

REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA, 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.  
PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

|   |                   |                                |   |   |  |
|---|-------------------|--------------------------------|---|---|--|
| 1. REPORT DATE (DD-MM-YYYY)<br>16-10-2017   |                   | 2. REPORT TYPE<br>Final Report |   | 3. DATES COVERED (From - To)<br>15-May-2014 - 14-May-2017 |  |
| 4. TITLE AND SUBTITLE<br>Final Report: Theoretical Chemistry: Theoretical Studies of "Roaming" Chemical Reactions   |                   |                                | 5a. CONTRACT NUMBER<br>W911NF-14-1-0208 |   |  |
|   |                   |                                | 5b. GRANT NUMBER                        |   |  |
|   |                   |                                | 5c. PROGRAM ELEMENT NUMBER<br>611102    |   |  |
| 6. AUTHORS  |                   |                                | 5d. PROJECT NUMBER                      |   |  |
|   |                   |                                | 5e. TASK NUMBER                         |   |  |
|   |                   |                                | 5f. WORK UNIT NUMBER                    |   |  |
| 7. PERFORMING ORGANIZATION NAMES AND ADDRESSES<br>Emory University<br>1599 Clifton Road NE, 4th Floor<br>1599-001-1BA<br>Atlanta, GA 30322 -4250  |                   |                                |   | 8. PERFORMING ORGANIZATION REPORT NUMBER                  |  |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)<br>U.S. Army Research Office<br>P.O. Box 12211<br>Research Triangle Park, NC 27709-2211  |                   |                                |   | 10. SPONSOR/MONITOR'S ACRONYM(S)<br>ARO                   |  |
|   |                   |                                |   | 11. SPONSOR/MONITOR'S REPORT NUMBER(S)<br>65324-CH.12     |  |
| 12. DISTRIBUTION AVAILABILITY STATEMENT<br>Approved for public release; distribution is unlimited.  |                   |                                |   |   |  |
| 13. SUPPLEMENTARY NOTES<br>The views, opinions and/or findings 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. |                   |                                |   |   |  |
| 14. ABSTRACT  |                   |                                |   |   |  |
| 15. SUBJECT TERMS   |                   |                                |   |   |  |
| 16. SECURITY CLASSIFICATION OF:   |                   |                                | 17. LIMITATION OF ABSTRACT<br>UU        | 15. NUMBER OF PAGES                                       | 19a. NAME OF RESPONSIBLE PERSON<br>Joel M Bowman |
| a. REPORT<br>UU   | b. ABSTRACT<br>UU | c. THIS PAGE<br>UU             |   |   | 19b. TELEPHONE NUMBER<br>404-727-6592            |

**RPPR Final Report**  
as of 12-Jun-2018

Agency Code:

Proposal Number: 65324CH

**Agreement Number: W911NF-14-1-0208**

**INVESTIGATOR(S):**

**Name:** Joel M Bowman  
**Email:** jmbowma@emory.edu  
**Phone Number:** 4047276592  
**Principal:** Y

Organization: **Emory University**

Address: 1599 Clifton Road NE, 4th Floor, Atlanta, GA 303224250

Country: USA

DUNS Number: 066469933

EIN: 580566256

**Report Date:** 14-Feb-2017

Date Received: 16-Oct-2017

**Final Report** for Period Beginning 15-May-2014 and Ending 14-May-2017

**Title:** Theoretical Chemistry: Theoretical Studies of "Roaming" Chemical Reactions

**Begin Performance Period:** 15-May-2014

**End Performance Period:** 14-Nov-2017

**Report Term:** 0-Other

Submitted By: Joel M Bowman

Email: jmbowma@emory.edu

Phone: (404) 727-6592

**Distribution Statement:** 1-Approved for public release; distribution is unlimited.

**STEM Degrees:** 0

**STEM Participants:** 0

**Major Goals:** Theoretical reaction dynamics including studies of roaming

**Accomplishments:** Numerous publications and the training of graduate students and postdocs

**Training Opportunities:** Training of postdocs and graduate students

**Results Dissemination:** Numerous publications

**Honors and Awards:** Nothing to Report

**Protocol Activity Status:**

**Technology Transfer:** Nothing to Report

**PARTICIPANTS:**

**Participant Type:** PD/PI

**Participant:** Joel Bowman

**Person Months Worked:** 12.00

**Funding Support:**

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

**Participant Type:** Faculty

**Participant:** Paul Houston

**Person Months Worked:** 12.00

**Funding Support:**

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

**RPPR Final Report**  
as of 12-Jun-2018

Other Collaborators:

**Participant Type:** Graduate Student (research assistant)

**Participant:** Kee Wang

**Person Months Worked:** 12.00

**Funding Support:**

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Yimin Wang

**Person Months Worked:** 3.00

**Funding Support:**

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

**Participant Type:** Graduate Student (research assistant)

**Participant:** Chen Qu

**Person Months Worked:** 6.00

**Funding Support:**

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

## Publications 2015-2017

1. Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation, P. L. Houston, R. Conte, and J. M. Bowman, *J. Phys. Chem. A*, **120**, 5103-5114 (2016). DOI: 10.1021/acs.jpca.6b00488
2. Unimolecular dissociation dynamics of vibrationally activated CH<sub>3</sub>CHOO Criegee intermediates to OH radical products, N. M. Kidwell, H. Li, X. Wang, J. M. Bowman, and M. I. Lester, *Nature Chem.*, **8**, 509-514 (2016) DOI:10.1038/nchem.2488
3. Calculating Feshbach resonances in HCO using an extension of Qim-path theory, X. Wang and J. M. Bowman, *Int. J. Quantum Chem.*, **117**, 139-145 (2016). 10.1002/qua.25286.
4. Two Pathways for Dissociation of Highly Energized syn-CH<sub>3</sub>CHOO to OH Plus Vinyloxy, X. Wang and J. M. Bowman, *J. Phys. Chem. Lett.* **7**, 3359-3364 (2016). 10.1021/acs.jpcllett.6b01392
5. Velocity map imaging of OH radical products from IR activated (CH<sub>3</sub>)<sub>2</sub>COO Criegee intermediates, H. Li, N. M. Kidwell, M. I. Lester, X. Wang, and J. M. Bowman, *J. Chem. Phys.* **145**, 104307 (2016). 10.1063/1.4962361
6. A new (multi-reference configuration interaction) potential energy surface for H<sub>2</sub>CO and preliminary studies of roaming, X. Wang, J. M. Bowman, and P. L. Houston, *Philos Trans A Math Phys. Eng. Sci.* **375** (2017). DOI: 10.1098/rsta.2016.0194
7. Formaldehyde roaming dynamics: Comparison of quasi-classical trajectory calculations and experiments, P. L. Houston, X. Wang, A. Ghosh, J. M. Bowman, M. S. Quinn, and S. H. Kable, *J. Chem. Phys.* **147**, 013936 (2017). 10.1063/1.4982823.
8. Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH<sub>4</sub>, C. Qu and J. M. Bowman, *J. Phys. Chem. A.*, **120**, 4988-4993 (2016).
9. Pruning the Hamiltonian Matrix in MULTIMODE: Test for C<sub>2</sub>H<sub>4</sub> and Application to CH<sub>3</sub>NO<sub>2</sub> Using a New Ab Initio Potential Energy Surface, X. H. Wang, S. Carter, and J. M. Bowman, *J. Phys. Chem. A* **119**, 11632-11640 (2015). DOI: 10.1021/acs.jpca.5b09816
10. Visible/Infrared Dissociation of NO<sub>3</sub>: Roaming in the Dark or Roaming on the Ground?, R. Fernando, A. Dey, B. M. Broderick, B. N. Fu, Z. Homayoon, J. M. Bowman, and A. G. Suits, *J. Phys. Chem. A* **119**, 7163-7168 (2015). DOI:

10.1021/jp509902d.

11. Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene? R. Fernando, C. Qu, J. M. Bowman, R. W. Field, and A. G. Suits, *J. Phys. Chem. Lett.*, 6, 2457-2462 (2015). DOI: 10.1021/acs.jpcllett.5b01031