

Hypergolic Ignition of Ionic Liquids

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IGNITION TEAM

Personnel and Support



TEAM LEADER



Tom Hawkins

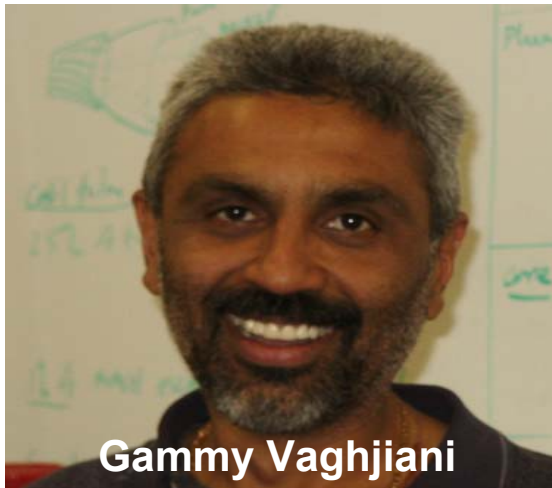


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Gammy Vaghjiani



Stefan Schneider



Angelo Alfano



Hypergolic Ignition of Ionic Liquids



■ IGNITION SURVEY DOCUMENT WRITTEN

- EVALUATED 13 IGNITION TECHNIQUES FOR IL APPLICATIONS & REVIEWED PUBLISHED/FUNDED WORK
- EXPERIMENTAL/COMPUTATIONAL FOCUS ON IL HYPERGOLIC IGNITION; TWO YR (FY05-06) PLAN WRITTEN

■ HYPERGOLIC IGNITION WORK HAS BEGUN

- OVER 50 VISUAL IGNITION TESTS OF WFNA, IRFNA, and N_2O_4 WITH HYDRAZINES, AMINES, STRAINED-RING HYDROCARBONS, TRIAZOLES, TRIAZOLIUM SALTS, AND FORMULATIONS
- AB INITIO CALCULATIONS OF DECOMPOSITION OF HYDRAZINES, 1,2,3 AND 1,2,4 TRIAZOLES AND THEIR AMINATED DERIVATIVES BY N_2O_4 .

■ RESONANT PHOTOPHYSICAL IGNITION OF HAN-BASED PROPELLANTS

- SINGLE PULSE CO_2 LASER IGNITION DEMONSTRATED DURING AFRL INTERNAL PROJECT





Hypergolic Ignition of Ionic Liquids



GOAL: Develop Capability to Experimentally Determine and Theoretically Validate Hypergolic Ignition Mechanisms in ILs

Technical Challenge:

Chemical dynamics and mixing dynamics strongly influence hypergolicity and must be decoupled →

Dozens of simultaneous, unmeasured reaction rates have the potential to control the ignition delay →

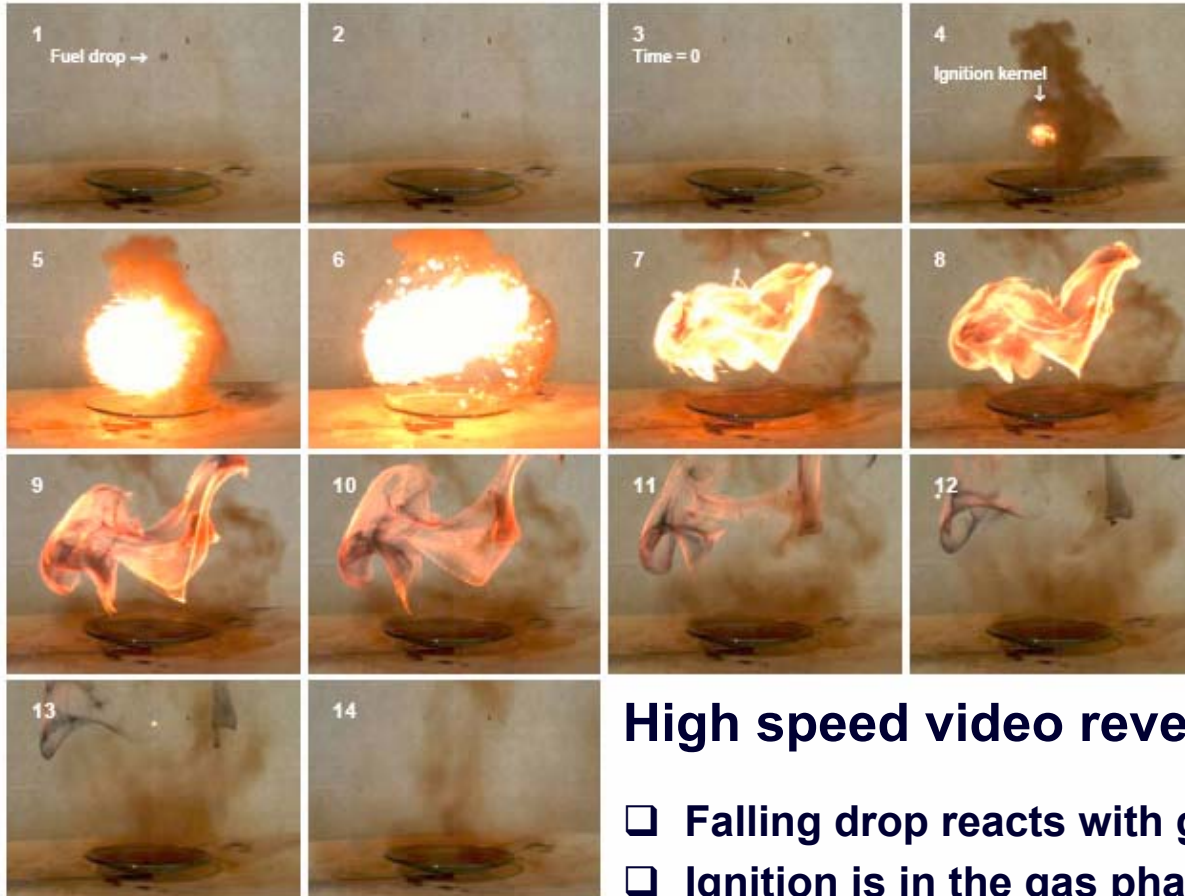
Approach:

Combine time-resolved techniques (FTIR, emission spectrosc., laser probing, ...) with novel reactant mixing strategies

Combine and extend quantum chemical and kinetics codes to focus experimental search for key transients and rate limiting steps



High Speed Video Highlights Complexity

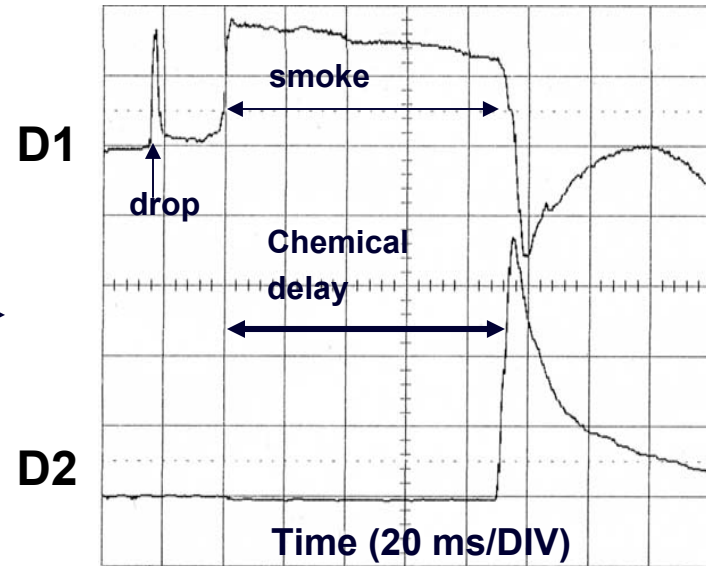
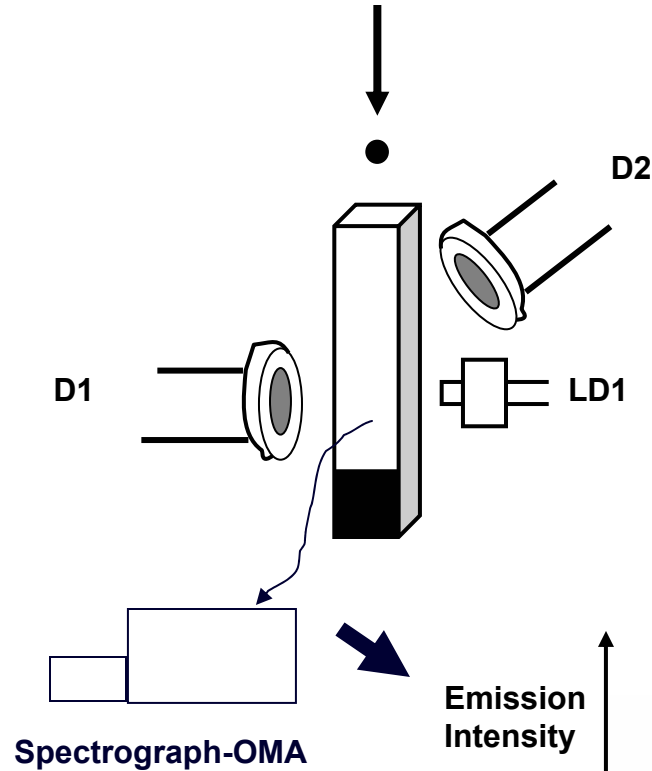


High speed video reveals:

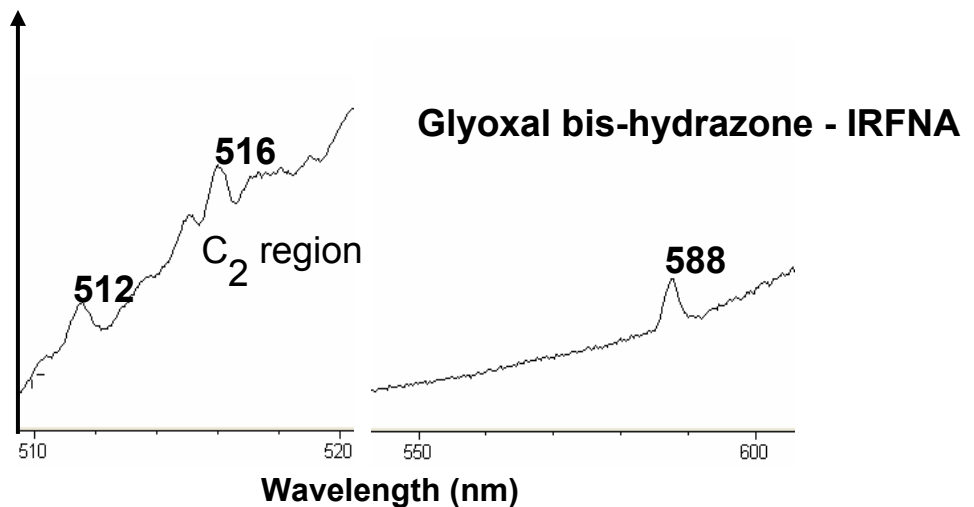
- ☐ Falling drop reacts with gas environment
- ☐ Ignition is in the gas phase
- ☐ Gas phase and liquid phase chemistry is connected
- ☐ Spatially indiscriminate information will not be sufficient for mechanistic understanding



Spatially Resolved Approach Required



COMPLEXITY HIGHLIGHTED IN
HIGH SPEED VIDEO IGNORED





Current Focus

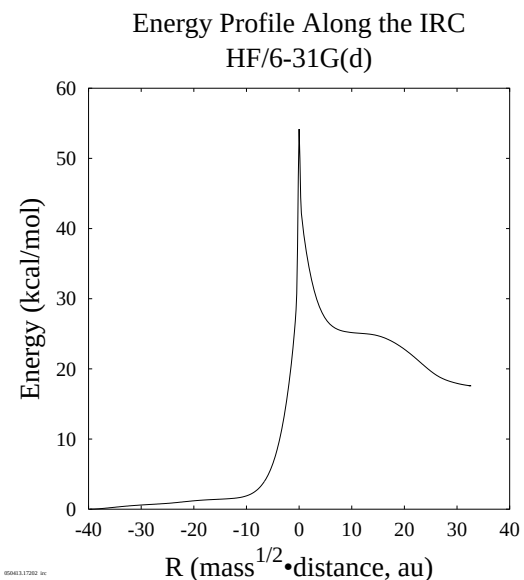
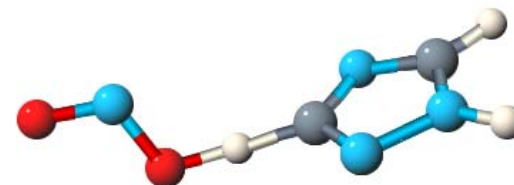


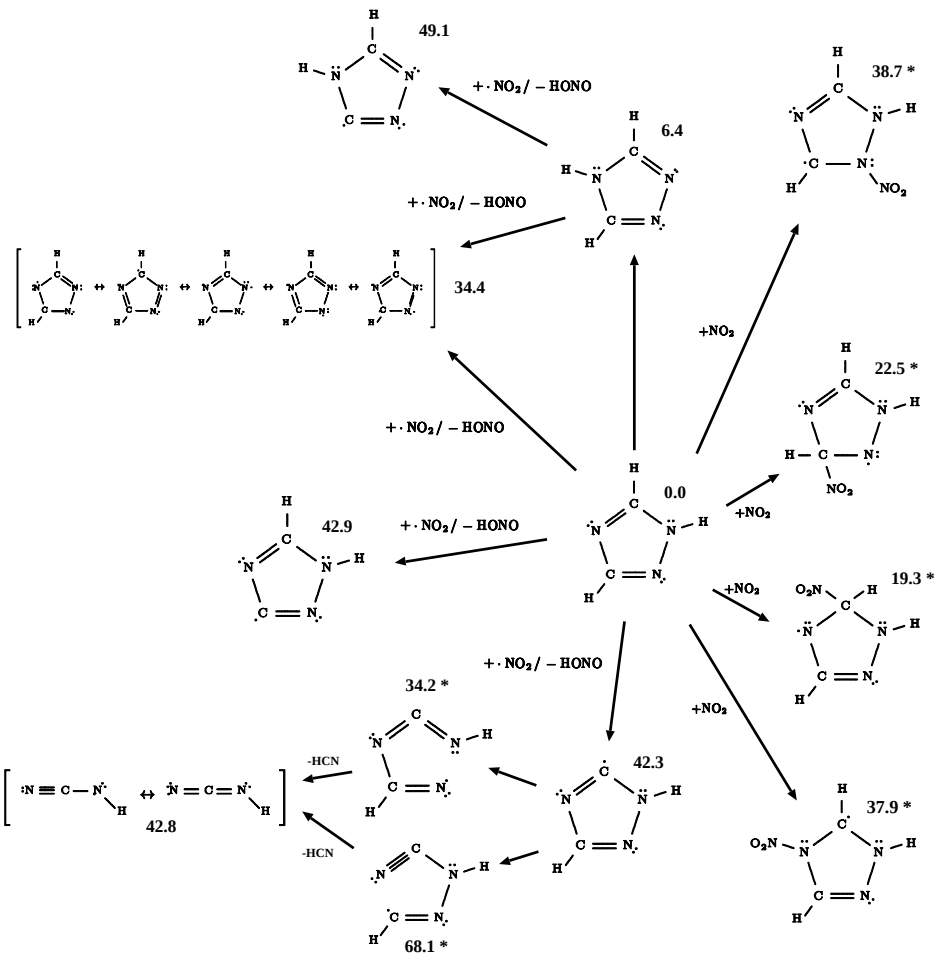
- **SIMPLIFY PROBLEM TO LIQUID PLUS GAS**
- **APPLY SPECTROSCOPIC TOOLS IN THIS REGIME**
 - **FTIR (RAPID & STEP SCAN)**
 - **TIME-RESOLVED RAMAN**
 - **TIME-RESOLVED EMISSION**
 - **HIGH SPEED VIDEO**



Theory and Modeling

- **Kinetic Parameters** → **Kinetic Model**
- **PES** → **Kinetic Parameters**
- **Reaction Step** → **PES**
- **Net Rxn Enthalpy** → **Reaction Step**
- **Trial Rxn Step** → **Net Rxn Enthalpy**

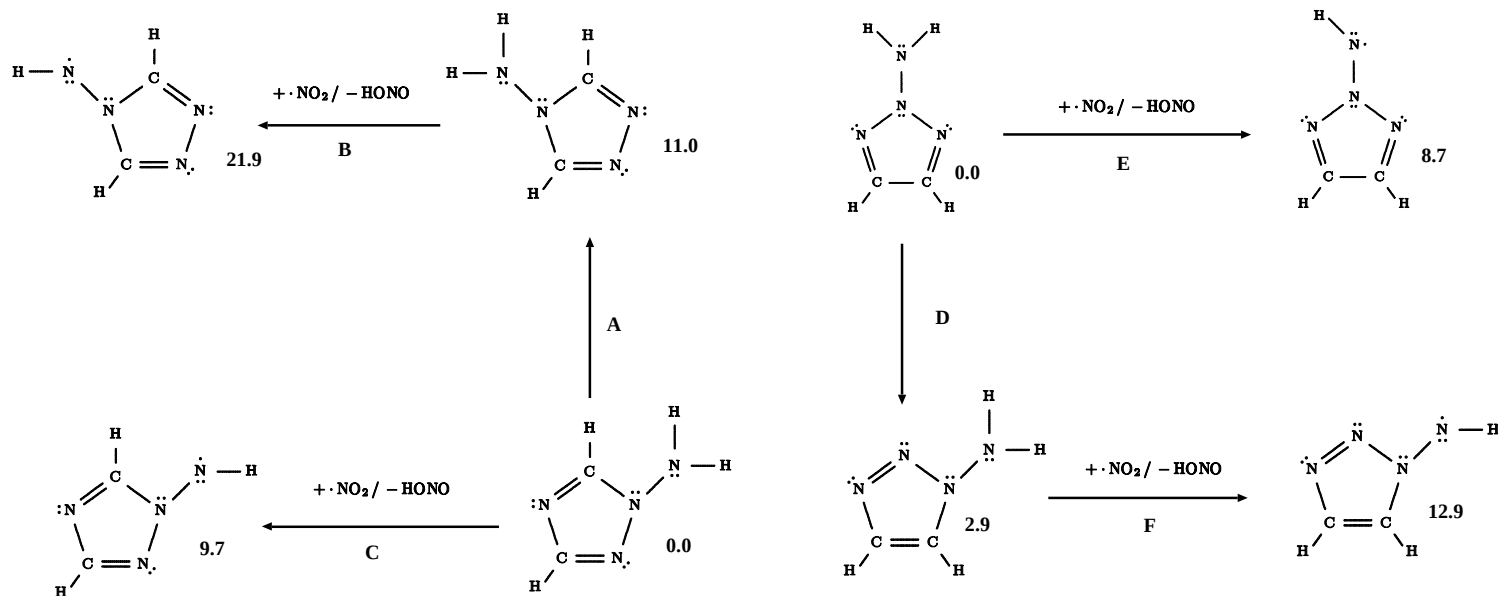




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Amino-Triazoles + N₂O₄



- Reaction Enthalpies Slightly Above Hydrazine and MMH
- Reaction Enthalpies Correlate with Visual Ignition Tests



Plan



Develop Capability to Experimentally Determine and Theoretically Validate Hypergolic Ignition Mechanisms in ILs

- To provide a roster of hypergolicity of IL-oxidizer pairs
- To provide ignition mechanisms for a reference set of IL-oxidizer reactions with time-resolved spectroscopic techniques
- To provide theoretical validation/prediction for experimental results
- To provide a predictive model to suggest targets and screen IL synthesis candidates



Back-up Slides



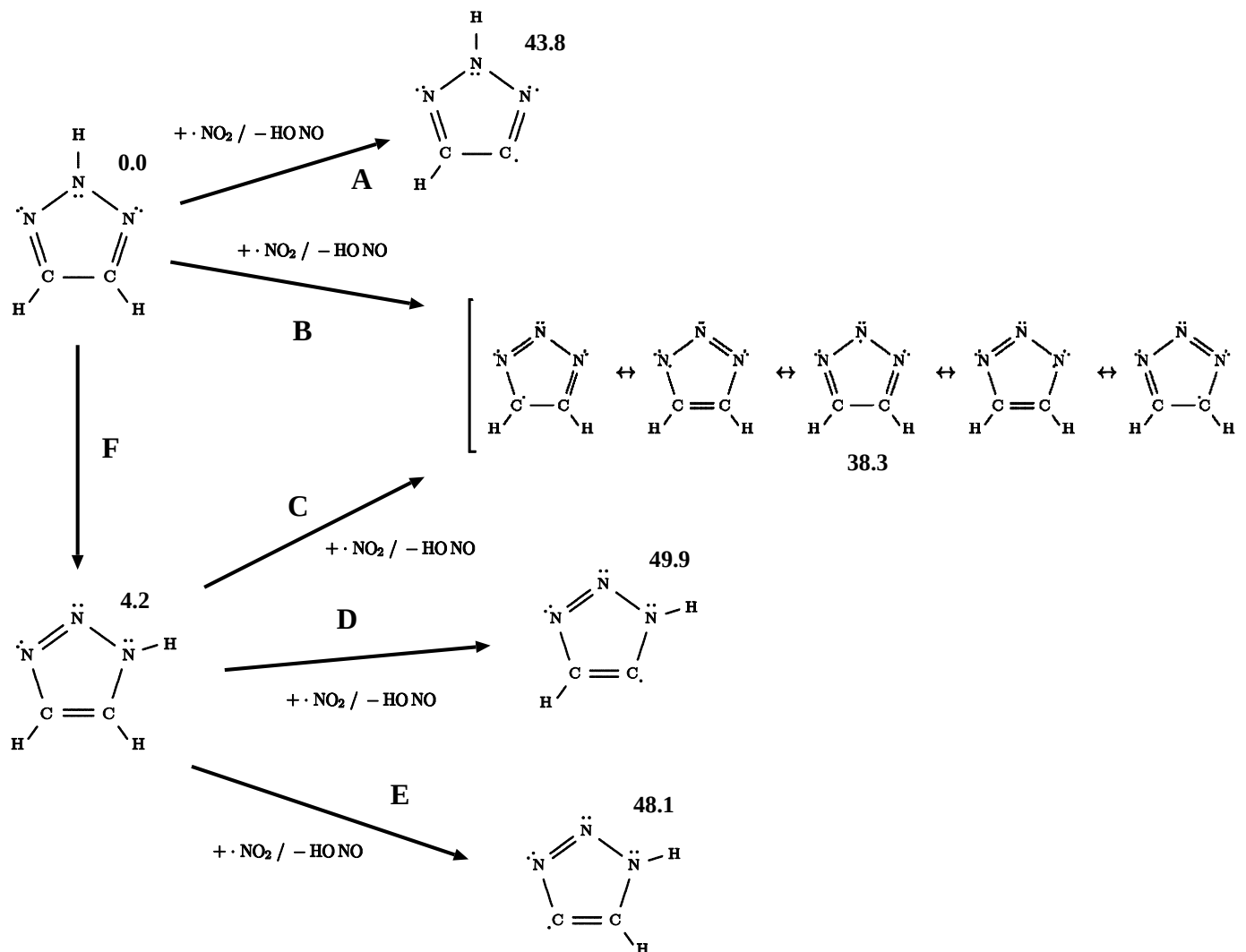
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1,2,3-Triazoles + N₂O₄





Hydrazine and MMH

