Advanced Energetic Material Synthesis

David E. Chavez

Los Alamos National Laboratory

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Outline

- Holy Grail Question
- Paths Foward
- Emerging Technologies
- Efficient Screening Methods
- Small-Scale Testing Investment
- Past Investments
- Material Selection

Holy Grail?

- **Answer is Needed**
  - Justify Investment
  - Results-based science funding
  - There is a metrics-based answer
- **Is this a "right" question**
  - Too many different application
  - Certainly not for propellants
  - Molecule centric
- **What might be a better question?**
  - Capability-centric, High-Level viewpoint
- **Breakthrough Technologies**
  - Always inspired through basic research
  - Not necessarily "planned"

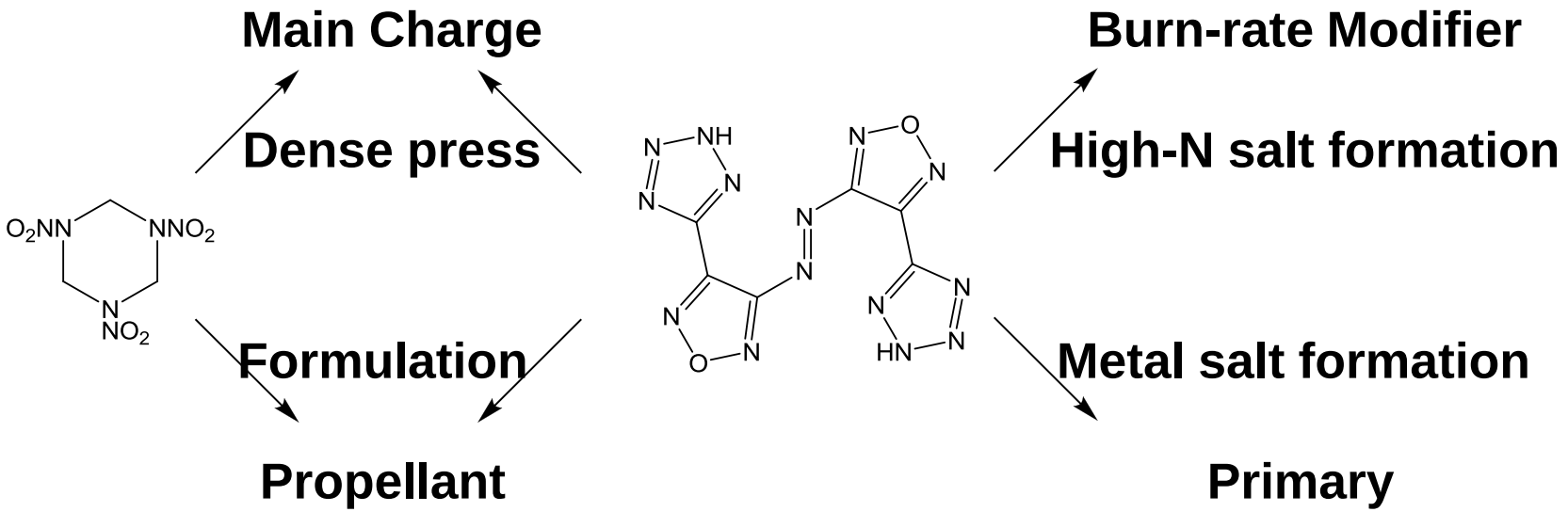
EM Research Funded Last 50 years: Results?

- **Answer from a molecule standpoint:**
  - Justification requirements have increased over time
  - Shows the difficulty of the field
  - EM Chemist are fighting a losing battle
- **Answer From a Material Standpoint**
  - Gun Propellant improvements
  - Reactive Materials, MIC, IM
- **Answer From Capability Viewpoint**
  - Modeling and Simulation
  - National capability to address national security
- **Historical Goals and Objectives**
  - More successful from a materials viewpoint
  - Less so from a molecule viewpoint

Paths Forward

- **View EM as Materials**
- **Training and Mentoring**
- **Consider overall cost**
  - Reduced environmental clean up costs
  - Improved safety for troops
- **Paradigm Shifts in Energetics?**
  - Autonomous Systems change the game
  - Example: Structural Energetics
- **New Concepts in Materials Properties**

Strategic Approach to EM Development

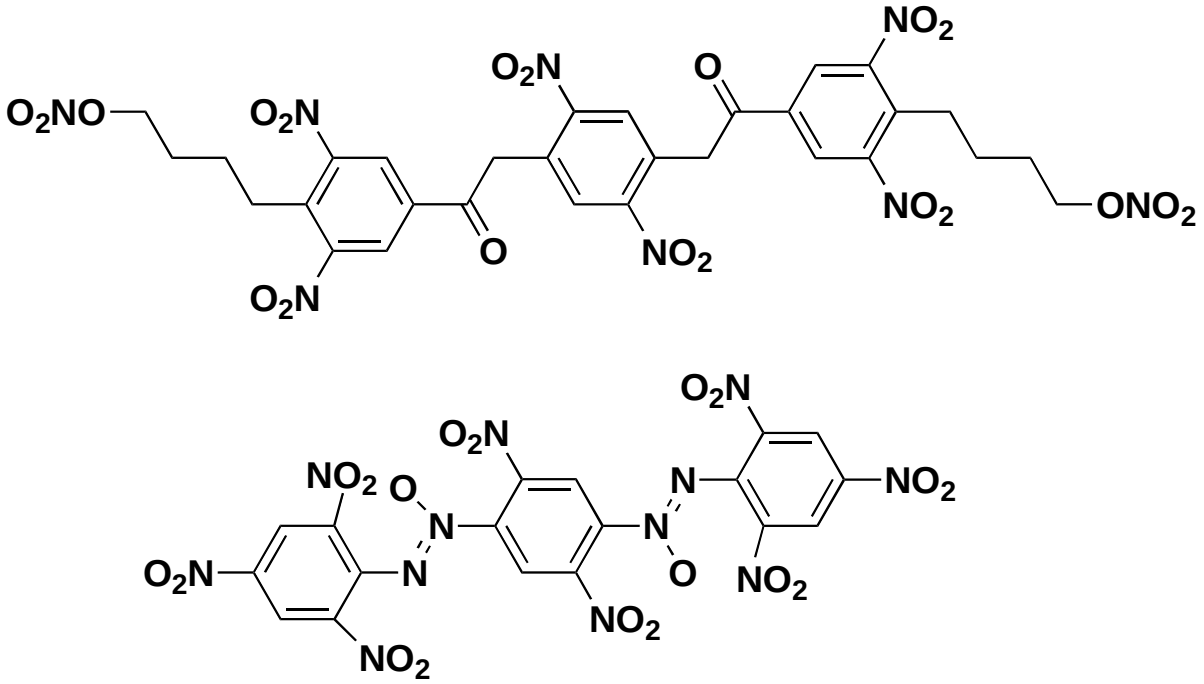


- Synthesize molecules tailorable for different applications through chemical specialization
- RDX is a current example of one material being used in both main-charge and propellant formulations
- Advantage of reduced infrastructure for HE production

Emerging Technologies

- **Tunable materials (on/off materials)**
  - Can we control sensitivity
  - Optical tuning
  - Other methods
- **Drug Discovery Capabilities**
  - Co-crystallization
  - Modification of sensitivity
- **Microreactor Technology**
  - Ease of Scale-up
  - Heat/volume concerns reduced

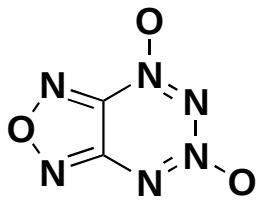
Liquid Crystalline Explosives



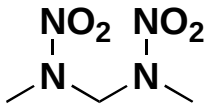
Sensitivity control through liquid crystalline properties?

Millar, R. et al., **2008**, patent application, WO2008/102111A2

Co-Crystallization to adjust sensitivity



FTDO



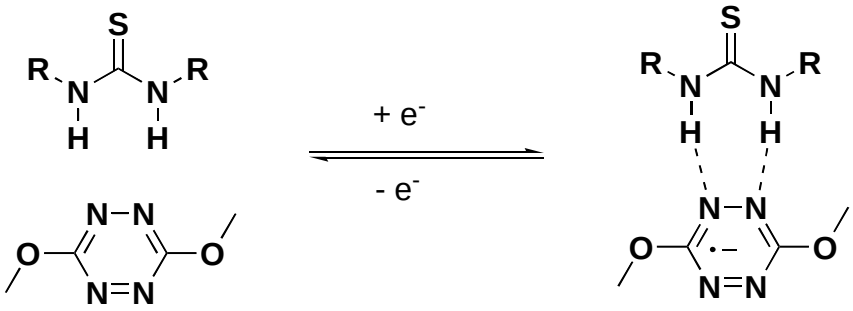
DNAP

-FTDO has sensitivity similar to Lead Azide
-FTDO forms a co-crystal with DNAP
-Studies on the sensitivity of the co crystal have been done

Zarko, V. E.; Simonenko, V. N.; Kalmykov, P. I.; Kvasov, A. A.; Chesnokov, E. N.; Kuper, K. E. *Combustion, Explosion and Shock Waves*, **2009**, *45*, 752.

Tetrazine On/Off Co-Crystallization

Redox controlled on/off switching



Clavier, G, et al., *Chem. Rev.* **2010**, 3299

-Literature precedent for on/off complexation switching
-Can we use a similar concept for on/off sensitization?

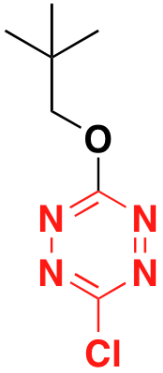
On/Off Fluorescence switching

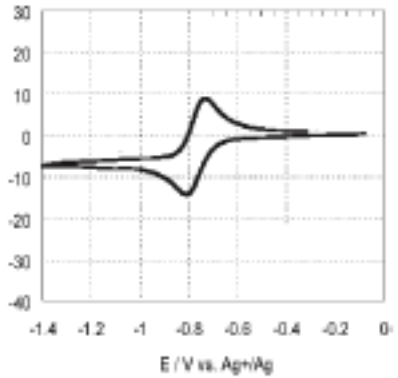
-Tetrazines are highly colored and small

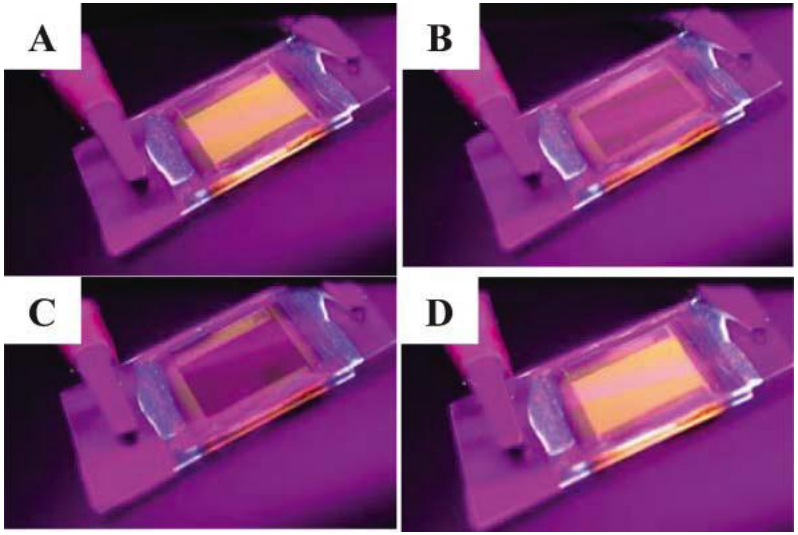
-Tetrazines are energetic

-Tetrazines are highly electroactive

-Studies have shown that tetrazine fluorescence can be turn on/off electronically







An on/off fluorescent window made from a tetrazine compound

Clavier, G, et al., *Chem. Rev.* **2010**, 3299

New Material Issues

- **Transition of Materials**
  - Scale-up
  - Funding to transition
- **Small-Scale Tests**
  - More small scale testing needed
  - Justification for scale-up
- **Environmental Fate and Toxicity**
  - When should materials be tested
  - Predictive capability
- **Safety, Aging and Life Cycle Concerns**
  - Small-scale methods

Technical Limitations

- **Availability of Small-Scale Tests**
  - Justification needed to invest in scale-up
  - Tests need to reliably estimate large scale
- **Energy/Sensitivity Tradeoff**
  - Need to justify investment
- **Scale-up Capability**
  - Synthesis and scale-up
- **Aging and Life Cycle Concern**
  - Small-scale methods

Efficient Screening Methods

- **Need small scale test methods**
  - Modeling and simulation to extrapolate
- **Chemical compatibility**
  - Need rapid methods to identify incompatibility
  - Need rapid aging test methods
- **Newer techniques**
  - Rapid environmental testing capability
  - Needs to be relatively inexpensive

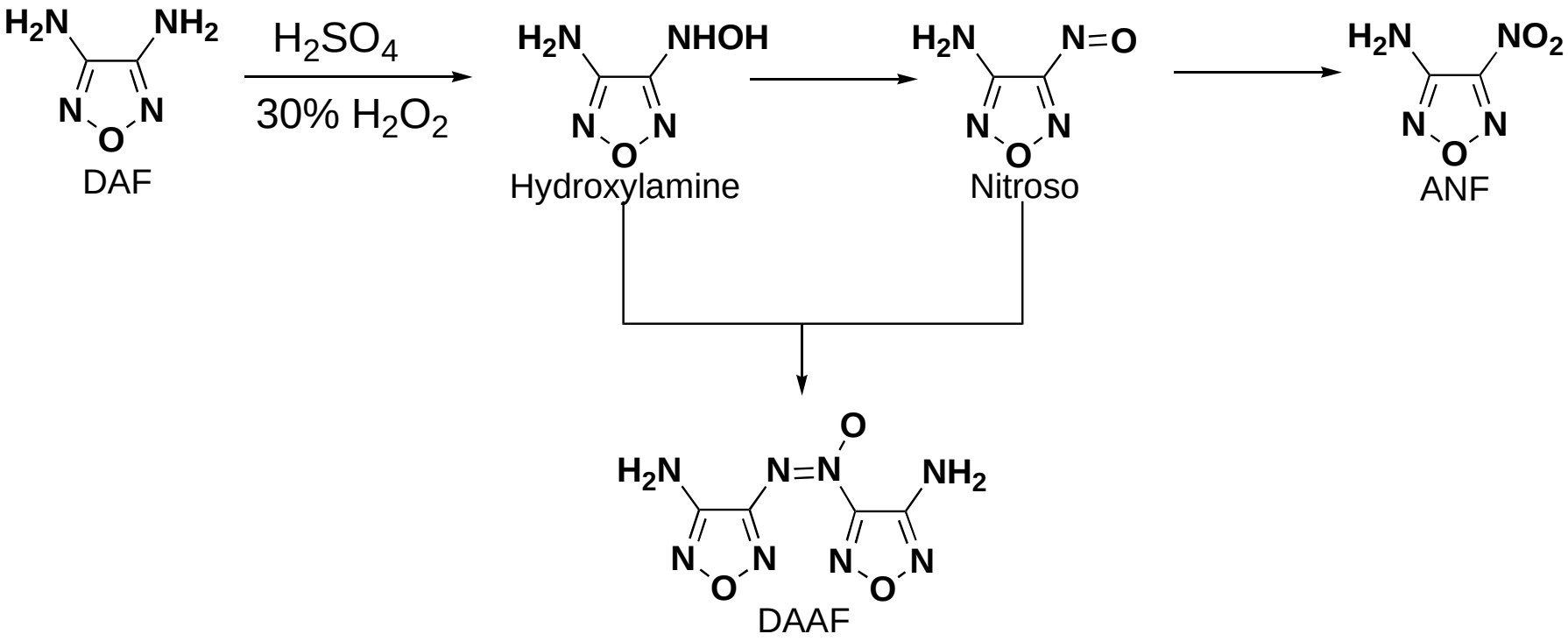
Small Scale Testing Investment

- **Rapid, cheap, safety and performance testing**
  - Need small scale test methods
  - Need info. on performance
  - Need info. on shock sensitivity, materials properties
  - Modeling and simulation to extrapolate
- **Mapping small scale to large scale phenomenon**
  - Test which extrapolate from small to large scale
  - Must be fast and inexpensive

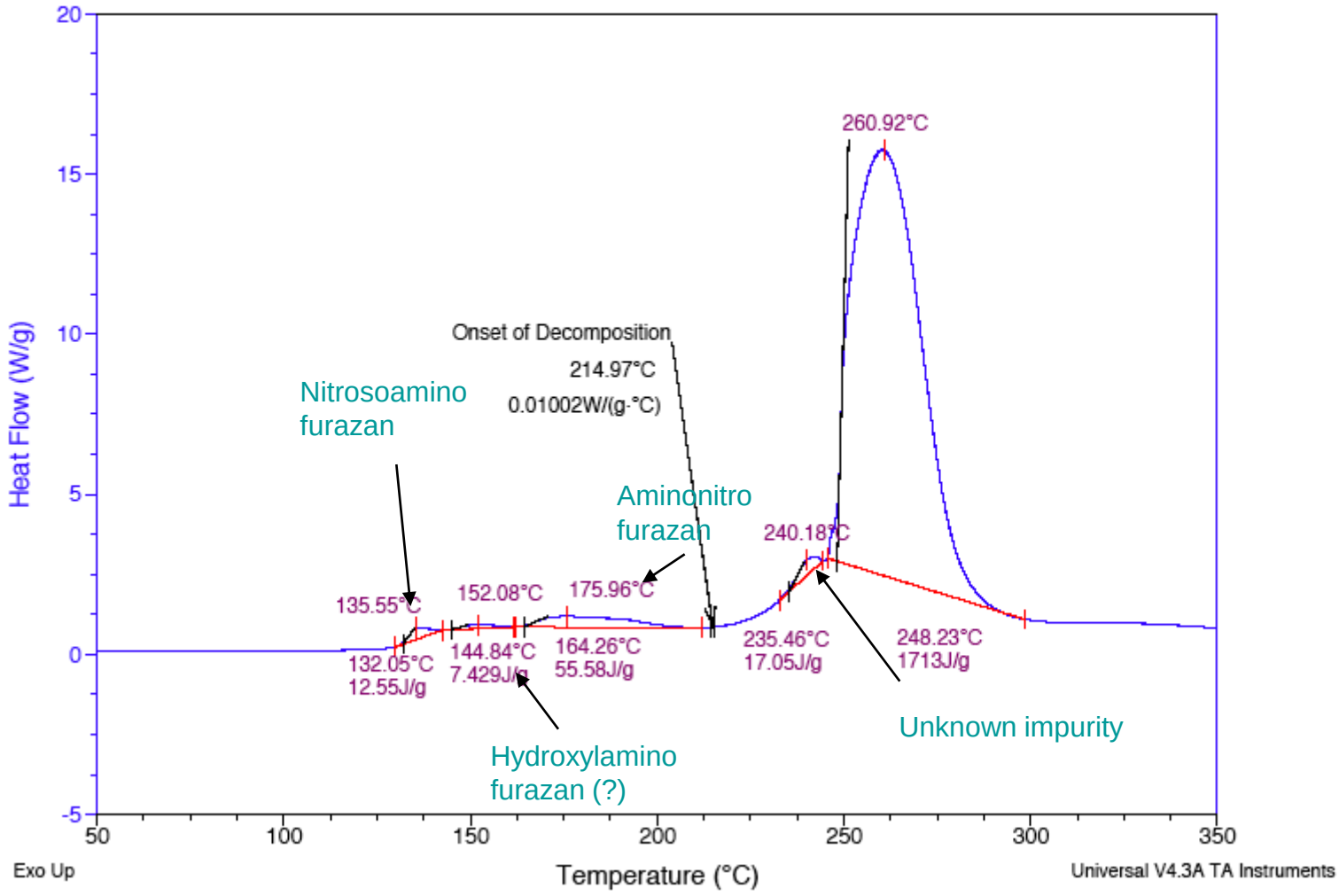
Past Investments

- **Many Materials Have Been Synthesized**
  - Did not meet requirements
  - Difficult to Synthesize
- **Reinvestigation is Worthwhile**
  - Environmental Considerations
  - New Synthesis Techniques
- **Critical Information**
  - Transfer of Prior Knowledge is Key
  - Must not repeat
- **Example: Synthesis of DAAF**

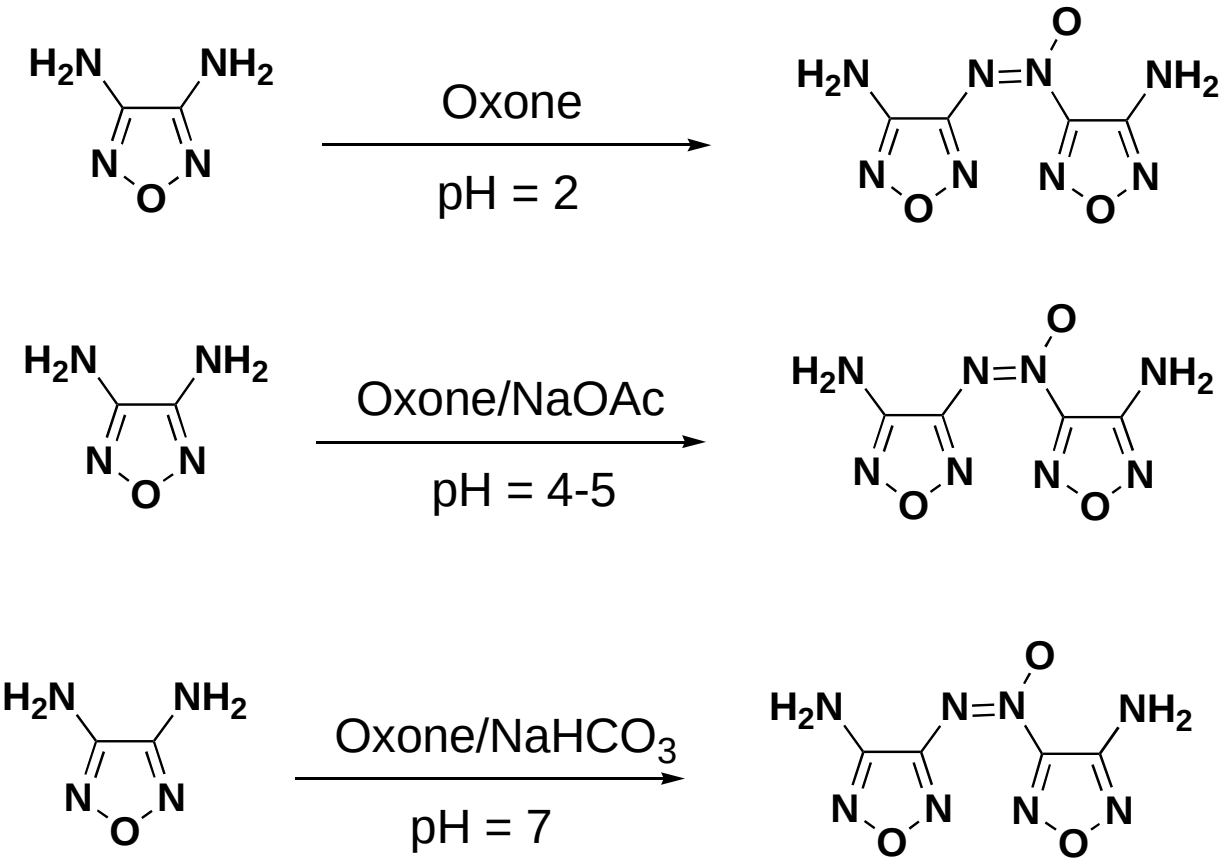
Synthesis of DAAF



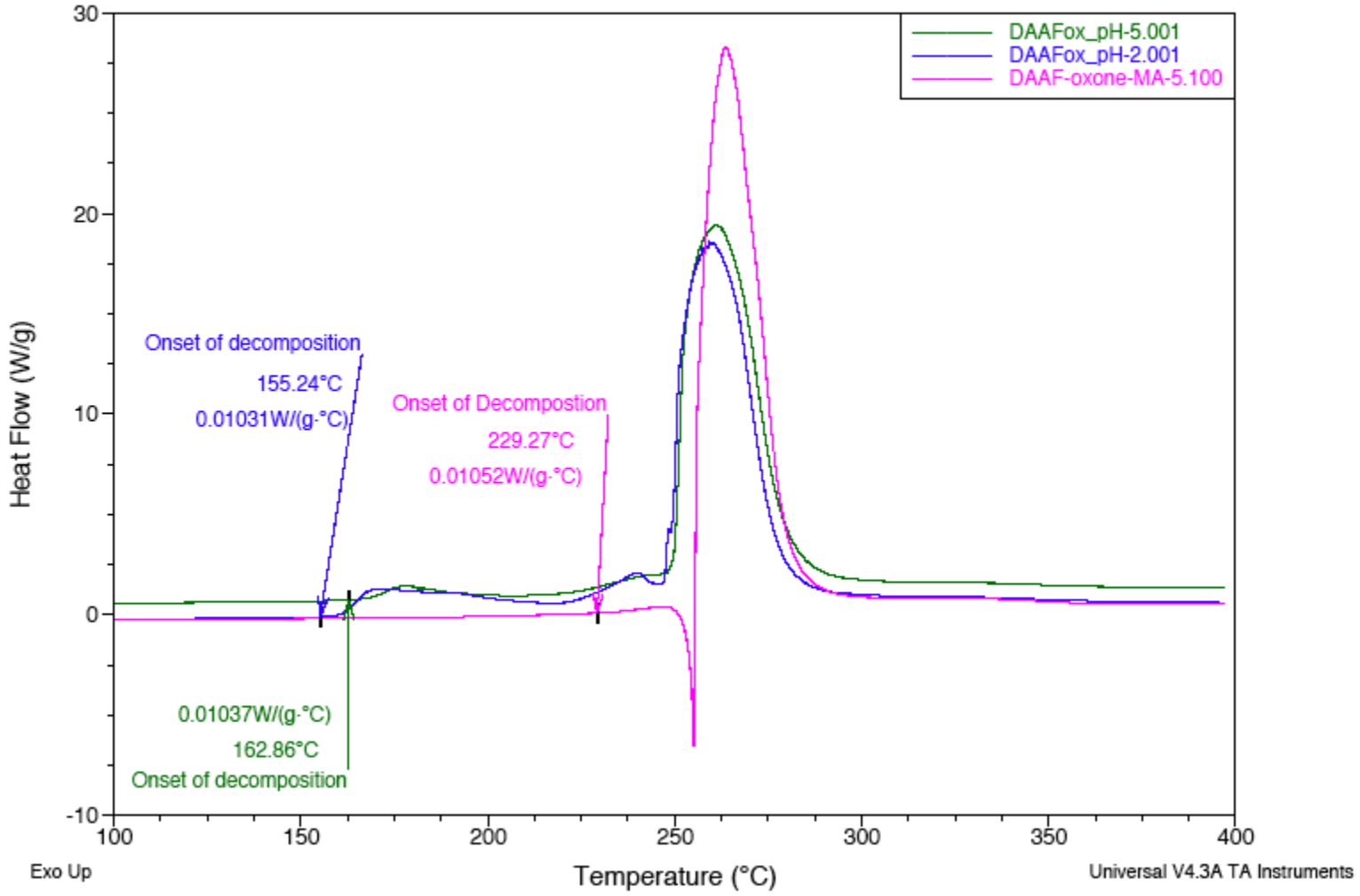
Impurity identification



New Approach to DAAF



DSC: pH Comparison



Purity Effect on ODTX

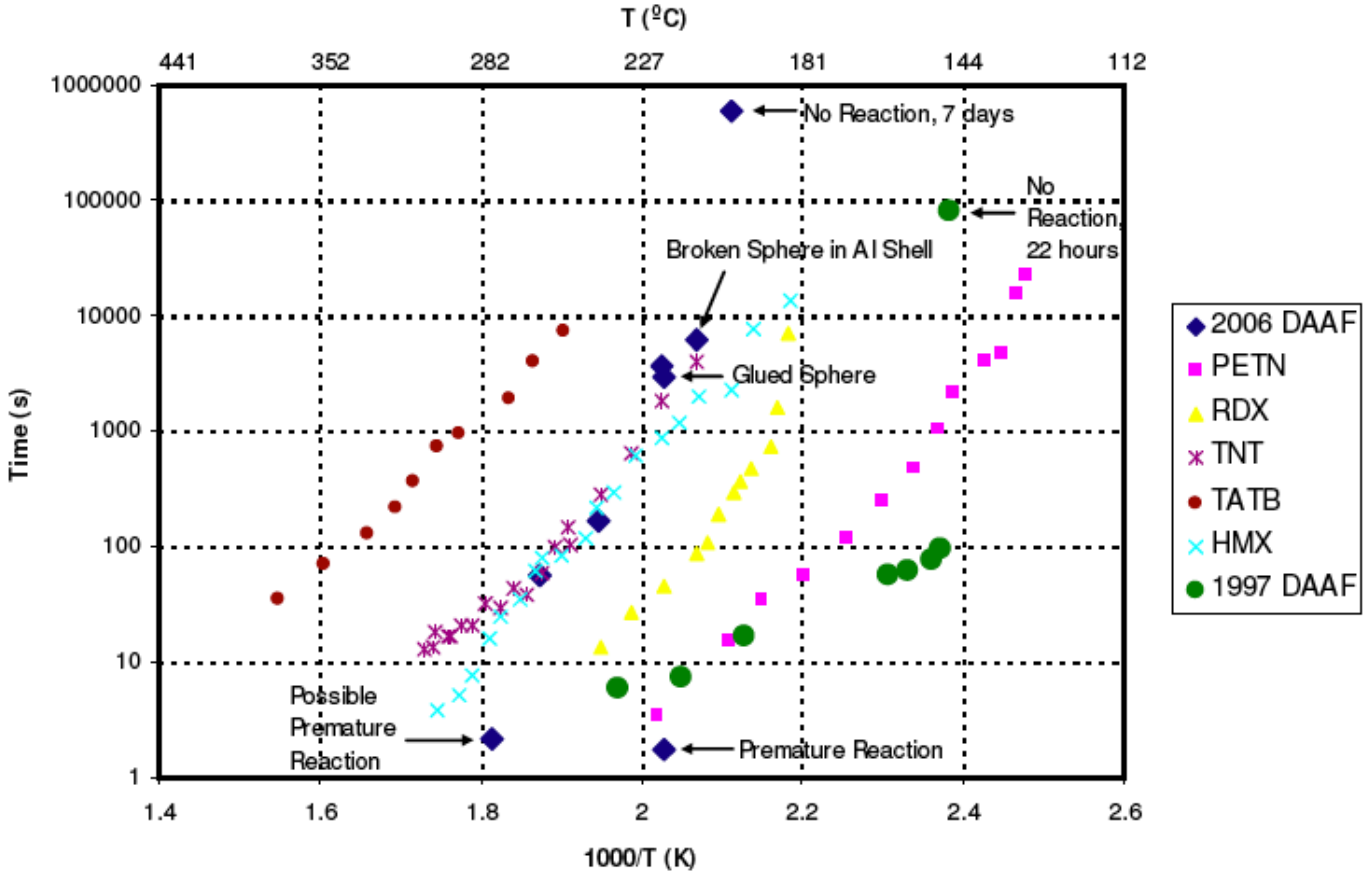


Figure A-2. ODTX comparing DAAF 2006 to DAAF from 1997-1998 along with other common explosives

Courtesy of J. Maienschein (LLNL)

Material Selection

- **Novel materials**
  - High Risk/ High Payoff
  - Requires long term investment
- **On/Off switchable materials**
  - High Risk/ High Payoff
  - Long term investment
- **Ease of Synthesis**
  - 3 steps of fewer
  - Environmentally Friendly
  - No energetic intermediates

Acknowledgments

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