

RONALD SAMUEL FRIEDMAN

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Indiana University Purdue University Fort Wayne
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EDUCATION

- 1989 PhD in Chemistry - Harvard University
Thesis : Coupled Equation Description of Molecular Perturbations
(Supervisor : Professor Alexander Dalgarno)
- 1986 A.M. in Chemistry - Harvard University
- 1984 B.S. in Chemistry with highest distinction - University of Virginia

EXPERIENCE

- 2004 - present: PROFESSOR and CHAIR of Chemistry at Indiana University Purdue University Fort Wayne.
- 1997 - 2004: ASSOCIATE PROFESSOR of Chemistry at Indiana University Purdue University Fort Wayne.
- 1999: VISITING ASSOCIATE PROFESSOR of Chemistry at the Technion - Israel Institute of Technology, sabbatical January - June, working in collaboration with Prof. Nimrod Moiseyev on chemical reaction dynamics and scattering theory using the complex coordinate method.
- 1997: VISITING ASSOCIATE PROFESSOR of Chemistry at the University of Michigan teaching Physical Chemistry II (Chemistry 461) May-June.
- 1996: VISITING ASSISTANT PROFESSOR of Chemistry at the University of Michigan teaching Physical Chemistry II (Chemistry 469) May-June.
- 1993 - 1998: FACULTY ADVISOR to the Student Affiliates of the American Chemical Society IPFW Chapter.
- 1991 - 1997: ASSISTANT PROFESSOR of Chemistry at Indiana University Purdue University Fort Wayne.
- 1989 - 1991: POSTDOCTORAL RESEARCH ASSOCIATE with Donald G. Truhlar at the University of Minnesota studying quantum mechanical reaction dynamics on a Cray-2 Supercomputer.

1984 - 1989: RESEARCH ASSISTANT with Alexander Dalgarno at the Harvard-Smithsonian Center for Astrophysics analyzing molecular perturbations using scattering theory.

1984 - 1985: TEACHING ASSISTANT at Harvard University responsible for recitation sections and laboratory instruction in General Chemistry.

1981 - 1984: UNDERGRADUATE RESEARCH STUDENT with Lester Andrews at the University of Virginia performing experiments in matrix-isolation spectroscopy of organic cations.

HONORS

2003 Inclusion in 2003 edition of *United Who's Who Executive and Professional Registry, 2003*

2002 Inclusion in seventh edition of *Who's Who Among America's Teachers, 2002*

1995 Sigma Xi Chapter of Fort Wayne Researcher of the Year

1990 Minnesota Supercomputer Institute Research Scholar

1985 Award for Outstanding Teaching as a Teaching Fellow

1985 Monsanto Fellow, Harvard University

1984 Gregory Paul Baxter Scholarship Prize, Harvard University

1984 Hugh Miller Spencer Scholarship Prize in Chemistry, University of Virginia

1983 Phi Beta Kappa

1983 MIT Material Processing Center Summer Scholarship

1981 Echols Scholar, University of Virginia

1981 CRC Press Freshman Chemistry Achievement Award

RESEARCH/TRAVEL GRANTS

2004 Awarded American Chemical Society Petroleum Research Fund Type B grant;
1/1/04 - 8/31/07

2002 Awarded Purdue Research Foundation International Travel Grant

2001 Awarded American Chemical Society Petroleum Research Fund Type B grant;
1/1/01 - 8/31/03; extended to 8/31/04

2001 Awarded IPFW Summer Grant for Research

2000 Awarded IPFW International Conference Fund Grant

2000 Awarded Purdue Research Foundation International Travel Grant

1997 Awarded American Chemical Society Petroleum Research Fund Type B grant;
9/1/97 - 8/31/99; extended to 8/31/01

1997 Awarded and accepted Purdue Research Foundation (PRF) Summer Faculty Grant

1997 Awarded IPFW Summer Grant for Research (declined in lieu of PRF grant)

1993 Awarded American Chemical Society Petroleum Research Fund Type GB grant;
9/1/93 - 8/31/95; extended to 8/31/96

1993 Awarded IPFW Summer Grant for Research

1992 Awarded and accepted Purdue Research Foundation (PRF) Summer Faculty Grant

1992 Awarded IPFW Summer Grant for Research (declined in lieu of PRF grant)

SOCIETY MEMBERSHIPS

American Chemical Society, American Physical Society, Phi Beta Kappa.

DEPARTMENTAL AND SPECIALTY SEMINARS

Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, March, 1988. "Effects of Shallow Attractive Wells at Large Internuclear Distances in Diatomic Potential Energy Curves."

Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, June, 1988. "Level Shifts in the B³_u State of Molecular Oxygen" and "Band Oscillator Strengths of the Schumann-Runge Absorption Bands of Molecular Oxygen."

Harvard-Smithsonian Center for Astrophysics, March, 1989. "Solving Scattering Problems using Molecular Potentials Inferred from Spectroscopic Data."

University of Minnesota, Chemistry Department, September 1989. "Multichannel Eigenvalue Problems."

University of Minnesota, Chemistry Department, January, 1991. "Global Control of Suprathreshold Reactivity by Quantized Transition States."

Indiana University Purdue University Fort Wayne, Chemistry Department Seminar, April, 1993. "Can Classical Transition States Be Described Quantum Mechanically?"

Indiana University Purdue University Fort Wayne, Sigma Xi Brown bag talk, February 1996. "Searching for the Holy Grail of Chemical Reactions."

Indiana University Purdue University Fort Wayne, Chemistry Department Seminar, December, 1996. "The Effects of Coupled Potential Energy Barriers on Chemical Reactivity: Model Studies."

Indiana University Purdue University Fort Wayne, Chemistry Department Seminar, November, 1999. "Quantum Mechanics, Israeli Style: Everything's Complex!"

University of Colorado at Denver, Chemistry Department Seminar, December, 2001. "Resonances of Conically-Intersecting Electronic States"

Indiana University Purdue University Fort Wayne, Chemistry Department Seminar, February, 2002. "Resonances of Conically-Intersecting Electronic States"

Elizabethtown College, Elizabethtown, PA, Chemistry Department Seminar, March, 2002. "Resonances arising from Conically Intersecting Electronic States"

Rhodes College, Memphis, TN, Chemistry Department Seminar, February, 2003. "Resonances and Bound States arising from Conical Intersections"

CONFERENCE PRESENTATIONS

“The Magnetic Dipole Photodissociation of Molecular Oxygen” by *R.S. Friedman* and A. Dalgarno, **Atomic, Molecular and Optical Physics Division Meeting**, Cambridge, MA, May 1987.(Poster presentation.)

“Level Shifts in the $B^3 \Sigma^-$ State of Molecular Oxygen” by *R.S. Friedman* and A. Dalgarno, **Atomic, Molecular and Optical Physics Division Meeting**, Baltimore, MD, April 1988.(Poster presentation.)

“Quantal Calculations of O^+ -O Scattering” by A. Dalgarno and *R.S. Friedman*, **American Geophysical Union Spring Meeting**, Baltimore, MD, May 1988.(Invited Oral presentation.)

“Level Shifts in the $B^3 \Sigma^-$ State of Molecular Oxygen” by *R.S. Friedman* and A. Dalgarno; and “Band Oscillator Strengths of the Schumann-Runge Absorption Bands of Molecular Oxygen” by *R.S. Friedman*, **Symposium on Molecular Spectroscopy**, Ohio State University, Columbus, Ohio, June 1988.(Oral presentations.)

“Inelastic Scattering of Low Energy Oxygen Atoms” by *R.S. Friedman* and A. Dalgarno, **Sixteenth International Conference on the Physics of Electronic and Atomic Collisions**, New York, NY, July 1989.(Poster presentation.)

“Quantal Dynamics Calculations of Scattering of Excited Sodium Atoms by Molecular Hydrogen” by *R.S. Friedman*, P. Halvick, D.C. Chatfield, D.G. Truhlar and D.W. Schwenke; and “Global Control of Suprathreshold Reactivity by Quantized Transition States” by D.C. Chatfield, *R.S. Friedman*, D.G. Truhlar, B.C. Garrett and D.W. Schwenke, **XXIII Midwest Theoretical Chemistry Conference**, University of Wisconsin, Madison, WI, May 1990.(Poster presentations.)

“Global Control of Suprathreshold Reactivity by Quantized Transition States” by D.C. Chatfield, *R.S. Friedman*, D.G. Truhlar, B.C. Garrett and D.W. Schwenke, **1990 Gordon Research Conference on Atomic and Molecular Interactions**, Salve Regina College, Newport, RI, July 1990.(Poster presentation.)

“Global Control of Suprathreshold Reactivity by Quantized Transition State” by D.C. Chatfield, *R.S. Friedman*, D.G. Truhlar, B.C. Garrett and D.W. Schwenke, **Symposium on Polymer Theory/Pragerfest**, University of Minnesota, October 1990. (Poster presentation.)

“Characterization of Reactive Transition States in the Reaction $O + H_2 \rightarrow OH + H$ ” by *D.C. Chatfield*, *R.S. Friedman*, D.G. Truhlar, G.C. Lynch and D.W. Schwenke, **Faraday Discussion 91: Structure and Dynamics of Reactive Transition States**, University of Nottingham, Nottingham, England, March 1991.

“Quantum Dynamics of $Na(3p^2P) + H_2$ collisions” by G.J. Tawa, S.L. Mielke, *R.S. Friedman*, P. Halvick, *D.G. Truhlar* and D.W. Schwenke, **203rd ACS National Meeting**, San Francisco, CA,

April 1992.

“Chemical Reaction Thresholds are Scattering Resonances” by *R.S. Friedman* and D.G. Truhlar, **1993 Conference on the Dynamics of Molecular Collisions**, Helen, Georgia, June 1993. (Poster presentation.)

“Problems involving nonideal resonances: Quantal scattering by one-dimensional potentials” by *R.S. Friedman*, **Institute for Mathematics and its Applications (IMA) Workshop on Multiparticle Quantum Scattering with Applications to Nuclear, Atomic and Molecular Physics**, University of Minnesota, Minneapolis, MN, June 1995. (Invited Oral presentation.)

“The Role of Resonances in Chemical Reactivity: Quantal Studies of Model 1-D Coupled Potentials” by *R.S. Friedman*, V.D. Hullinger, and D.J. Kaufman, **38th American Chemical Society Central Regional Meeting**, Dayton, OH, June, 1996.(Oral presentation.)

“Nonadiabatic Effects on Chemical Reactivity: One-Dimensional Quantum Mechanical Model Studies” by *R.S. Friedman*, V.D. Hullinger, D.J. Kaufman, and P.M. Small, **31st Midwest Theoretical Chemistry Conference**, Purdue University, West Lafayette, IN, May, 1998. (Oral presentation.)

“Funnel Resonances in Chemical Reaction Dynamics: The Nonadiabatic Tunneling Case Associated with an Avoided Crossing at a Saddle Point” by *R. S. Friedman*, **Winter-school and Workshop on Resonance Phenomena in Chemical Physics**, Technion - Israel Institute of Technology, Haifa, Israel, February 1999. (Poster presentation.)

“Resonance States in Nonadiabatic Systems:Reduced-Dimensionality Quantal Studies Using the Complex Coordinate Method” by *R.S. Friedman*, V.M. Ryaboy and N. Moiseyev, **2000 Gordon Research Conference on Atomic and Molecular Interactions**, Colby-Sawyer College, New London, NH, July 2000.(Poster presentation.)

“Resonance States in Nonadiabatic Systems: Reduced-Dimensionality Quantal Studies Using the Complex Coordinate Method” by *R.S. Friedman*, V.M. Ryaboy and N. Moiseyev, **MOLEC 2000: 13-th European Conference on Dynamics of Molecular Collisions**, Kibbutz Ramat Rachel, Jerusalem, Israel, September 2000.(Poster presentation.)

“Resonances of Conically Intersecting Electronic States: A Quantal Study Using the Complex Coordinate Method” by *R.S. Friedman*, L.S. Cederbaum, V.M. Ryaboy and N. Moiseyev, **2001 Conference on the Dynamics of Molecular Collisions**, Copper Mountain, CO, July 2001.(Poster presentation.)

“Resonances of Conically Intersecting Electronic States: A Quantal Study Using the Complex Coordinate Method” by *R.S. Friedman*, I. Podzielinski, L.S. Cederbaum, V.M. Ryaboy and N. Moiseyev, **34th Midwest Theoretical Chemistry Conference**, University of Minnesota, Minneapolis, MN, October 2001.(Poster presentation.)

“Vibronic Resonances Arising from Conically Intersecting Electronic States” by *R.S. Friedman*, I. Podzielinski, L.S. Cederbaum, V.M. Ryaboy and N. Moiseyev, **4th Congress of the International Society for Theoretical Chemical Physics**, INJEP, Marly-le-Roi, France, July 2002. (Poster presentation.)

“Bound Molecular States Embedded in the Continuum and Arising from Conical Intersections” by *R.S. Friedman*, L.S. Cederbaum, V.M. Ryaboy, and N. Moiseyev, **XIXth Conference on the Dynamics of Molecular Collisions**, Lake Tahoe, CA, July 2003.(Poster presentation.)

“Resonances and bound states arising from conical intersections” by *R. S. Friedman*, D. Villavicencio, S. A. Langmeyer, , L. S. Cederbaum, V. M. Ryaboy and N. Moiseyev, **Gordon Research Conference on Atomic and Molecular Interactions**, Colby-Sawyer College, New London, NH, July 2004. (Poster Presentation)

PUBLICATIONS: Journal Articles and Book Chapters

Vibronic Absorption Spectra of Dichloro- and Dibromobenzene Cations in Solid Argon at 20 K, R.S. Friedman, B.J. Kelsall, and L. Andrews, *J. Phys. Chem.* **88**, 1944, 1984.

Photochemical Rearrangements of o- and m-Dichlorobenzene Cations to p-Dichlorobenzene Cation in Solid Argon, R.S. Friedman and L. Andrews, *J. Am. Chem. Soc.* **107**, 822, 1985.

Vibronic Absorption Spectra of Condensed Ring Aromatic Cation Systems in Solid Argon, L. Andrews, R.S. Friedman, and B.J. Kelsall, *J. Phys. Chem.* **89**, 4016, 1985.

Vibronic Absorption Spectra of Dimethylnaphthalene Cations in Solid Argon, L. Andrews, R.S. Friedman, and B.J. Kelsall, *J. Phys. Chem.* **89**, 4550, 1985.

The CH²⁺ Cation, R. Friedman, S. Preston, and A. Dalgarno, *Chem. Phys. Lett.* **141**, 469, 1987.

High Resolution Absorption Cross-Sections and Band Oscillator Strengths of the Schumann-Runge Absorption Bands of Isotopic Oxygen, ¹⁸O₂, at 79 K, K. Yoshino, D.E. Freeman, J.R. Esmond, R.S. Friedman, and W.H. Parkinson, *Planet. Space Sci.* **36**, 1201, 1988.

The Magnetic Dipole Photodissociation Cross Section of Molecular Oxygen, R. Friedman and A. Dalgarno, *J. Quant. Spectrosc. Radiat. Transfer* **42**, 137, 1989.

The Schumann-Runge Absorption Bands of ¹⁶O¹⁸O in the Wavelength Region 175-205 nm and Spectroscopic Constants of Isotopic Oxygen Molecules, A.S.-C. Cheung, K. Yoshino, D.E. Freeman, R.S. Friedman, A. Dalgarno, and W.H. Parkinson, *J. Mol. Spectrosc.* **134**, 362, 1989.

High Resolution Absorption Cross-Sections and Band Oscillator Strengths of the Schumann-Runge Absorption Bands of Isotopic Oxygen, ¹⁶O¹⁸O, at 79 K, K. Yoshino, D.E. Freeman, J.R. Esmond, R.S. Friedman, and W.H. Parkinson, *Planet. Space Sci.* **37**, 419, 1989 .

Model Potentials for Multichannel Eigenvalue Problems, R.S. Friedman and M.J. Jamieson, *Computer Phys. Comm.* **55**, 137, 1989.

Comment on "Predissociation of the d^1_g Rydberg State in O_2 : Nature of the Rydberg-Valence Interactions," R.S. Friedman and A. Dalgarno, *J. Chem. Phys.* **90**, 7606, 1989.

Oscillator Strengths of the Schumann-Runge Bands of Isotopic Oxygen Molecules, R.S. Friedman, *J. Quant. Spectrosc. Radiat. Transfer* **43**, 225, 1990.

On the Numerical Solution of Coupled Eigenvalue Differential Equations Arising in Molecular Spectroscopy, R.S. Friedman, M.J. Jamieson, and S.C. Preston, *Computer Phys. Comm.* **58**, 17, 1990.

The C^3_g Rydberg and 1^3_g Valence States of O_2 , R.S. Friedman and A. Dalgarno, *J. Chem. Phys.* **93**, 2370, 1990.

Predissociation channels of the C^3_g Rydberg state of O_2 , R.S. Friedman, M.L. Du, and A. Dalgarno, *J. Chem. Phys.* **93**, 2375, 1990.

A Note on Solving Coupled Second-Order Linear Differential Equations, R.S. Friedman and M.J. Jamieson, *Computer Phys. Comm.* **62**, 53, 1991.

Global Control of Suprathreshold Reactivity by Quantized Transition States, D.C. Chatfield, R.S. Friedman, D.G. Truhlar, B.C. Garrett, and D.W. Schwenke, *J. Am. Chem. Soc.* **113**, 486, 1991.

Rotational Dependence of the Rydberg-Valence Interactions in the 1_g States of Molecular Oxygen, A. Sur, R.S. Friedman, and P.J. Miller, *J. Chem. Phys.* **94**, 1705, 1991.

Quantum-dynamical Characterization of Reactive Transition States, D.C. Chatfield, R.S. Friedman, D.G. Truhlar, and D.W. Schwenke, *Faraday Discuss. Chem. Soc.* **91**, 289, 1991.

Remarks on the Photodetachment Spectra of $ClHCl^+$, IHI^+ , and IDI^+ , D.C. Chatfield, R.S. Friedman, G.C. Lynch, and D.G. Truhlar, *Faraday Discuss. Chem. Soc.* **91**, 398, 1991.

Chemical Reaction Thresholds are Resonances, R.S. Friedman and D.G. Truhlar, *Chem. Phys. Lett.* **183**, 539, 1991.

Quantized Transition-State Structure in the Cumulative Reaction Probabilities for the $Cl + HCl$, $I + HI$, and $I + DI$ reactions, D. C. Chatfield, R.S. Friedman, G.C. Lynch, and D.G. Truhlar, *J. Phys. Chem.* **96**, 57, 1992.

Control of Chemical Reactivity by Quantized Transition States, D.C. Chatfield, R.S. Friedman, D.W. Schwenke, and D.G. Truhlar, *J. Phys. Chem.* **96**, 2414, 1992.

Error Estimation in Molecular Vibrational Eigenenergies calculated by the Hartree and Numerov

Methods, M.J. Jamieson and R.S. Friedman, *Computer Phys. Comm.* **70**, 53, 1992.

High-Energy State-to-State Quantum Dynamics for $D+H_2 (v=j=1) \rightarrow HD (v'=1, j') + H$, S.L. Mielke, R.S. Friedman, D.G. Truhlar, and D.W. Schwenke, *Chem. Phys. Lett.* **188**, 359, 1992.

Collisional excitation of metastable oxygen $O(^1D)$ atoms through the $B^3 \Sigma_u^-$ channel of O_2 , M.J. Jamieson, M. Finch, R.S. Friedman, and A. Dalgarno, *Planet. Space Sci.* **40**, 1719, 1992.

The Nature and Role of Quantized Transition States in the Accurate Quantum Dynamics of the Reaction $O+H_2 \rightarrow OH+H$, D.C. Chatfield, R.S. Friedman, G.C. Lynch, D.G. Truhlar, D.W. Schwenke, *J. Chem. Phys.* **98**, 342, 1993.

Converged Quantum Mechanical Calculations of Electronic-to-Vibrational, Rotational Energy Transfer Probabilities in a System with a Conical Intersection, D.W. Schwenke, S.L. Mielke, G.J. Tawa, R.S. Friedman, P. Halvick, D.G. Truhlar, *Chem. Phys. Lett.* **203**, 565, 1993.

On Johnson's Log-Derivative Algorithm for a Single Equation, R.S. Friedman and M.J. Jamieson, *Computer Phys. Comm.* **85**, 231, 1995.

Scattering by a Pair of Potential Energy Barriers: Tests of Numerical Software, R.S. Friedman and M.J. Jamieson, *Computer Phys. Comm.* **85**, 382, 1995.

Quantum Mechanical Threshold Resonances for Unsymmetric Potential Energy Barriers, R.S. Friedman, V.D. Hullinger, and D.G. Truhlar, *J. Phys. Chem.* **99**, 3184, 1995.

Large-Scale Calculations of the Quantum Dynamics of Molecular Collisions and Reactions, D.G. Truhlar, D.W. Schwenke, S.L. Mielke, M.S. Reeves, R.W. Numrich, D.M. Briesemeister, D.C. Chatfield, R.S. Friedman, M. Kalke, G.J. Tawa, and M.J. Unekis, *Conference Proceedings of Toward Teraflop Computing and New Grand Challenge Applications*, Louisiana State University, February 10-12, 1994; published by Nova Science Publishers, Inc., New York, 1995.

Computational Spectroscopy of the Transition State, D.C. Chatfield, R.S. Friedman, S.L. Mielke, G.C. Lynch, T.C. Allison, D.G. Truhlar, and D.W. Schwenke, *Dynamics of Molecules and Chemical Reactions*, Ed. R.E. Wyatt and J.Z.H. Zhang, Marcel Dekker, New York, 323-386, 1996.

Barrier Resonances and Chemical Reactivity, R.S. Friedman and D.G. Truhlar, *Program Proceedings of the Institute of Mathematics and its Applications (IMA) Workshop "Multiparticle Quantum Scattering with Applications to Nuclear, Atomic and Molecular Physics"*, Ed. D.G. Truhlar and B. Simon, Springer-Verlag, 243-281, 1997.

Exciplex Funnel Resonances in Chemical Reaction Dynamics, R.S. Friedman, T.C. Allison, and D.G. Truhlar, *Physical Chemistry Chemical Physics* **1**, 1237, 1999.

Error Estimation in Molecular Vibrational Energies Calculated by Johnson's Log-Derivative

Method, M.J. Jamieson and R.S. Friedman, *Computer Phys. Comm.* **118**, 145, 1999.

Scattering Matrix Determination by Asymptotic Analysis of Complex Scaled Resonance Wavefunctions: Model Cl + H₂ Nonadiabatic Dynamics, R.S. Friedman, V.M. Ryaboy, and N. Moiseyev, *J. Chem. Phys.* **111**, 7187, 1999.

Analysis of the Resonance in H + D₂ HD(v'=3) + D, T.C. Allison, R.S. Friedman, D.J. Kaufman, and D.G. Truhlar, *Chem. Phys. Lett.*, **327**, 439, 2000.

Vibronic Resonances Arising from Conically Intersecting Electronic States, R.S. Friedman, I. Podzielinski, L.S. Cederbaum, V.M. Ryaboy and N. Moiseyev, *J. Phys. Chem. A*, **106**, 4320, 2002.

Conical Intersections and Bound Molecular States Embedded in the Continuum, L.S. Cederbaum, R.S. Friedman, V.M. Ryaboy and N. Moiseyev, *Phys. Rev. Lett.* **90**, 013001, 2003.

PUBLICATIONS: Textbooks

Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, Oxford University Press, Oxford/New York, 3rd ed., 1997.

Solutions Manual for Molecular Quantum Mechanics Third Edition, P.W. Atkins and R.S. Friedman, Oxford University Press, Oxford/New York, 3rd ed., 1997.

Meccanica Quantistica Molecolare, P.W. Atkins and R.S. Friedman, Zanichelli, Bologna, 1st (Italian) ed., 2000.