

Timothy S. Zwier

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EDUCATION

B.S. in Chemistry	Calvin College	1977
Ph.D. in Chemical Physics	University of Colorado-Boulder	1981
Thesis advisors:	Professor Stephen R. Leone	
	Professor G. Barney Ellison	

POSITIONS HELD

Postdoctoral Research Associate	The University of Chicago	1981-83
Research advisor:	Donald H. Levy	
Assistant, Associate Professor of Chemistry,	Calvin College	1983-88
Assistant Professor of Chemistry,	Purdue University	1988-93
JILA Visiting Fellow		1994-95
Associate Professor of Chemistry,	Purdue University	1993-97
Associate Department Head,	Purdue University	2001-03

PRESENT POSITION

Professor of Chemistry, Purdue University	1997- present
Department Head, Department of Chemistry	2004- present

AWARDS AND HONORS

Purdue University Faculty Scholar	1999-2004
Fellow of the American Physical Society	2000
Alfred P. Sloan Research Fellow	1989 - 1991

PROFESSIONAL SERVICE

Journal editorships and editorial boards

Senior editor, <i>The Journal of Physical Chemistry</i>	2003-present.
Co-editor, <i>International Reviews in Physical Chemistry</i>	1998-2003
Member of Editorial Board, <i>Molecular Physics</i>	2001-present

Advisory roles (recent)

Combustion Research Facility Advisory Board, Sandia Nat'l Laboratories	2004-present
Councilor-at-Large, Division of Chemical Physics, APS	2002-05
National Research Council Research Associateship Review Panel, Chemical Sciences Panel	1999-2005
Advisory Committee, Research Corp. Science Advancement Programs	1996-01, 03-04.
NASA Planetary Atmospheres Review Panel	2000, 03, 04
External Advisory Committee for Research Corporation evaluation, James Madison University	2005 – present.

Conference organization (recent)

International Advisory Committee, Ohio State Molecular Spectroscopy Conference (Chairman 2002-04)	2000-present
Chairman, Gordon Conference on Molecular and Ionic Clusters	2004
Vice-chairman/Chairman, Gordon Conference on Electronic Spectroscopy and Dynamics	2006/2009
Co-organizer of Symposium, Physical Chemistry Division, ACS "Hydrogen Bonding: Developments in Experiment and Theory"	2005

PROFESSIONAL AND SCHOLARLY ASSOCIATIONS

American Chemical Society
 American Physical Society
 American Astronomical Society (Division of Planetary Sciences)
 American Association for the Advancement of Science

RESEARCH INTERESTS

Development and application of new laser-based methods for mapping out potential energy surfaces of flexible molecules with many conformational minima; single-conformation spectroscopy; hydrogen bonding and solvation effects; intramolecular H-atom tunneling; energy flow and isomerization rates in large molecules; electronic coupling and energy transfer in multichromophore molecules; laboratory measurements of photochemical processes of importance in planetary atmospheres.

RESEARCH PUBLICATIONS

1. R.L. DeKock, A.J. Kromminga, and T.S. Zwier, "The Symmetry of Atomic States and Atomic Orbitals", *J. Chem. Ed.* **56**, 510 (1979).
2. T.S. Zwier, V.M. Bierbaum, G.B. Ellison, and S.R. Leone, "Vibrational product state distributions of ion-molecule reactions by infrared chemiluminescence: $\text{Cl}^- + \text{HBr}, \text{HI} \rightarrow \text{HCl}(\nu) + \text{Br}^-, \text{I}^-$ ", *J. Chem. Phys.* **72**, 5426 (1980).
3. T.S. Zwier, M.M. Maricq, C.J.S.M. Simpson, V.M. Bierbaum, G.B. Ellison, and S.R. Leone, "Direct detection of the product vibrational state distribution in the associative detachment reaction $\text{Cl}^- + \text{H} \rightarrow \text{HCl}(\nu) + \text{e}^-$ ", *Phys. Rev. Lett.* **44**, 1050 (1980).
4. J.C. Weisshaar, T.S. Zwier, and S.R. Leone, "Nascent product vibrational state distributions of ion-molecule reactions: The proton transfer reactions: $\text{F}^- + \text{HX} \rightarrow \text{HF}(\nu) + \text{X}^-$, $\text{X} = \text{Cl}, \text{Br}, \text{and I}$ ", *J. Chem. Phys.* **75**, 4873 (1981).
5. T.S. Zwier, J.C. Weisshaar, and S.R. Leone, "Nascent product vibrational state distributions of ion-molecule reactions: The $\text{H} + \text{F}^- \rightarrow \text{HF}(\nu) + \text{e}^-$ associative detachment reaction", *J. Chem. Phys.* **75**, 4885 (1981).
6. C.E. Hamilton, M.A. Duncan, T.S. Zwier, J.C. Weisshaar, G.B. Ellison, V.M. Bierbaum, and S.R. Leone, "Product vibrational analysis of ion-molecule reactions by laser-induced fluorescence in a flowing afterglow: $\text{O}^- + \text{HF} \rightarrow \text{OH}(\nu=0,1) + \text{F}^-$ ", *Chem. Phys. Lett.* **94**, 4 (1983).
7. T.S. Zwier, E. Carrasquillo M., and D.H. Levy, "The spectroscopy and single vibronic level fluorescence quantum yields of jet-cooled trans-stilbene and its van der Waals complexes", *J. Chem. Phys.* **78**, 5493 (1983).
8. E. Carrasquillo M., T.S. Zwier, and D.H. Levy, "The Multiphoton Ionization Spectrum of Complexes of Benzene and Acetylene", *J. Chem. Phys.* **83**, 4990 (1985).

9. C.A. Taatjes, W.B. Bosma, and T.S. Zwier, "Mode-Selective Broadening in Low Frequency Modes of *trans*-stilbene van der Waals Complexes", Chem. Phys. Lett. **128**, 127-132 (1986).
10. L.H. Spangler, R. van Zee, and T.S. Zwier, "Assignment of Low Frequency Modes in *trans*-stilbene. Evidence for Planarity in the Isolated Molecule", J. Phys. Chem. **91**, 2782-2786 (1987).
11. L.H. Spangler, R.D. van Zee, S.C. Blankespoor, and T.S. Zwier, "Additional Evidence for Planarity in isolated *trans*-stilbene: A study of α -Deuterio-*trans*-stilbene", J. Phys. Chem., **91**, 6077-6079 (1987).
12. M.-C. Duval, B. Soep, R.D. van Zee, W.B. Bosma, and T.S. Zwier, "Half Collision Studies of the Hg-NH₃ Excimer", J. Chem. Phys. **88**, 2148-2158 (1988).
13. R. van Zee, W.B. Bosma, T. Zwier, M.C. Duval, and B. Soep, "Intermolecular Potential and Dissociation of Excited State Mercury Ammonia Complexes", in *Large Finite Systems*, ed. J. Jortner, A. Pullman and B. Pullman (Reidel, Dordrecht, 1987) Vol. 20, pp. 101-112.
14. R.D. van Zee, S.C. Blankespoor, and T.S. Zwier, "Direct Spectroscopic Determination of the Ground State Hg₂ Bond Length and an Analysis of the 2540 Å Band", J. Chem. Phys. **88**, 4650 - 4654 (1988).
15. L.H. Spangler, W.B. Bosma, R.D. van Zee, and T.S. Zwier, "Hindered Internal Rotation in some singly methylated *trans*-Stilbenes", J. Chem. Phys. **88**, 6768- 6777 (1988).
16. D.O. DeHaan, A.L. Holton, and T.S. Zwier, "State Mixing and Vibrational Predissociation in Large-Molecule van der Waals Complexes: *trans*-stilbene-X complexes where X = He, H₂, Ne, and Ar", J. Chem. Phys. **90**, 3952-3966(1989).
17. T.S. Zwier, "State Mixing and Internal Rotation Predissociation in Large-Molecule van der Waals Complexes: p-methyl-*trans*-stilbene-X complexes where X = He, H₂", J. Chem. Phys. **90**, 3967-3980 (1989).
18. D.O. DeHaan and T.S. Zwier, "Hindered internal rotation and *ortho*-H₂ enrichment in *trans*-stilbene-H₂/D₂ complexes", J. Chem. Phys., **90**, 1460-1468 (1989).
19. R.D. van Zee, S.C. Blankespoor, and T.S. Zwier, "Spectroscopic Studies of the Hg-He and Hg-Ar₂ van der Waals' Complexes: The Hg Vapor Fluorescence Filter", Chem. Phys. Lett. **158**, 306-311 (1989).
20. J.R. Gord, A.W. Garrett, R.E. Bandy, and T.S. Zwier, "REMPI Fragmentation as a Probe of Hydrogen Bonding in Aromatic-X Clusters", Chem. Phys. Lett. **171**, 443-450 (1990).
21. A.J. Gotch and T.S. Zwier, "Half-Collision Studies of π -Hydrogen Bonding interactions in Benzene-HCl and Toluene-HCl Complexes", J. Chem. Phys. **93**, 6977-6986 (1990).

22. A.J. Gotch, A.W. Garrett, D.L. Severance, and T.S. Zwier, "The Structure and Photophysics of Clusters of Immiscible Liquids: $C_6H_6-(H_2O)_n$ ", Chem. Phys. Lett. **178**, 121-129 (1991).
23. R.E. Bandy, J. Nash, and T.S. Zwier, "The Spectroscopic and Photophysical Effects of the Position of Methyl Substitution: 1. 4- and 5-methylpyrimidine", J. Chem. Phys. **95**, 2317-2335 (1991).
24. A.J. Gotch, A.W. Garrett, and T.S. Zwier, "The Ham Bands Revisited: The Spectroscopy and Photophysics of the $C_6H_6-CCl_4$ complex", J. Phys. Chem. **95**, 9699-9707 (1991).
25. R.E. Bandy, A.W. Garrett, H.D. Lee, and T.S. Zwier, "The Spectroscopic and Photophysical Effects of the Position of Methyl Substitution: 2. 2-methylpyrimidine", J. Chem. Phys. **96**, 1667-1676 (1992).
26. A.J. Gotch and T.S. Zwier, "Multiphoton Ionization Studies of Clusters of Immiscible Liquids: 1. $C_6H_6-(H_2O)_n$, $n=1,2$ ", J. Chem. Phys. **96**, 3388-3401(1992).
27. A.W. Garrett and T.S. Zwier, "Multiphoton Ionization Studies of Clusters of Immiscible Liquids: 2. $C_6H_6-(H_2O)_n$, $n=3-8$ and $(C_6H_6)_2-(H_2O)_{1,2}$ ", J. Chem. Phys. **96**, 3402-3410 (1992).
28. A.W. Garrett, D.L. Severance, and T.S. Zwier, "Multiphoton Ionization Studies of $C_6H_6-(CH_3OH)_n$ Clusters: I. Comparisons with $C_6H_6-(H_2O)_n$ Clusters", J. Chem. Phys. **96**, 7245-7258 (1992).
29. A.W. Garrett and T.S. Zwier, "Multiphoton Ionization Studies of $C_6H_6-(CH_3OH)_n$ Clusters: II. Intracluster Ion-Molecule Reactions", J. Chem. Phys. **92**, 7259 - 7267 (1992).
30. R.E. Bandy, C. Lakshminarayan, and T.S. Zwier, "Spectroscopy and Photophysics of the $^1\Delta_u \leftarrow ^1\Sigma_g^+$ Transition of Jet-Cooled C_4H_2 , C_4HD , and C_4D_2 ", J. Phys. Chem. **96**, 5337-5343 (1992).
31. J.D. Augspurger, C.E. Dykstra, and T.S. Zwier, "Hydrogen Bond Swapping in the Benzene-Water Complex. A Model Study of the Interaction Potential", J. Phys. Chem. **96**, 7252 - 7257 (1992).
32. A.W. Garrett and T.S. Zwier, "The Spectroscopy of Mixed-Solvent Clusters: $C_6H_6-(H_2O)_n-(CH_3OH)_m$ ", J. Phys. Chem. **96**, 9710-9718 (1992).
33. R.E. Bandy, C. Lakshminarayan, R.K. Frost, and T. S. Zwier, "Direct Detection of C_4H_2 Photochemical Products: Possible Routes to Complex Hydrocarbons in Planetary Atmospheres", Science **258**, 1630-1633 (1992).
34. J.D. Augspurger, C.E. Dykstra, and T.S. Zwier, "A Model Study of the Structures and Stabilities of $C_6H_6-(H_2O)_{2-12}$ Clusters", J. Phys. Chem. **97**, 980-984 (1993).

35. R.E. Bandy, C. Lakshminarayan, R.K. Frost, and T.S. Zwier, "The Ultraviolet Photochemistry of Diacetylene: Direct Detection of Primary Products of the Metastable $C_4H_2^* + C_4H_2$ Reaction", *J. Chem. Phys.* **98**, 5362-5374 (1993).
36. F.A. Ensminger, J. Plassard and T.S. Zwier, "Electronic substituent and Amino Torsional Coupling Effects on Intramolecular Proton Tunneling in 5-aminotropolone", *J. Phys. Chem.* **97**, 4344-4353 (1993).
37. F.A. Ensminger, Jason Plassard, and T.S. Zwier, "Vibronically State-Selective Photoisomerization in 5-hydroxytropolone", *J. Chem. Phys.* **99**, 8341 (1993).
38. A.J. Gotch, R.N. Pribble, F.A. Ensminger, and T.S. Zwier, "The Spectroscopy and Photophysics π Hydrogen-bonded Complexes: $C_6H_6-CHCl_3$ ", *Laser Chemistry* **13**, 187-205 (1994).
39. R.N. Pribble and T.S. Zwier, "Size-Specific Infrared Spectra of Benzene- $(H_2O)_n$ with $n=1-7$: Evidence for the Transition from Cyclic to Non-cyclic $(H_2O)_n$ structures", *Science* **265**, 75-79 (1994).
40. R.N. Pribble and T.S. Zwier, "Probing Hydrogen Bonding in Benzene- $(water)_n$ Clusters using Resonant Ion-Dip Infrared Spectroscopy", *Faraday Discuss.* **97**, 229 (1994).
41. K. Kim, K.D. Jordan, and T.S. Zwier, "Low-energy Structures and Vibrational Frequencies of the Water Hexamer: Comparison with Benzene $(H_2O)_6$ ", *J. Am. Chem. Soc.* **116**, 11568-9 (1994).
42. A.W. Garrett and T.S. Zwier, "Resonant Two-Photon Ionization Studies of Benzene (solvent) $_n$ Clusters", a review chapter in *Advances in Multiphoton Processes and Spectroscopy*, ed. S.H. Lin, A.A. Villaeys, and Y. Fujimara (World Scientific), Vol. 8, Part 2, pp. 129-188 (1994) .
43. R.K. Frost, G. Zavarin, and T.S. Zwier, "The Ultraviolet Photochemistry of Diacetylene: The Metastable $C_4H_2^*+C_2H_2$ Reaction in Helium and Nitrogen", *J. Phys. Chem.* **99**, 9408-9415 (1995).
44. F.A. Ensminger, J. Plassard, T.S. Zwier, and S. Hardinger, "Mode-selective Photo-isomerization in 5-hydroxytropolone: I. Experiment", *J. Chem. Phys.* **102**, 5246-5259 (1995).
45. J.J. Nash, T.S. Zwier, and K.D. Jordan, "Mode-selective Photoisomerization in 5-hydroxytropolone: II. Theory", *J. Chem. Phys.* **102**, 5260-5270 (1995).
46. R.N. Pribble, A.W. Garrett, K. Haber, and T.S. Zwier, "Resonant Ion-dip Infrared Spectroscopy of Benzene- H_2O and Benzene-HOD", *J. Chem. Phys.* **103**, 531-544 (1995).
47. S. Fredericks, K.D. Jordan, and T.S. Zwier, "Theoretical Characterization of the Structures and Vibrational Spectra of Benzene- $(H_2O)_n$, $n=1-3$, Clusters", *J. Phys. Chem.* **100**, 7810-7821 (1996).

48. R.K. Frost, C.A. Arrington, C. Ramos, and T.S. Zwier, "The Ultraviolet Photochemistry of Diacetylene: The Metastable $C_4H_2^*$ Reaction with ethene, propene, and propyne", *J. Am. Chem. Soc.* **118**, 4451-4461 (1996).
49. R.K. Frost, F. Hagemester, C.A. Arrington, T.S. Zwier, and K.D. Jordan, "Fluorescence-dip infrared spectroscopy of Tropolone and Tropolone-OD", *J. Chem. Phys.* **105**, 2595-2604 (1996).
50. R.K. Frost, F. Hagemester, C.A. Arrington, D. Schleppenbach, T.S. Zwier, and K.D. Jordan, "Fluorescence-dip infrared spectroscopy of the tropolone- H_2O complex", *J. Chem. Phys.* **105**, 2605-17 (1996).
51. D.T. Anderson, S. Davis, T.S. Zwier, and D.J. Nesbitt, "An intense slit discharge source of jet-cooled molecular ions and radicals ($T_{rot} < 30$ K)", *Chem. Phys. Lett.* **258**, 207-12 (1996).
52. T.S. Zwier and M. Allen, "Metastable diacetylene reactions as routes to large hydrocarbons in Titan's atmosphere", *Icarus* **123**, 578-583 (1996).
53. R.K. Frost, F. Hagemester, C. Arrington, D. Schleppenbach, G. Laurence, and T.S. Zwier, "Fluorescence-dip infrared spectroscopy of 5-hydroxytropolone", *J. Phys. Chem.* **100**, 16835-16842 (1996).
54. T.S. Zwier, "The Spectroscopy of Solvation in Hydrogen-bonded Aromatic Clusters", *Ann. Rev. Phys. Chem.* **47**, 205-241 (1996).
55. R.N. Pribble, C. Gruenloh, and T.S. Zwier, "Resonant ion-dip infrared spectroscopy of benzene-(methanol)_n clusters with n=1-6", *J. Chem. Phys.* **106**, 2145-2157 (1997).
56. R.N. Pribble, C. Gruenloh, and T.S. Zwier, "The ultraviolet and infrared spectroscopy of (benzene)₂-(CH₃OH)₃ isomeric clusters" *Chem. Phys. Lett.* **262**, 627-632 (1996).
57. T.S. Zwier, "The Infrared Spectroscopy of Hydrogen-bonded clusters: Chains, cycles, cubes, and three-dimensional networks", to appear in *Advances in Molecular Vibrations and Collision Dynamics*, J.M. Bowman ed., (JAI, Greenwich, 1998), pp. 249-280.
58. S.Y. Fredericks, J.M. Pedulla, K.D. Jordan, and T.S. Zwier, "OH stretch IR spectra of (H₂O)₃ and benzene-(H₂O)₃", *Theor. Chem. Acc.* **96**, 51-55 (1997).
59. C.J. Gruenloh, J.R. Carney, C.A. Arrington, T.S. Zwier, S.Y. Fredericks, and K.D. Jordan, "Infrared Spectrum of a Molecular Ice Cube: The S₄ and D_{2d} Water Octamers in Benzene-(water)₈", *Science* **276**, 1678-1681 (1997).
60. F. Hagemester and T.S. Zwier, "Density functional theory calculations of the structures, binding energies, and infrared spectra of methanol clusters", *J. Phys. Chem. A* **102**, 82-94 (1998).

61. J.R. Carney, F.C. Hagemeister, and T.S. Zwier, "The hydrogen-bonding topologies of indole-(water)_n clusters from resonant ion-dip infrared spectroscopy", *J. Chem. Phys.* **108**, 3379-3382 (1998).
62. F.C. Hagemeister, C.A. Arrington, B.J. Giles, B. Quimpo, L. Zhang, and T.S. Zwier, "Cavity ringdown methods for studying intramolecular and intermolecular dynamics", chapter in "Cavity ring-down spectroscopy – An Ultratrace-Absorption Measurement Technique", ed. K.S. Busch and M.A. Busch, ACS Symposium Series 720, Chap. 14, pp. 210-232.
63. C.A. Arrington, C. Ramos, A.D. Robinson, and T.S. Zwier, "Aromatic Ring-Forming Reactions of Metastable Diacetylene with 1,3-butadiene", *J. Phys. Chem. A* **102**, 3315-3322 (1998).
64. C.J. Gruenloh, J.R. Carney, F.C. Hagemeister, C.A. Arrington, T.S. Zwier, S.Y. Fredericks, J.T. Wood III, and K.D. Jordan, "Resonant ion-dip infrared spectroscopy of the S₄ and D_{2d} water octamers in benzene-(water)₈ and benzene₂-(water)₈", *J. Chem. Phys.* **109**, 6601-6614 (1998).
65. F.C. Hagemeister, C.J. Gruenloh, and Timothy S. Zwier, "Resonant ion-dip infrared spectroscopy of benzene-(water)_n(methanol)_m clusters with n+m=4,5", *Chem. Phys.* **239**, 83-96 (1998).
66. Christopher J. Gruenloh, Gina M. Florio, Joel R. Carney, Fredrick C. Hagemeister, and Timothy S. Zwier, "C-H Stretch Modes as a Probe of H-bonding in Methanol-containing Clusters", *J. Phys. Chem. A* **103**, 496-502 (1999).
67. Christopher J. Gruenloh, Fredrick C. Hagemeister, Joel R. Carney, and Timothy S. Zwier, "Resonant ion-dip infrared spectroscopy of ternary benzene-(water)_n (methanol)_m hydrogen-bonded clusters", *J. Phys. Chem. A* **103**, 503-513 (1999).
68. C.A. Arrington, C. Ramos, A.D. Robinson, and T.S. Zwier, "The ultraviolet photochemistry of diacetylene with alkynes and alkenes: Spectroscopic characterization of the products", *J. Phys. Chem. A* **103**, 1294-1299 (1999).
69. Joel R. Carney and Timothy S. Zwier, "The Infrared and Ultraviolet Spectroscopy of water-containing clusters of indole, 1-methylindole, and 3-methylindole", *J. Phys. Chem. A* **103**, 9943-9957 (1999).
70. C.J. Gruenloh, F.C. Hagemeister, and T.S. Zwier, "Size and Conformation-selective infrared spectroscopy of neutral hydrogen-bonded clusters", *Recent Theoretical and Experimental Advances in Hydrogen-Bonded Clusters*, NATO Advanced Study Institute, edited by S.S. Xantheas (Kluwer, The Netherlands), 83-99 (2000).
71. Christopher J. Gruenloh, Joel R. Carney, Fredrick C. Hagemeister, Timothy S. Zwier, John T. Wood III, and Kenneth D. Jordan, "Resonant ion-dip infrared spectroscopy of benzene-(water)₉: Expanding the cube", *J. Chem. Phys.* **113**, 2290-2303 (2000).

72. Charles S. McEnally, Allison G. Robinson, Lisa D. Pfefferle, and Timothy S. Zwier, "Aromatic Hydrocarbon Formation in Nonpremixed Flames Doped with Diacetylene, Vinylacetylene, and Other Hydrocarbons: Evidence for Pathways Involving C₄ Species", *Combustion and Flame* **123**, 344-357 (2000).
73. Joel R. Carney and Timothy S. Zwier, "The Infrared and Ultraviolet Spectra of Individual Conformers of Biomolecules: Tryptamine", *J. Phys. Chem. A* **104**, 8677-8688 (2000).
74. Allison G. Robinson, Paul R. Winter, Christopher Ramos, and Timothy S. Zwier, "Ultraviolet Photochemistry of Diacetylene: Reactions with Benzene and Toluene", *J. Phys. Chem. A* **104**, 10312-10320 (2000).
75. Gina M. Florio, Christopher J. Gruenloh, Robert C. Quimpo, and Timothy S. Zwier, "The Infrared Spectroscopy of Hydrogen-Bonded Bridges: I. 2-pyridone-(water)_n and 2-hydroxypyridine-(water)_n, n=1,2", *J. Chem. Phys.* **113**, 11143-11153 (2000).
76. Joel R. Carney, Andrei Fedorov, John R. Cable, and Timothy S. Zwier, "The Infrared Spectroscopy of H-bonded bridges stretched across the cis-amide group: I. Water bridges", *J. Phys. Chem. A*, **105**, 3487-3497 (2001).
77. Gina M. Florio, Edwin L. Sibert III, and Timothy S. Zwier, "Fluorescence-dip infrared spectra of jet-cooled benzoic acid dimer in its ground and first excited singlet states", *Faraday Discussion* **118** (Cluster Dynamics), pp. 315-330 (2001).
78. Andrei Fedorov, John R. Cable, Joel R. Carney, and Timothy S. Zwier, "The Infrared Spectroscopy of H-bonded bridges spanning the cis-amide group: II. Ammonia and mixed ammonia/water bridges", *J. Phys. Chem. A* **105** (35), 8162-8175 (2001).
79. Joel R. Carney and Timothy S. Zwier, "Conformational Flexibility in small biomolecules: Tryptamine and 3-indole-propionic acid", *Chem. Phys. Lett.* **341**, 77-85 (2001).
80. Joel R. Carney, Brian C. Dian, Gina M. Florio, and Timothy S. Zwier, "The role of water bridges in directing the conformational preferences of 3-indole-propionic acid and tryptamine", *J. Am. Chem. Soc.* **123**, 5596-5597 (2001).
81. Timothy S. Zwier, "Laser Spectroscopy of Jet-Cooled Biomolecules and their Water-Containing Clusters: Water Bridges and Molecular Conformation", *J. Phys. Chem. A* **105**, 8827-8839 (2001).
82. C. Ramos, Paul R. Winter, Timothy S. Zwier, and Stephen T. Pratt, "Photoelectron Spectroscopy via the 1¹Δ_g state of Diacetylene", *J. Chem. Phys.* **116**, 4011 (2002).
83. Allison G. Robinson, Paul R. Winter, and Timothy S. Zwier, "The singlet-triplet spectroscopy of 1,3-butadiene using cavity ring-down spectroscopy", *J. Chem. Phys.* **116** (18): 7918-7925 (2002).

84. Allison G. Robinson, Paul R. Winter, and Timothy S. Zwier, "The Ultraviolet Photochemistry of Diacetylene with Styrene", *J. Phys. Chem. A* **106** (24): 4789-4796 (2002).
85. Brian C. Dian, Asier Longarte, and Timothy S. Zwier, "Conformational Dynamics in a Dipeptide After Single-Mode Vibrational Excitation", *Science* **296** (5577): 2369-2373 (2002).
86. David R. Borst, Joseph R. Roscioli, David W. Pratt, Gina M. Florio, Timothy S. Zwier, Andreas Müller and Samuel Leutwyler, "Hydrogen bonding and tunneling in the 2-pyridone-2-hydroxypyridine mixed dimer. Effect of electronic excitation", *Chemical Physics* **283**: 341-354 (2002).
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93. Christopher Ramos, Paul R. Winter, Jaime A. Stearns, and Timothy S. Zwier, "The spectroscopic consequences of C-H \cdots π H-bonding: C₆H₆-(C₄H₂)_n clusters with n=1 and 2", *J. Phys. Chem. A* **107**, 10280-10287 (2003).
94. Jaime A. Stearns and Timothy S. Zwier, "The infrared and ultraviolet spectroscopy of jet-cooled *ortho*-, *meta*-, and *para*-diethynylbenzene", *J. Phys. Chem. A* **107**, 10717-10724 (2003).
95. Brian C. Dian, Asier Longarte, Paul R. Winter, and Timothy S. Zwier, "The Dynamics of Conformational Isomerization in Flexible Biomolecules: Hole-filling spectroscopy of N-acetyl tryptophan methyl amide and N-acetyl tryptophan amide", *J. Chem. Phys.* **120**, 133-147 (2004).

96. David Evans, David Wales, Brian C. Dian, and Timothy S. Zwier, "The Dynamics of Conformational Isomerization in Flexible Biomolecules: Simulating isomerizations in a supersonic expansion with master equation dynamics", *J. Chem. Phys.* **120**, 148-157 (2004).
97. Jaime A. Stearns, Alope Das, and Timothy S. Zwier, Hydrogen atom dislocation in the excited state of anthranilic acid: Probing the carbonyl stretch fundamental and the effects of water complexation", *Physical Chemistry-Chemical Physics* **6**, 2605-2610 (2004).
98. Brian C. Dian, Jasper R. Clarkson, and Timothy S. Zwier, "Infrared-induced conformational isomerization dynamics and vibrational relaxation in melatonin and 5-methoxy-N-acetyl tryptophan methyl amide", *J. Chem. Phys.* **120** (19): 9033-9046 (2004).
99. Brian C. Dian, Jasper R. Clarkson, and Timothy S. Zwier, "Direct Experimental Measurement of the Energy Thresholds to Conformational Isomerization in Tryptamine", *Science* **303**, 1169-1173 (2004).
100. Timothy S. Zwier, "The Structure of Protonated Water Clusters", *Science* **304** (5674): 1119-1120 (2004).
101. Cathrine A. Southern, Donald H. Levy, Jaime A. Stearns, Gina M. Florio, Asier Longarte, and Timothy S. Zwier, "The Spectroscopic Consequences of Localized Electronic Excitation in Anthranilic Acid Dimer", *J. Phys. Chem. A* **108**(21) 4599-4609 (2004).
102. Jasper R. Clarkson, Esteban Baquero, V. Alvin Shubert, Evgeniy M. Myshakin, Kenneth D. Jordan, and Timothy S. Zwier, "Laser-Driven Shuttling of a Water Molecule between H-bonding sites", *Science* **307**, 1443-1446 (2005).
103. Bruce C. Garrett, David A. Dixon, Donald M. Camaioni, Daniel M. Chipman, Mark A. Johnson, Charles D. Jonah, Gregory A. Kimmel, John H. Miller, Thomas N. Rescigno, Peter J. Rossky, Sotiris S. Xantheas, Steven D. Colson, Allan H. Laufer, Douglas Ray, Paul F. Barbara, David M. Bartels, Kurt H. Becker, Kit H. Bowen, Stephen E. Bradforth, Ian Carmichael, James V. Coe, L. Rene Corrales, James P. Cowin, Michel Dupuis, Kenneth B. Eisenthal, James A. Franz, Maciej S. Gutowski, Kenneth D. Jordan, Bruce D. Kay, Jay A. LaVerne, Sergei V. Lymar, Theodore E. Madey, C. William McCurdy, Dan Meisel, Shaul Mukamel, Anders R. Nilsson, Thomas M. Orlando, Nikolay G. Petrik, Simon M. Pimblott, James R. Rustad, Gregory K. Schenter, Sherwin J. Singer, Andrei Tokmakoff, Lai-Sheng Wang, Curt Wittig, and Timothy S. Zwier, "The Role of Water on Electron-Initiated Processes and Radical Chemistry: Issues and Scientific Advances", *Chemical Reviews* **105**, 355-389 (2005).
104. Jasper R. Clarkson, Brian C. Dian, Loïck Moriggi, Albert DeFusco, Valerie McCarthy, Kenneth D. Jordan, and Timothy S. Zwier, "Direct Measurement of the Energy Thresholds to Conformational Isomerization in Tryptamine: Experiment and Theory", *J. Chem. Phys.* **122**, Art. No. 214311 (2005), 15 pages.
105. Jasper R. Clarkson, Esteban Baquero, and Timothy S. Zwier, "Direct Measurement of the Energy Thresholds to Conformational Isomerization: II. 3-indole propionic acid and its water-containing complex", *J. Chem. Phys.* **122**, Art. No. 214312 (2005), 8 pages.

106. Talitha M. Selby, Jasper R. Clarkson, Diane Mitchell, James A.J. Fitzpatrick, H. Daniel Lee, David W. Pratt, and Timothy S. Zwier, "Conformation-specific Spectroscopy and Conformational Isomerization Energetics of *ortho*-, *meta*-, and *para*-Ethynylstyrenes", *J. Phys. Chem. A* **109**, 4484-96 (2005).
107. Talitha M. Selby and Timothy S. Zwier, "Conformation-specific spectroscopy of 4-phenyl-1-butyne and 5-phenyl-1-pentyne", *J. Phys. Chem. A* **109**(38) 8487-8496 (2005).
108. Talitha M. Selby, Alope Das, T. Bekele, H. Daniel Lee, Timothy S. Zwier, "Conformation-specific Spectroscopy of 3-benzyl-1,5-hexadiyne", *J. Phys. Chem. A* **109**(38), 8497-8506 (2005).
109. Timothy S. Zwier, "Laser probes of Conformational Isomerization in Flexible Molecules and Complexes", *J. Phys. Chem. A* **110**(12) 4133-4150 (2006). Feature article.

SUBMITTED MANUSCRIPTS

110. Dieter Cremer, Elfrieda Kraka, Jaime A. Stearns, and Timothy S. Zwier, "Exploration of the potential energy surface for Rearrangement and Decomposition Reactions of Vinylacetylene : A Computational Study", PCCP (submitted).
111. Jaime A. Stearns, Dieter Cremer, Elfrieda Kraka, and Timothy S. Zwier, "The Gas-phase photochemistry of vinylacetylene", PCCP (submitted).

MANUSCRIPTS IN PREPARATION

1. Jaime A. Stearns, Nathan R. Pillsbury, Alope Das, Talitha M. Selby, David F. Plusquellic, and Timothy S. Zwier, "Phenyl ring torsion and Excitonic Interaction in Diphenylmethane", (in preparation).
2. Talitha M. Selby, W. Leo Meerts, and Timothy S. Zwier, "Isomer-specific Ultraviolet Spectroscopy of *meta*- and *para*-divinylbenzene", (in preparation).
3. Talitha M. Selby and Timothy S. Zwier, "Laser-initiated conformational isomerization of *meta*-divinylbenzene: Barrier heights and pathways", (in preparation).
4. V. Alvin Shubert, Esteban E. Baquero, Jasper R. Clarkson, William H. James, Jeffrey A. Turk, Alissa A. Hare, Mark Lipton, and Timothy S. Zwier, "Laser spectroscopy of a doubly-substituted aromatic with two flexible side chains: Intrachain and interchain conformational preferences" (in preparation).
5. Esteban E. Baquero, V. Alvin Shubert, Tracy M. LeGreve, Jasper R. Clarkson, William H. James III, and Timothy S. Zwier, "Single-conformation spectroscopy of a flexible bichromophore: 3-(4-hydroxyphenyl)-N-benzyl-propionamide" (in preparation).
6. Jasper R. Clarkson and Timothy S. Zwier, "Infrared photodissociation of a water molecule from a flexible molecule-H₂O complex: Rates and conformational product yields following XH stretch excitation", (in preparation).

7. Nathan R. Pillsbury, David Plusquellic, W. Leo Meerts, and Timothy S. Zwier, "Conformational effects on excitonic interactions in a prototypical H-bonded bichromophore: bis-(2-hydroxyphenyl)methane", (in preparation).
8. Tracy LeGreve, Jasper R. Clarkson, and Timothy S. Zwier, "Conformer-specific, single vibronic-level fluorescence spectra of tryptamine and melatonin: Duschinsky mixing and anharmonic coupling", (in preparation).
9. Tracy LeGreve, Esteban E. Baquero, and Timothy S. Zwier, "The infrared and ultraviolet spectral signatures and conformational preferences of jet-cooled Serotonin", (in preparation).

INVITED LECTURES

1. Physical Chemistry Seminar, University of Chicago, 1981.
2. Chemistry Dept. Seminar, Calvin College, 1981.
3. Physical Chemistry Seminar, University of California at Irvine, Irvine, California, 1983.
4. Chemistry Dept. Seminar, Hope College, Holland, Michigan, 1984.
5. Physical Chemistry Seminar, Michigan State University, Lansing, Michigan, 1984.
6. University of Colorado Chemical Physics Seminar, Boulder, Colorado, 1985.
7. Physical Chemistry Seminar, Northwestern University, Evanston, Illinois, 1986.
8. Chemistry Dept. Seminar, Grand Valley State University, Allendale, Michigan, 1986.
9. Physical Chemistry Seminar, University of Michigan, Ann Arbor, Michigan, 1986.
10. XVIIth Informal Photochemistry Conference, Boulder, Colorado, 1986.
11. Physical Chemistry Seminar, Wayne State University, Detroit, Michigan, 1986.
12. Physical Chemistry Seminar, Universite Paris-Sud, Orsay, France, 1987.
13. Physical Chemistry Seminar, Purdue University, West Lafayette, Indiana, 1987.
14. Physical Chemistry Seminar, Ohio State University, Columbus, Ohio, 1988.
15. Physical Chemistry Seminar, University of California at Santa Barbara, Santa Barbara, California, 1988.
16. Physical Chemistry Seminar, Rice University, Houston, Texas, 1988.
17. Physical Chemistry Seminar, Oregon State University, Corvallis, Oregon, 1988.
18. Chemistry Department Seminar, Calvin College, Grand Rapids, Michigan, 1989.
19. Chemistry Department Seminar, Hope College, Holland, Michigan, 1989.
20. Physical Chemistry Seminar, Colorado State University, March, 1990.
21. Physical Chemistry Seminar, University of Utah, March, 1990.
22. JILA Chemical Physics Seminar, University of Colorado, March, 1990.
23. XIXth Informal Conference on Photochemistry, Ann Arbor, Michigan, June 25-29, 1990.
24. National American Chemical Society Meeting, Washington, D.C., August 1990. (Invited talk in Symposium on Intermolecular Potentials, Physical Chemistry Division).
25. Physical Chemistry seminar, University of Wisconsin, Madison, Wisconsin, February, 1991.
26. Physical Chemistry Seminar, Indiana University, Bloomington, Indiana, February, 1991.
27. Telluride Summer Research Conference on Intermolecular Interactions, July 1991, Telluride, Colorado.
28. Dean's Honors Seminar, Sept. 1991, Purdue University.
29. Chemistry Dept. Seminar, Sept. 1991, Bowling Green State University.
30. Chemistry Dept. Seminar, Oct., 1991, Bradley University.
31. Physical Chemistry Seminar, University of Rochester, Oct., 1991.
32. Physical Chemistry Seminar, Cornell University, Oct., 1991.
33. Chemistry Department Seminar, IUPUI, Nov., 1991.
34. Chemical Physics Seminar, University of California at Los Angeles, Dec, 1991.
35. Physical Chemistry Seminar, University of California at Irvine, Dec., 1991.

36. Chemical Physics Seminar, University of Southern California, Dec., 1991.
37. Physical Chemistry Seminar, University of Pittsburgh, Feb., 1992.
38. Physical Chemistry Seminar, Pennsylvania State University, Feb., 1992.
39. Physical Chemistry Seminar, University of Pennsylvania, March, 1992.
40. Physical Chemistry Seminar, Princeton University, March, 1992.
41. Chemical Structure and Dynamics Seminar, Molecular Sciences Research Center, Battelle Pacific Northwest Laboratories, Richland Washington, March, 1992.
42. *Atmospheric Photochemistry: Laser Techniques and What They Can Tell Us*, Earth and Atmospheric Sciences Departmental Seminar, Purdue University, March, 1992.
43. National American Chemical Society Meeting, San Francisco, California, April, 1992. (Invited talk as part of the Symposium on Intermolecular Potentials, Sponsored by the Physical Chemistry Division).
44. Co-organizer (with Prof. C.S. Parmenter) of the Telluride Summer Research Workshop on *Large-Amplitude Motions and Intramolecular Dynamics*, Telluride, Colorado, July, 1992.
45. Telluride Summer Research Workshop on *Large-Amplitude Motions and Intramolecular Dynamics*, Telluride, Colorado, July, 1992.
46. Optical Society of America / International Laser Science Symposium on High Resolution Spectroscopy and Dynamics, Albuquerque, New Mexico, Sept. 1992.
47. Latsis Symposium 1992 on Intramolecular Kinetics and Reaction Dynamics, ETH Zürich, Switzerland, Oct. 1992.
48. Institut für Physikalische und Theoretische Chemie der Technischen Universität München, Munich, Germany, Oct. 1992.
49. Institut für Anorganische, Analytische und Physikalische Chemie, Universität Bern, Bern, Switzerland, Oct. 1992.
50. Physical Chemistry seminar, University of Illinois at Champaign-Urbana, Nov. 1992.
51. Physical Chemistry seminar, Emory University, Dec. 1992.
52. Physical Chemistry seminar, Northwestern University, Jan. 1993.
53. Chemistry Dept. seminar, University of South Dakota, Jan. 1993.
54. Chemistry Dept. seminar, South Dakota State University, Jan. 1993.
55. Fifth Australian Conference on Chemical Reaction Dynamics, University of New England, Armidale, New South Wales, Australia, Feb. 1993.
56. Physical Chemistry seminar, University of Sydney, Sydney, Australia, Feb. 1993.
57. Physical Chemistry seminar, Macquarie University, Sydney, Australia, Feb. 1993.
58. Chemistry Department Colloquium, University of Iowa, Iowa City, Iowa, Sept. 24, 1993.
59. Physical Chemistry Seminar, Ohio State University, March 7, 1994.
60. Physical Chemistry Seminar, University of Toronto, March 24, 1994.
61. Physical Chemistry Seminar, University of Waterloo, March 25, 1994.
62. Faraday Division of the Royal Society of Chemistry Discussion No. 97 on Structure and Dynamics of van der Waals' Complexes", University of Durham, England, April, 1994.
63. Gordon Conference on Multiphoton Processes, New Hampshire, June, 1994.
64. Gordon Conference on Molecular Electronic Spectroscopy, New Hampshire, Aug., 1994.
65. Chemistry Dept. Seminar, Colorado State University, Fort Collins, Colorado, Oct. 1994.
66. Chemistry Dept. colloquium, Texas Tech University, Lubbock, Texas, Jan. 1995.
67. Gordon Conference on Molecular Clusters, Oxnard, California, Jan. 1995.
68. Physical chemistry seminar, University of Pittsburgh, Pittsburgh, Pennsylvania, Jan. 1995.
69. JILA Chemical Physics Colloquium, Boulder, Colorado, Feb. 1995.

70. Symposium on Proton Transfer of the Physical Chemistry Division, Fall 1995 National ACS meeting, Chicago, Illinois, Aug., 1995.
71. Symposium on Multiresonance Spectroscopy, International Laser Society - Optical Society of America National Meeting, Portland, Oregon, Sept., 1995.
72. Chemistry department colloquium, Virginia Commonwealth University, Richmond, Virginia, Nov. 1995.
73. Physical chemistry seminar, Tokyo Institute of Technology, Tokyo, Japan, Jan. 1996.
74. Physical chemistry seminar, University of Tokyo Komaba Campus, Tokyo, Japan, Jan. 1996.
75. Physical chemistry seminar, Keio University, Tokyo, Japan, Jan. 1996.

76. 47th Okazaki Conference on the Dynamics of Hydrogen Atom Transfer Reactions, Institute for Molecular Science, Okazaki, Japan, Jan. 1996.
77. Physical chemistry seminar, Tohoku University, Sendai, Japan, Jan. 1996.
78. Gordon Conference on Atomic and Molecular Processes, Session chair and introductory talk in session on Molecular Ionic Clusters, New London, New Hampshire, June 1996.
79. Physical Chemistry Seminar, University of Arizona, Tucson, Arizona, Oct. 1996.
80. New York University Chemistry Department Colloquium, New York, New York, Nov. 1996.
81. March Meeting of the American Physical Society, Kansas City, Missouri, March, 1997. Invited talk in symposium on "Molecular Clusters: From the dimer to the Condensed Phase".
82. Wabash College Chemistry Department Colloquium, Crawfordsville, Indiana, March 1997.
83. April Meeting of the American Physical Society, Washington D.C., April, 1997. Organizer of session on Cavity ring-down spectroscopy.
84. NATO Advanced Study Institute entitled "Recent Theoretical and Experimental Advances in Hydrogen-bonded Clusters", Heraklion, Crete, June 1997. Invited instructor.
85. Co-organizer of symposium on *Dynamics of Molecular Systems*, Fall National Meeting of the American Chemical Society, Las Vegas, Sept. 1997.
86. University of North Carolina-Chapel Hill, Chemistry Dept. Colloquium, Chapel Hill, North Carolina, Nov. 1997.
87. Gordon Conference on Molecular and Ionic Clusters, Ventura, California, January, 1998.
88. Oxford University, Physical Chemistry seminar, Oxford, England, March 1998.
89. University College-London, Physical Chemistry seminar, London, England, March 1998.
90. Ecole Polytechnique Federale de Lausanne, Seminar at the Laboratoire de chimie physique moleculaire, March 1998.
91. Spring meeting of the New Swiss Chemical Society, Invited speaker in a symposium entitled "Hydrogen bonds: From Structure and Dynamics to Molecular Recognition", Bern, Switzerland, March 1998.
92. Satellite Research Seminar to the Spring meeting of the New Swiss Chemical Society entitled "Hydrogen Bonds: Recent Research", Beatenberg, Switzerland, March 1998.
93. 31st Great Lakes Regional ACS meeting, invited speaker in symposium entitled "Molecular Dynamics in Gas and Condensed Phases", Milwaukee, Wisconsin, June 1998.
94. Plenary lecturer for the 53rd Ohio State University International Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1998.
95. International Conference on Water in the Gas Phase, sponsored by the French Ministry of Research and Education, Paris, France, June 1998.
96. Gordon Research Conference on Atomic and Molecular Interactions, New London, New Hampshire, June 1998.
97. Indiana University Northwest Campus Chemistry Department Seminar, Gary, Indiana, Nov. 1998.
98. Calvin College Chemistry Department Seminar, Grand Rapids, Michigan, Nov. 1998.

99. Indiana University Southeast Campus Chemistry Department Seminar, New Albany, Indiana, Feb. 1999.
100. Vanderbilt University Chemistry Department Seminar, Nashville, Tennessee, March 1999.
101. Symposium entitled "Molecular Clusters", Centennial Meeting of the American Physical Society Meeting, Atlanta, Georgia, March 1999.
102. International Symposium on Molecular Clusters, Niederpöcking, Germany, May 1999.
103. 18th International Symposium on Molecular Beams, Ameland, The Netherlands, May 1999.
104. Department of Energy – Office of Basic Energy Sciences Combustion Research Meeting, Tahoe City, California, June 1999.

105. Fall 1999 National Meeting of the American Chemical Society, in the Symposium on Water and Water Clusters, New Orleans, August 1999.
106. Telluride Summer Research Conference on Reaction Dynamics in Small Clusters, Telluride, Colorado, August 1999.
107. Hatfield Memorial Lecture, Georgetown College, Georgetown, Kentucky, Nov. 1999.
108. Chemistry Dept. Seminar, Southern Illinois University, Carbondale, Illinois, Nov. 1999.
109. *Modern Research on Water: What we know and don't know about Nature's Solvent*, Chemistry Dept. seminar, Butler University, Nov. 1999.
110. Physical Chemistry seminar, University of Michigan, January 2000.
111. Physical and Analytical Chemistry seminar, University of Texas-Austin, Austin, Texas, February, 2000.
112. Chemistry Dept. seminar, Wright State University, Dayton, Ohio, March 2000.
113. Gordon Research Conference on Multiphoton Processes, New London, NH, June 2000.
114. Telluride Workshop on Water in Confined Geometries, Telluride, CO, August 2000.
115. Calvin College Chemistry Dept. Seminar, September 2000.
116. Joint Meeting of the International Laser Science and the Optical Society of America, Providence, RI, October 2000.
117. Physical Chemistry Seminar, Massachusetts Institute of Technology, Cambridge, MA, Nov. 2000.
118. Physical Chemistry Seminar, Yale University, New Haven, Conn., Nov. 2000.
119. Chemistry Dept. seminar, Lawrence University, Appleton, WI, Nov. 2000.
120. Invited talk in symposium entitled 'Large Molecule Vibrational Dynamics,' ACS Pacificchem meeting, Honolulu, Hawaii, Dec. 2000.
121. Invited talk in symposium entitled 'Structure, Dynamics, and Reactions of Small Clusters,' ACS Pacificchem meeting, Honolulu, Hawaii, Dec. 2000.
122. Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, Maryland, March 2001.
123. Chemistry Departmental Seminar, Kent State University, Kent, Ohio, April 2001.
124. Chemistry Dept. seminar, Oakland University, Oakland, MI, April 2001.
125. Faraday Discussion 118 on Cluster Dynamics, University of Durham, UK, April 2001.
126. Lectureship for the Troisième Cycle of the Swiss Universities (5 lectures at 5 Swiss universities).
127. International Symposium on "Isolated Molecules of Biological Interest", Schloss Mickeln, Dusseldorf, Germany, June 2001.
128. Fall National ACS meeting, Chicago, IL, August 2001.
129. Chemistry Department Seminar, Valparaiso University, Valparaiso, IN, Sept. 2001.
130. Chemistry Department Seminar, Columbia University, New York, NY, Sept. 2001.
131. Okazaki Center-of-Excellence Symposium entitled "Reactions in Aqueous Media", Okazaki, Japan, October 2001.
132. Chemistry Department Seminar, Washington University, St. Louis, MO, Nov. 2001.
133. Chemistry Department Seminar, Swarthmore College, Philadelphia, PA, Nov. 2001.

134. Chemistry Department Seminar, University of Akron, Akron, OH, Jan. 2002.
135. Chemistry Department Seminar, College of William and Mary, Williamsburg, VA, Feb. 2002.
136. Chemical Physics Seminar, California Institute of Technology, Pasadena, CA, March 2002.
137. Chemistry Department Seminar, Johns Hopkins University, Baltimore, MD, April, 2002.
138. Department of Energy - Office of Basic Energy Sciences Combustion Research Meeting, Warrenton, VA, May 2002.
139. Gordon Conference on Atomic and Molecular Interactions, Bristol, RI, July 2002.
140. EURESCO conference entitled, "Molecules of Biological Interest in the Gas Phase", Wilbad Kreuth, Germany, 21-26 July 2002.
141. Invited talk in symposium on Biologically Relevant Molecules in the Gas Phase, Fall 2002 National ACS meeting, Boston, Massachusetts, Aug. 2002.
142. Chemistry Department Seminar, The University of Chicago, Chicago, IL, Jan., 2003.
143. University of Oregon Physical/Analytical Seminar, Eugene, Oregon, Feb., 2003.
144. Physical/Analytical Seminar, Indiana University, Bloomington, IN, Feb., 2003.
145. Chemistry Department Seminar, Pennsylvania State University, College Station, PA, April, 2003.
146. Chemistry Department Seminar, Princeton University, Princeton, NJ, April 28, 2003.
147. Chemical Division Seminar, Argonne National Laboratories, Argonne, IL, May 4, 2003.
148. Workshop on Photoactive Biomolecules in the gas phase, in liquids, and in vivo, sponsored by the European Science Foundation, June 2003, Aarhus, Denmark.
149. Gordon Research Conference on Electronic Spectroscopy and Dynamics, Lewiston, Maine, July, 2003.
150. XIXth Conference on the Dynamics of Molecular Collisions, Lake Tahoe, CA, July 13-18, 2003.
151. Gordon Conference on 'Biological Molecules in the Gas Phase', New London, Connecticut, July, 2003.
152. Telluride workshop on Potential Energy Landscapes, Telluride, CO, July, 2003.
153. XVth International Conference on Horizons in Hydrogen Bond research, Sept., 2003, Freie Universität Berlin, Germany.
154. CEA Saclay, Paris France, Sept., 2003.
155. CNRS Orsay, Paris France, Sept., 2003.
156. Symposium on Chemical Physics, Waterloo, Ontario, Oct., 2003.
157. University Pais Vasco, Bilbao, Spain, November, 2003.
158. Department of Chemistry, University of Pennsylvania, Dec., 2003.
159. Gordon Research Conference on Vibrational Spectroscopy, July, 2004.
160. Chemistry Departmental Colloquium, University of Kentucky, Lexington, KY, Oct., 2004.
161. Department of Chemistry, University of Southern California, Nov., 2004.
162. Department of Chemistry, University of California-Santa Barbara, Nov., 2004.
163. Department of Chemistry, University of Kansas, Nov., 2004.
164. Workshop on Unimolecular Processes, Gottingen, Germany, Dec., 2004.
165. Institute for Theoretical Physics, Trieste, Italy, Dec., 2004.
166. Spectroscopy and Dynamics Group Annual Meeting, Leicester, UK, Dec., 2004.
167. Modern Optics and Spectroscopy Seminar, Massachusetts Institute of Technology, Cambridge, MA, March, 2005.
168. Physical Chemistry Seminar, University of California-Berkeley, Berkeley, CA, April, 2005.
169. Workshop on Flexibility in Biomolecules, Tempe, Arizona, May, 2005.
170. 26th Annual Combustion Research Conference, DOE Basic Energy Sciences contractor's meeting, May 2005.

171. Symposium on Molecular Clusters, Fall 2005 National ACS Meeting, Washington, DC, August 2005.
172. Chemistry Dept. Seminar, Calvin College, Sept. 2005.
173. Chemistry Dept. Seminar, Hope College, Sept. 2005.
174. Chemical Physics Colloquium, University of Colorado-Boulder, Nov. 2005.
175. Symposium on Frontiers in Structural and Functional Studies of Atomic and Molecular Clusters and Nanoparticles, Pacificchem 2005, Honolulu, Hawaii, Dec. 2005.
176. McElvain Lecture, Department of Chemistry, Univ. of Wisconsin-Madison, Jan. 2006.
177. Physical Chemistry seminar, Department of Chemistry, Univ. of Illinois-Urbana-Champaign, Feb. 2006.
178. Frontiers in Spectroscopy Lectures, Department of Chemistry, The Ohio State University, Feb. 2006.
179. Gordon Research Conference on Molecular and Ionic Clusters, Ventura, CA, Feb. 2006.
180. Symposium on the Spectroscopy of Biomolecules, March Meeting of the American Physical Society, Baltimore, MD, March, 2006.
181. Tulip 2006 Summer School of Modern Developments in Spectroscopy, April, 2006, Noordwijk, The Netherlands.
182. Gordon Conference on Multiphoton Processes, Tilton, NH, June, 2006.
183. 61st International Symposium on Molecular Spectroscopy, Symposium on *Spectral Signatures of Molecular Dynamics*, Columbus, Ohio, June 2006.
184. ESF Research Conference on “Biomolecules – From Gas Phase Properties to Reactions relevant to Living Cells”, Innsbruck, Austria, June 2006.

RESEARCH SUPPORT

Current funding

1. NSF CHE 0551075 Experimental Physical Chemistry

T. Zwiier (PI), Single investigator 04/01/2006 – 03/30/2009 **\$513K total**
Laser Probes of the Spectroscopy and Dynamics of Flexible Molecules and Complexes

2. DE-FG01-96ER14656 Department of Energy, Chemical Sciences, Office of Basic Energy Sciences

T. Zwiier (PI), Single investigator 06/15/04 – 06/14/07 **\$428K total**
Experimental Characterization of the Potential Energy Surfaces for Conformational Isomerization in Aromatic Fuels

3. NASA 05-PATM-73 NASA Planetary Atmospheres program

T. Zwiier (PI), Single investigator 03/01/06 – 02/28/09 **\$345K total**
Laboratory Studies of Photochemical and Discharge-driven Pathways to Complex Molecule Formation in Titan's atmosphere

4. NSF MRI (Multi-investigator, Co-I)

\$225K total (Purdue \$25K)

Acquisition of a Transportable Pulsed Laser System to Enhance Undergraduate Research Programs

I served as co-PI on this proposal, spearheaded by Prof. S. Drucker (UW-Eau Claire). The grant supported the acquisition of a mobile YAG-pumped dye laser and associated optics/electronics, to be shared by PI's at four Midwest PUI's, with Purdue's Laser facility serving as a central support facility.

Pending proposals

None

Past funding, since 1995 (~\$4.6 M total to Zwiier group since 1995, including current funding)

1. National Science Foundation

CHE 9404716 T. Zwiier (PI) 05/01/94 – 04/30/97 **\$357K total**

CHE 9728636 T. Zwiier (PI) 12/15/97 – 12/14/2000 **\$364K total**

2-year creativity extension T. Zwiier (PI) 12/15/2000-12/14/2002 **\$238K total**

DMR 9413889 T. Zwiier (PI) 09/01/94 – 08/31/95 **\$360K total**

Equipment grant for a picosecond SFG apparatus, multi-investigator shared instrumentation housed in the Chemistry Department Laser Facility.

CHE 0242818 T. Zwiier (PI) 12/01/02 – 05/30/06 **\$441K total**

2. NASA Planetary Atmospheres

NAGW-3019 T. Zwiier (PI) 03/01/95 – 02/28/97 **\$125K total**

NAG5-4819 T. Zwiier (PI) 06/01/97 – 05/31/99 **\$118K total**

NGT5-50130 T. Zwiier (PI) 07/01/97 – 06/30/2000 **\$66K total**

Graduate Student Research Fellowship for Christopher Ramos

NAG5-8155 BASIC T. Zwiier (PI) 06/01/99 – 05/31/2002 **\$324K total**

NAG5-12098 T. Zwiier (PI) 05/01/2002 – 04/30/2005 **\$304K total**

NGT5-50336 T. Zwiier (PI) 07/01/2001 – 06/30/2004 **\$66K total**

Graduate Student Research Fellowship for Jaime Stearns

3. Department of Energy, Basic Energy Sciences

DE-FG02-96ER14656 T. Zwiier (PI) 09/15/96 – 06/14/99 **\$315K total**

06/15/99 – 06/14/2002 **\$344K total**

06/15/02 – 06/14/04 **\$220K total**

4. Petroleum Research Fund, Type AC

35988-AC6 T. Zwiier (PI) 09/01/2000 – 08/31/02 **\$60K total**

INVOLVEMENT IN EDUCATIONAL PROGRAMS

CURRENT RESEARCH GROUP

Post-doctoral research associate

Dr. Ching-Ping Liu Began 2/1/2006, funded by Taiwan Fellowship

Graduate students

Jasper Clarkson 5th year graduate student, graduation August 2006.
 Talitha Selby 5th year graduate student, graduation August 2006.
 Esteban Baquero 4th year graduate student
 V. Alvin Shubert 4th year graduate student
 Nathan Pillsbury 3rd year graduate student
 Tracy LeGreve 3rd year graduate student
 William James 2nd year graduate student
 Joshua Newby 2nd year graduate student
 Chirantha Rodrigo 1st year graduate student

Undergraduates

Melissa Brink Sophomore
 Paul Carey Senior

FORMER GROUP MEMBERS

Graduate Students

Albert J. Gotch Ph.D. 1991
 Thesis: Probing solute/solvent interactions: A study of benzene-small molecule van der Waals' complexes.

Ralph E. Bandy Ph.D. 1992
 Thesis: The laser spectroscopy and dynamics of methylprmidines and diacetylene

Aaron W. Garrett Ph.D. 1993
 Thesis: Multiphoton ionization studies of π -hydrogen bonded molecular clusters containing benzene

Frederick A. Ensminger Ph.D. 1994
 Thesis: Laser-induced fluorescence spectroscopy of intramolecular hydrogen bonding in tropolone derivatives

R. Nathaniel Pribble Ph.D. 1996
 Thesis: Resonant ion-dip infrared spectroscopy of hydrogen-bonding molecular clusters containing benzene

Rex K. Frost Ph.D. 1996
 Thesis: Ultraviolet photochemistry of gas phase diacetylene and infrared spectroscopy of jet-cooled tropolone derivatives and their complexes with water

Frederick C. Hagemeister Ph.D. 1999
 Thesis: Experimental and theoretical studies of hydrogen-bonded systems : Tropolone and its water-containing clusters together with methanol and water clusters.

Christopher J. Gruenloh Ph.D. 1999
 Thesis: Shedding light on the nature of hydrogen-bonding in jet-cooled aromatic_m-(solvent)_n clusters using multiresonant laser spectroscopic methods

Allison G. Robinson Ph.D. 2001
 Thesis: Reactions of metastable diacetylene with aromatic molecules and the singlet-triplet spectroscopy of butadiene

Jason P. Overdorf M.S. 2001
 Thesis: Vibrational Sum-frequency Spectroscopy of short aliphatic dicarboxylic acids at the air-water interface

Joel R. Carney Ph.D. 2001
 Thesis: The infrared and ultraviolet spectroscopy of tryptophan analogs and their small water clusters : contributing to the understanding of tryptophan photophysics

Christopher Ramos Ph.D. 2002

Thesis: Photochemistry and photophysics of diacetylene and cyanoacetylene : Applications to the atmosphere of Titan.

Gina M. Florio Ph.D. 2002

Thesis: Probing the structure and dynamics of jet-cooled biomolecules: Laser spectroscopy of water bridges, hydrogen-bonded dimers, and conformationally flexible molecules

Brian C. Dian Ph.D. 2003

Thesis: The spectroscopy and dynamics of flexible biomolecules in the gas phase

Jaime A. Stearns Ph.D. 2005

Thesis: The Fate of Electronically Excited Molecules: Photochemical Reactivity and Excitonic Interaction

Post-doctoral research associates

Dr. Chitra Lakshminaryan 1992-3

Dr. Caleb Arrington 1996-8

Dr. Asier Longarte 2000-02

Dr. Aloke Das 2003-05

Undergraduates: ~1 per year in laboratory

TEACHING (2000-present)

Semester & Year	Course Number Credit Hour & Type	Title of Course	# of Students	Student Classification	Evaluation Scale: 0-5.0 Lowest-highest
Fall 2000	CHM 671 3 credits, lecture	Quantum Chemistry	6	Graduate	5.0 Course 5.0 Instructor
Spring 2001	CHM 376, 2 credits, laboratory	Physical Chemistry laboratory	63	Undergraduate	3.6 Course 3.5 Instructor
Fall 2001	CHM 671, 3 credits, lecture	Quantum Chemistry	14	Graduate	5.0 Course 5.0 Instructor
Spring 2002	CHM 376, 2 credits, laboratory	Physical Chemistry laboratory	71	Undergraduate	3.7 Course 3.6 Instructor
Fall 2002	CHM 671, 3 credits, lecture	Quantum Chemistry	14	Graduate	4.8 Course 4.9 Instructor
Spring 2003	CHM 376, 2 credits, laboratory	Physical Chemistry laboratory	73	Undergraduate	3.7 Course 3.9 Instructor
Fall 2003	Research Leave (Assoc. Head / JPC editor course reduction)				
Spring 2004	CHM 696A, 3 credits, lecture	Molecular Spectroscopy	10	Graduate	4.9 Course 4.9 Instructor
Fall 2004 - present	No teaching as department head				

UNIVERSITY SERVICE (recent)

Chemistry Department Head, Fall 2004 - present

Associate Department Head, 2001-2003

Chemistry Department Strategic Planning Committee, Chair, 2002-03

Chair, Graduate Recruiting and Admissions (as part of associate head duties), 2001-03

College of Science Strategic Planning Committee, 2002

Search Committee, Director of the Birck Nanotechnology Center

University Laser Safety Committee, 2000-2004