FINAL PROGRESS REPORT (ORIGINAL AND TWO COPIES REQUIRED)

CONTRACT/GRANT NUMBER: DAAH04-95-1-0185
PERIOD COVERED BY REPORT: 15 April 1995 – 1 July 1998
TITLE OF PROPOSAL: Rydberg States of Energetic Materials
NAME OF INSTITUTION: Colorado State University
AUTHOR OF REPORT: Elliot R. Bernstein

STATEMENT OF PROBLEM

In this work we studied the fragmentation, reactions, and dynamics of model energetic compounds (methyl amines, azaaromatics, radicals) with high excitation energies. The general idea was to characterize the behavior of electronically excited energetic materials and to understand the beginnings of the decomposition processes.

SUMMARY OF MOST IMPORTANT RESULTS

The main results of the last three years are well represented in the Technical Progress Reports already submitted. These studies show that radicals and Rydberg states play an important role in the fragmentation behavior and dynamics of many energetic materials model systems. We have generated new and never-before studied radicals of substituted cyclopentadienyls (CN, F, CH₃) and lutidyl and picolyl and have shown that their excited electronic states are much more reactive than their ground states. We have demonstrated their reactivity toward small substituted methanes, water, alcohol, ammonia, and others. We have developed new published algorithms for the theoretical description of such behavior.

The latest progress of the last six months of this effort (since our last comprehensive report of results and progress) has been for laser ablation of RDX and related materials. We have now constructed a supersonic nozzle that can be used with laser ablation of matrix isolated materials. The nozzle works well with large molecules and metal oxide systems, and we can observe the original molecule as well as its fragments in the mass spectrum of the ablated material. We have observed V₂O₅, Ti₃O₇, tyramine, tryptamine, dopamine, and other large involatile molecules as well as their fragments in this manner. Covariance mapping of these ablation plumes has given us good information on how molecules and clusters can fragment.

All of these results are published, with the exception of the metal oxide and organic molecule ablation results. These are reported here for the first time. The fact that we can now access such diverse systems from matrices for mass spectroscopy and covariance mapping is a major step forward for our program with ARO.

LIST OF PUBLICATIONS AND TECHNICAL REPORTS

Interim Progress Report for 1/1/97 – 12/31/97 period
Interim Progress Report for 1/1/96 – 12/31/96 period
Interim Progress Report for 4/15/95 – 12/31/95 period


M. Foltin, G. Stueber, and E. R. Bernstein, "Dynamics of Neutral Cluster Growth and Cluster Ion Fragmentation for Toluene/Water, Aniline/Argon, and 4-


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**REPORT DOCUMENTATION PAGE**

1. AGENCY USE ONLY (Leave blank)
2. REPORT DATE
   10/13/98
3. REPORT TYPE AND DATES COVERED
   Final Report – 4/15/95 – 7/1/96

4. TITLE AND SUBTITLE
   Rydberg State of Energetic Materials

5. FUNDING NUMBERS
   DAAH04-95-1-0185

6. AUTHOR(S)
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
   U.S. Army Research Office
   P.O. Box 12211
   Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
    ARO 32 569.21-CH

11. SUPPLEMENTARY NOTES
    The views, opinions and/or finding contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12a. DISTRIBUTION / AVAILABILITY STATEMENT
    Approved for public release; distribution unlimited

12b. DISTRIBUTION CODE

12. ABSTRACT (Maximum 200 words)
   Energetic materials are modeled experimentally and theoretically with regard to possible excited electronic Rydberg state reactivity and dissociation. The systems of methyl and ethyl alkyl amines have been studied. We show that these Rydberg states can be both highly reactive and dissociative. Thus, excited Rydberg states are a possible route to radicals and other reactive species for these model systems. We are presently expanding our experimental capabilities to allow study of broad spectra of model energetic materials such as nitramines and nitro compounds in general.

   Studies employing covariance spectroscopy of clusters are used to demonstrate the importance of this technique for finding parent/daughter relations in fragmentation studies. Radical behavior is investigated as it relates to fragments of energetic materials.

14. SUBJECT TERMS
   Energetic materials, RDX, Rydberg states, radicals, covariance mapping, fragmentation studies, laser ablation

15. NUMBER OF PAGES
   4

16. PRICE CODE

17. SECURITY CLASSIFICATION
    OR REPORT
    UNCLASSIFIED

18. SECURITY CLASSIFICATION
    OF THIS PAGE
    UNCLASSIFIED

19. SECURITY CLASSIFICATION
    OF THIS PAGE
    UNCLASSIFIED

20. LIMITATION OF ABSTRACT
    I11

NSN 7540-01-280-5500

Enclosure 1

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. 239-16