Bryan C. Hathorn

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EDUCATION

California Institute of Technology, Pasadena, California
Ph.D. in Theoretical Chemistry — June 1999
Thesis advisor: Dr. R. A. Marcus

Haverford College, Haverford, Pennsylvania
B.A., Chemistry and Mathematics — May 1991

Maine–Endwell Senior High School, Endwell, New York
Graduated with Merit and Honors — June 1987

HONORS and AWARDS

Journal of Physical Chemistry.
Article and artwork featured on cover.
B.C. Hathorn *et al.*, *J. Phys. Chem.*, October 10, 2002.

Materials Science Corner of ScienceDirect
Paper selected as an outstanding contribution:
B.C. Hathorn *et al. Polymer*, **43**, 3115 (2002).

Oak Ridge National Laboratory
Seed Money Grant
Community Service Award, 2001

California Institute of Technology
James Glanville Postdoctoral Fellowship

Haverford College
Magna Cum Laude
High Honors in Chemistry
Honors in Mathematics
Phi Beta Kappa
George Peirce Prize in Chemistry
Freshman Prize in Mathematics

EXPERIENCE

Adjunct Professor: 2002-present
Maryville College, Maryville, TN

Consultant: 2002-present
HemoSaga Diagnostics Corporation, San Diego, CA

Postdoctoral Scholar in Computer Science and Mathematics: 2000-present
with Drs. D.W. Noid and B.G. Sumpter at the Oak Ridge National Laboratory, Oak Ridge, Tennessee. Application of statistical theories to large molecular systems. Molecular Dynamics simulations of large scale polymer systems. Normal mode calculations in large systems. Applications of semiclassical methods in quantum mechanics.

Postdoctoral Scholar in Chemistry: 1999-2000
with Dr. R.A. Marcus at the California Institute of Technology, Pasadena, California. Elaboration of simple models which describe mass-independent isotopic enrichments in ozone.

Graduate Research Assistant: 1991-1999
with Dr. R. A. Marcus at the California Institute of Technology, Pasadena, California. Investigation of the rates of ozone formation using statistical reaction rate theories, and the extension to the non-mass dependent isotopic enhancement of heavy isotopes of oxygen in ozone.

Undergraduate Research:
with Dr. J.P. Chesick at Haverford College, Haverford, Pennsylvania. 1990-1991
Synthesis and characterization of transition metal complexes with encapsulating ligands.

with Dr. W. Epstein at the University of Utah, Salt Lake City, Utah. 1990
Synthesis of naturally occurring terpene compounds and their precursors.

TEACHING EXPERIENCE

Maryville College 2002-present

Physical Chemistry I. (Adjunct Professor)
Advanced course in physical, chemical and dynamical properties of chemical systems. Central themes include chemical/statistical thermodynamics and kinetics.

Physical Chemistry II. (Adjunct Professor)
Advanced course in physical and molecular properties of chemical systems. Topics include quantum theory, spectroscopy, and symmetry analysis.

California Institute of Technology 1991-1999

General Chemistry. (Head Grader)
Introductory course in the undergraduate chemistry sequence.

The Physical Description of Chemical Systems. (Teaching Assistant)
Junior level physical chemistry course. Covered basics of physical chemistry, quantum mechanics, statistical mechanics and kinetic theory.

The Elements of Quantum Chemistry. (Teaching Assistant)
Graduate level course in quantum mechanics, including operator theory, time dependent and time independent perturbation theory, spectroscopy and group theory.

Chemical Dynamics. (Teaching Assistant)
Graduate level course treating molecular interactions and reactions. Subtends a wide variety of modern chemical research from kinetic theory to molecular collision theory.

Introduction to Statistical Thermodynamics. (Teaching Assistant)
Graduate level course in statistical mechanics. Includes relationships between quantum energy levels and thermodynamic functions, and applications to various systems.

Electron Transfer Reactions in Chemistry and Biology. (Teaching Assistant)
Graduate level topics course in the theory and applications of Marcus' theory of electron transfer.

Haverford College 1987-1991

Physical Chemistry Laboratory. (Teaching Assistant)
Elementary physical chemistry laboratory. Experimental techniques include examples such as electrochemistry, kinetics and calorimetry.

Advanced Organic Chemistry Laboratory. (Teaching Assistant)
Advanced organic chemistry laboratory. Students performed synthesis and purification of organic compounds, and performed elementary spectroscopic techniques.

Introductory Organic Chemistry Laboratory. (Teaching Assistant)
First course in organic laboratory techniques for undergraduates. Covers synthesis and purification of organic compounds.

Introductory Calculus. (Teaching Assistant)
First course in the undergraduate mathematics sequence. Covers differentiation, integration and applications.

Linear Algebra. (Teaching Assistant)
Sophomore level course introducing matrices and linear algebra techniques.

SELECTED PUBLICATIONS AND PRESENTATIONS

B.C. Hathorn and R.A. Marcus, An intramolecular theory of the mass-independent isotope effect for ozone. I. *Journal of Chemical Physics*, **111**, 4087 (1999).

Conference Internationale Sur Les Isotopes Stables et Les Effets Isotopiques, Carry le Rouet, France. *An Intramolecular Theory of the Mass-Independent Isotope Effect for Ozone.*

B.C. Hathorn and R.A. Marcus, An intramolecular theory of the mass-independent isotope effect for ozone. II. Numerical applications at low pressures using a loose transition state, *Journal of Chemical Physics*, **113**, 9497 (2000).

B.C. Hathorn and R.A. Marcus Estimation of vibrational frequencies and vibrational densities of states in isotopically substituted nonlinear triatomic molecules, *Journal of Physical Chemistry A*, **105**, 5586 (2001).

B.C. Hathorn, B.G. Sumpter, and D.W. Noid, Comparison of transition state theory rate constants for internal conformational motion with those obtained from Molecular Dynamics simulations. *Polymer*, **43**, 615 (2002).

B.C. Hathorn, B.G. Sumpter, and D.W. Noid, On the distribution of fragment sizes in the thermal decomposition of polymers, *Macromolecular Theory and Simulations,* **10**, 581 (2001).

B.C. Hathorn, B.G. Sumpter, and D.W. Noid, On the contribution of restricted rotors to quantum sieving of hydrogen isotopes, *Phys. Rev. A.*, **64**, 022903 (2001).

B.C. Hathorn, B.G. Sumpter, and D.W. Noid, Theory of Unimolecular Reactions in Confined Volumes. *accepted, Computer Modelling in Engineering & Sciences.*

B.C. Hathorn, B.G. Sumpter, M.D. Barnes and D.W. Noid, Molecular Dynamics simulation of collinear nanoparticle collisions: reaction and scattering. *J. Phys. Chem. B*, **105**, 11468 (2001).

B.C. Hathorn, B.G. Sumpter, M.D. Barnes and D.W. Noid, Molecular Dynamics simulation of nanoparticle collisions: internal reorganization and translation-vibration coupling *Macromolecules*, **35**, 1102 (2002).

B.C. Hathorn, B.G. Sumpter, M.D. Barnes and D.W. Noid Molecular Dynamics simulation of nanoparticle collisions: orbital angular momentum effects, *Polymer*, **43**, 3115 (2002).

B.C. Hathorn, B.G. Sumpter, D.W. Noid, R.E. Tuzun, and C. Yang, Vibrational normal modes of polymer nanoparticle dimers using the time averaged normal coordinate analysis method, *in press. Journal of Physical Chemistry.*

S.M. Mahurin, A. Mehta, B.C. Hathorn, B.G. Sumpter, D.W. Noid, K. Runge, and M.D. Barnes, Photonic "polymers": A new class of photonic wire structure from intersecting polymer-blend microspheres. *Optics Letters*, **27**, 610 (2002).

B.C. Hathorn, B.G. Sumpter, and D.W. Noid, Simulation of soft nanoparticles with hard surfaces, Conference Proceedings, 6th World Multiconference on Systemics, Cybernetics and Informatics, 2002.

B.C. Hathorn, B.G. Sumpter, D.W. Noid and M.D. Barnes, Vibrational normal modes of polymer nanoparticle systems using the time averaged normal coordinate analysis method, Conference Proceedings, 6th World Multiconference on Systemics, Cybernetics and Informatics, 2002.

B.C. Hathorn, B.G. Sumpter, D.W. Noid, R.E. Tuzun, and C. Yang, Computational Simulation of Polymer Particle Structures: Vibrational Normal Modes Using the Time Averaged Normal Coordinate Analysis Method, *in press*, *Polymer*.

M.D. Barnes, K. Runge, B.C. Hathorn, S. Mahurin, B.G. Sumpter, and D.W. Noid, Manipulation with molecules, *Materials Today*, September 2002, p. 20.

B.C. Hathorn, B.G. Sumpter, D.W. Noid, R.E. Tuzun, and C. Yang, Surface contact force constants of polymer nanoparticle dimers, *in preparation*

B.C. Hathorn, B.G. Sumpter, D.W. Noid, M.D. Barnes, R.E. Tuzun, and C. Yang, Multibody vibrations in large scale polymer particle superstructures, *in preparation.*

R.E. Tuzun, B.C. Hathorn, B.G. Sumpter, D.W. Noid, Facile conversion of internal to cartesian coordinates in polymer chains, *in preparation*

B.C. Hathorn and R.A. Marcus, An intramolecular theory of the mass-independent isotope effect for ozone. III. effect of pressure on recombination rate constant ratios, *in preparation.*