 50 atm, $[C_6H_5I]_0$ = 50.6 ppm, Reaction Time = 1.24 – 1.99 ms
o : $P_{nominal}$ = 25 atm, $[C_6H_5I]_0$ = 54.2 ppm, Reaction Time = 1.33 – 2.08 ms
o : $P_{nominal}$ = 50 atm, $[C_6H_5I]_0$ = 26.6 ppm, Reaction Time = 1.34 – 2.15 ms

Identification of Target Species

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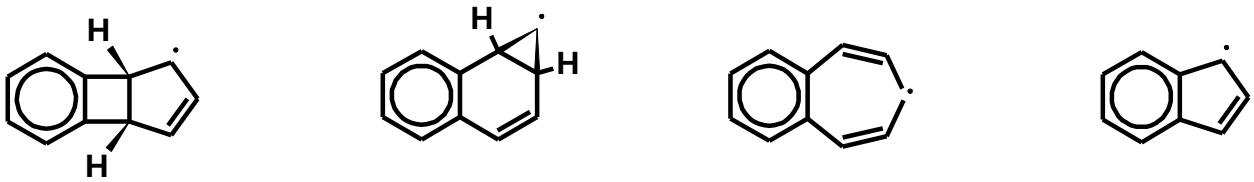
Radical PAH intermediates



- "Radical/π-Bond Addition between o-Benzyne and Cyclic C5 Hydrocarbons", Comandini, A.; Brezinsky, K.; submitted, Journal of Physical Chemistry A

Summary

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Extremes: Pressure, Molecular Size/Weight

- "Chemistry of PAHs Formation from Phenyl Radical Pyrolysis and Phenyl + Acetylene Reaction" Comandini, A.; Malewicki, T.; Brezinsky, K.; submitted, Journal of Physical Chemistry A
- "Online and Offline Experimental Techniques for PAHs Recovery and Measurement", Comandini, A.; Malewicki, T.; Brezinsky, K.; to be submitted
- "Radical/π-Bond Addition between o-Benzyne and Cyclic C5 Hydrocarbons", Comandini, A.; Brezinsky, K.; submitted, Journal of Physical Chemistry A
- "Theoretical Study of the Formation of Naphthalene from the Radical/π-Bond Addition between Single-Ring Aromatic Hydrocarbons", Comandini, A.; Brezinsky, K.; J. Phys. Chem., 115(22), 5547-5559, 2011

Extreme Gradients

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- Lyle Pickett (CRF) *Diagnostics for Fuel Spray Research at High Pressure and Temperature*; refractive index gradients
- Jesse Kroll (MIT) *Measuring Particle Formation, Growth, and Chemistry Using Advanced Aerosol Mass Spectrometry Techniques*; in the atmosphere
- Michael Drake (GM) *Ignition and Flame Growth in Steep Gradients in a Spray-Guided Gasoline Engine*; stratified mixtures
- Break
- Volker Sick (Michigan) *High-Speed, High Resolution Imaging near Surfaces*; wall and near wall conditions
- Nabiha Chaumeix (CNRS-Orleans) *Soot Formation from Diesel Type of Fuels at Engine-like Conditions using Shock Tubes: a Decade of Studies*; engine-like conditions
- Discussion