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**Josh J. Newby - Physical Chemistry**  
Assistant Professor, Department of Chemistry  
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## Education

Ph. D., Physical Chemistry, Purdue University, 2004 - 2009  
Advisor: Prof. Timothy S. Zwier  
Dissertation: "Spectroscopy and Excited State Dynamics of Aromatic Species Relevant to the Atmosphere of Titan."

B. S., Chemistry, Eastern Illinois University, 1999 - 2004  
Advisor: Prof. Sean A. Peebles and Prof. Daniel J. Sheeran

B. S., Secondary Education, Eastern Illinois University, 1999 - 2004  
Certificates in chemistry and physics

## Professional Experience

Assistant Professor, Hobart and William Smith Colleges 2014 - present

Visiting Assistant Professor, Swarthmore College 2011 - 2014

Postdoctoral Associate, Purdue University 2009 - 2011  
Advisor: Prof. Mary J. Wirth

## Courses Taught

CHEM 110: Introductory General Chemistry (lecture)  
CHEM 190: Accelerated General Chemistry (lab)  
CHEM 280: Introductory General Chemistry (lecture)  
CHEM 320: Physical Chemistry I (lecture)  
CHEM 322: Physical Chemistry II (lecture, lab)  
CHEM 425: Advanced Integrated Lab  
CHEM 426: Advanced Topics in Chemistry: Computational Chemistry

CHEM 005 (Swarthmore): It's a small world after a... (first year seminar)  
CHEM 010 (Swarthmore): General Chemistry (lecture, lab)  
CHEM 044 (Swarthmore): Physical Chemistry I (lecture, lab)  
CHEM 045 (Swarthmore): Physical Chemistry II (lecture, lab)

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## External Grant Activity

P.I. - XSEDE (TG-CHE150016) 2015 - 2016  
(130,000 S.U.) *Computational studies of weakly bound molecular systems.*

P.I. - GridChem (ID 547, Project 558) 2012 - 2013  
(30,000 S.U.) *Ab initio investigation of astronomically relevant species*

## Internal Grant Activity

HWS Faculty Research Grant 2015 - 2016  
*Matrix isolation studies of flavor components and their weakly-bound clusters.*

HWS Faculty Startup Grant 2014 - 2017  
*Matrix isolation and computational studies of weakly-bound cluster systems.*

Swarthmore Projects for Educational Exploration and Development 2014  
*Enhancing chemistry labs with digital video.*

Swarthmore College Faculty Research Grant 2013 - 2014  
*Spectroscopic investigations of natural product molecules.*

Summer Educational eProject Development (Swarthmore College) 2013  
*Readiness for Chemistry at Swarthmore College.*

Summer Educational eProject Development (Swarthmore College) 2012  
*Enhancing physical chemistry labs with digital video.*

Swarthmore College Faculty Research Grant 2011 - 2013  
*Spectroscopic investigations of astrochemically relevant species.*

## Undergraduate Research Students

Keshihito Murphy (William Smith '17) May 2015  
*Spectroscopic and computational studies of furan clusters.*

Jackleen Nesheiwat (William Smith '17) May 2015  
*Spectroscopic and computational studies of anthole clusters.*

Schuyler Lockwood (Hobart '16) May 2015  
*Spectroscopic and computational studies of thiophene clusters.*

Sooyun Choi (Swarthmore '17) May 2014 - Aug 2014  
*Spectroscopic and computational studies of vinylanisole isomers*

Melissa A. Trofa (Swarthmore '16) May 2014 - Aug 2014  
*Spectroscopic and computational studies of isoeugenol*

Dawei (David) Ding (Swarthmore '16) May 2013 - Aug 2013  
*Spectroscopic and computational studies of cis-anethole*

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Joseph D. Hagedorn (Swarthmore '15) <i>Spectroscopic and computational studies of isosafrole</i>	May 2013 - Aug 2013
Madeline R. Amodio (Swarthmore) <i>Spectroscopic and computational studies of anethole</i>	May 2012 - Aug 2012
Victoria P. Barber (Swarthmore '13) <i>Spectroscopic and computational studies of anethole</i>	May 2012 - May 2013

## Service

NASA Postdoctoral Program Reviewer	2013
Swarthmore College Institutional Animal Care and Use	2013 - 2014
Swarthmore College Departmental Assessment Liaison	2012 - 2014
Purdue University Graduate Student Advisory Board	2005 - 2007

## Professional Memberships

American Chemical Society	2004 - present
American Physical Society	2009 - present

## Peer-Reviewed Publications

(undergraduate coauthors in **bold**)

1. **V. P. Barber**, J. J. Newby, Jet-cooled fluorescence spectroscopy of a natural product: anethole. *J. Phys. Chem. A*, **2013**, 117, 12831 - 12841.
2. J. J. Newby, M. A. Legg, B. Rogers, M. J. Wirth, Annealing of silica to reduce the concentration of isolated silanols and peak tailing in reverse phase liquid chromatography. *J. Chromatogr. A*. **2011**, 1218, 5131 - 5135.
3. J. J. Newby. Spectroscopy and Excited State Dynamics of Aromatic Species Relevant to the Atmosphere of Titan. Ph. D. Dissertation. Purdue University, West Lafayette, IN, December **2009**.
4. C. W. Müller, J. J. Newby, C. P. Liu, C. P. Rodrigo, T. S. Zwier. Duschinsky mixing between four non-totally symmetric normal coordinates in the S<sub>1</sub>-S<sub>0</sub> vibronic structure of phenylvinylacetylene: A quantitative analysis. *Phys. Chem. Chem. Phys.* **2010**, 12, 2331-2343.
5. J. J. Newby, C. P. Liu, C. W. Müller, W. H. James III, E. G. Buchanan, H D. Lee, T. S. Zwier, Spectroscopy and Photophysics of Structural Isomers of Naphthalene: Z-Phenylvinylacetylene, *J. Phys. Chem. A.*, **2010**, 114, 3190-3198.
6. J. J. Newby, C. W. Müller, C. P. Liu, H. D. Lee, T. S. Zwier, Probing E/Z isomerization of the C<sub>10</sub>H<sub>8</sub> potential energy surface with ultraviolet population transfer spectroscopy, *J. Am. Chem. Soc.*, **2010**, 132, 1611-1620.

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7. J. J. Newby, C. Müller, C. P. Liu, T. S. Zwier, Jet-cooled vibronic spectroscopy of potential intermediates along the pathway to PAH: Phenylcyclopentadi-1,3-ene, *Phys. Chem. Chem. Phys.*, **2009**, 11, 8316-8329.
  8. J. J. Newby, C. P. Liu, C. Müller, T. S. Zwier, Jet-cooled vibronic spectroscopy and asymmetric torsional potentials of phenylcyclopentene, *Phys. Chem. Chem. Phys.*, **2009**, 11, 8330-8341.
  9. C. P. Liu, J. J. Newby, C. W. Müller, H. D. Lee, T. S. Zwier. Spectroscopic characterization of structural isomers of naphthalene: E- and Z-phenylvinylacetylene, *J. Phys. Chem. A.*, **2008**, 112, 9454-9466.
  10. J.J. Newby, J. A. Stearns, C. P. Liu, T. S. Zwier, Photochemical and discharge-driven pathways to aromatic products from 1,3-butadiene, *J. Phys Chem. A.*, **2007**, 111, 10914 -10927.
  11. S.A. Peebles, R.A. Peebles, J.J. Newby and M.M. Serafin, Tunneling Motions and the Barrier to Inversion in the Dimethyl Ether-CS<sub>2</sub> van der Waals Dimer, *Chem. Phys. Lett.*, **2005**, 410, 77-81.
  12. J.J. Newby, M.M. Serafin, R.A. Peebles and S.A. Peebles, Rotational Spectrum of the Dimethyl Ether-Acetylene Complex: Evidence for an Effective C<sub>2v</sub> Geometry, *J. Phys. Chem. A.*, **2005**, 109(24), 5316-5322.
  13. J.J. Newby, R.A. Peebles, S.A. Peebles, Heavy atom structure and conformer stabilities of cyclopropyl carbinol from rotational spectroscopy and ab initio calculations, *J. Mol. Struct.*, **2005**, 740, 133-142.
  14. J.J. Newby, M.M. Serafin, R.A. Peebles, S.A. Peebles, Rotational Spectrum, Structure and Modeling of the OCS-CS<sub>2</sub> van der Waals Dimer, *Phys. Chem. Chem. Phys.*, **2005**, 7, 487-492.
  15. J.J. Newby, R.A. Peebles, S.A. Peebles, The Structure of the Dimethyl Ether-CO<sub>2</sub> van der Waals Complex from Microwave Spectroscopy, *J. Phys. Chem. A.*, **2004**, 108, 11234-11240.
  16. J.J. Newby, R.A. Peebles, S.A. Peebles, The Dimethyl Ether-OCS Dimer: Rotational Spectrum, Structure and Ab Initio Calculations, *J. Phys. Chem. A.*, **2004**, 108, 7372-7378.

## Presentations

(undergraduate coauthors in **bold**)

1. **V. P. Barber**, J. J. Newby. Spectroscopic characterization of a natural product: anethole. Poster at the 246<sup>th</sup> American Chemical Society National Meeting, Indianapolis, IN, September 8-12, 2013
2. **V. P. Barber**, J. J. Newby. Spectroscopic characterization of a natural product: anethole. Talk at the 68<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 17-21, 2013.
3. J. J. Newby, M. A. Legg, B. Rogers, M. J. Wirth, Annealing of silica to reduce the concentration of isolated silanols and peak tailing in reverse phase liquid chromatography. Poster at the 42<sup>nd</sup> ACS Central Regional Meeting Indianapolis IN, June 8-10 2011.

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4. J. J. Newby, M. J. Wirth. Submicrometer particles for protein UHPLC. Poster at the Midwestern Universities Analytical Chemistry Conference, West Lafayette, IN, October 7-9, 2010.
  5. J. J. Newby, C. P. Liu, C. W. Müller, H D. Lee, T. S. Zwier. Excited State Isomerization of a Stilbene Analog: E / Z Phenylvinylacetylene. Poster at the Gordon Research Conference on Electronic Spectroscopy and Dynamics, Waterville, ME, July 19-24, 2009.
  6. J. J. Newby, C. P. Liu, C. W. Müller, H D. Lee, T. S. Zwier. Excited State Isomerization of a Stilbene Analog: E / Z Phenylvinylacetylene. Talk at the 64<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 22-26, 2009.
  7. J. J. Newby, C. P. Liu, C. W. Müller, W. H. James III, E. G. Buchanan, H D. Lee, T. S. Zwier. Characterization of Structural Isomers of Naphthalene: Electronic Spectroscopy of Z-Phenylvinylacetylene. Talk at the 64<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 22-26, 2009.
  8. E. G. Buchanan, C. P. Rodrigo, W. H. James III, J. J. Newby T. S. Zwier. Conformation-Specific Electronic and Vibrational Spectroscopy of Dibenzo-15-Crown-5 Ether in a Supersonic Jet. Talk at the 64<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 22-26, 2009.
  9. J. J. Newby, C. Müller, C. P. Liu, T. S. Zwier, Vibronic Spectroscopy Relevant to Planetary Atmospheres, Invited Talk at Eastern Illinois University Chemistry Seminar, Charleston, IL, January 21, 2009.
  10. J. J. Newby, T. S. Zwier, Conformation Specific Spectroscopy of p-dibenzylbenzene. Talk at the 63<sup>rd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 16-20, 2008.
  11. J. J. Newby, C. Müller, C. P. Liu, T. S. Zwier, Torsional Analysis of Phenylcyclopentenes. Talk at the 63<sup>rd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 16-20, 2008.
  12. C. W. Müller, C.P. Liu, J. J. Newby and T. S. Zwier, Duschinsky mixing between four non-totally symmetric normal coordinates in the  $S_1-S_0$  vibronic structure of phenylvinylacetylene: a quantitative analysis. Talk at the 63<sup>rd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 16-20, 2008.
  13. J. J. Newby, C.-P. Liu, C. Müller and T. S. Zwier, Vibronic spectroscopy of jet-cooled aromatics relevant to planetary atmospheres. Talk at the 22<sup>nd</sup> Austin Symposium on Molecular Structure, Austin, TX, March 1-4, 2008.
  14. J. J. Newby, C.-P. Liu, C. Müller and T. S. Zwier, The ultraviolet spectroscopy of phenylcyclopentene and phenylcyclopentadiene. Talk at the 62<sup>nd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 18-22, 2007.
  15. J. J. Newby, J. A. Stearns, C.-P. Liu and T. S. Zwier, Photochemical and Discharge-driven pathways to aromatics from 1,3-butadiene: Exploring aromatic production in Titan's atmosphere. Talk at the 62<sup>nd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 18-22, 2007.

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16. C.P. Liu, J. J. Newby, C. W. Müller and T. S. Zwier, Fluorescence Spectroscopy of Jet-Cooled 1-Phenyl-1-buten-3-yne in its Ground and First Excited States. Talk at the 62<sup>nd</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 18-22, 2007.
  17. J. J. Newby, R. A. Peebles, S. A. Peebles, Inversion Motions in the Dimethyl Ether-Carbon Disulfide Dimer. Talk at the 60<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 20-24, 2005.
  18. J. J. Newby, M. M. Serafin, Rebecca A. Peebles, Sean A. Peebles, Effective  $C_{2v}$  Symmetry in the Dimethyl Ether- Acetylene. Talk at the 60<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 20-24, 2005.
  19. R.A. Peebles, J.J. Newby, S.A. Peebles, Microwave Spectra, Heavy Atom Structure, and ab initio Calculations on Cyclopropyl Carbinol. Talk at the 59<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 21-25, 2004.
  20. J.J. Newby, R.A. Peebles, S.A. Peebles, Microwave Investigation of C-H Hydrogen Bonding Interactions in the Dimethyl Ether-OCS Dimer. Talk at the 59<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, OH, June 21-25, 2004.

## Video Productions

(undergraduate coauthors in **bold**)

1. **M. F. Silva**, K. P Howard, V. M. Heck, J. J. Newby, Absorption and emission spectroscopy of iodine, YouTube, <http://youtu.be/d6WlvapcSwI> Posted August 28, 2014.
2. **Z. Nakhoda**, M. Bednarz, V. M. Heck, J. J. Newby, Rovibrational spectroscopy, YouTube, <http://youtu.be/iLuGw6z2IJ0> Posted January 16, 2013.
3. **Z. Nakhoda**, M. Bednarz, V. M. Heck, J. J. Newby, HCl/DCl lab, YouTube, <http://youtu.be/EnE02tuyjsM> Posted January 16, 2013.
4. **Z. Nakhoda**, M. Bednarz, V. M. Heck, J. J. Newby, Calorimetry lab, YouTube, <http://youtu.be/GR9F3Ca4m6o> Posted January 16, 2013.