

Publications of William Hase

1. Hase, W. L.; Brieland, W. G.; Simons, J. W. Comparison of Methylene Radical Insertion Reactions with the Si–H Bond of Methylsilane, Dimethylsilane, and Trimethylsilane. *J. Phys. Chem.* **1969**, *73*, 4401–4403.
2. Johnson, R. L.; Hase, W. L.; Simons, J. W. Kinetics of Chemically Activated Isobutane and Neopentane from the 4358- and 3660-Å Photolysis of Diazomethane with Propane and Isobutane. *J. Chem. Phys.* **1970**, *52*, 3911–3919.
3. Hase, W. L.; Simons, J. W. Chemically Activated Tetramethylsilane from the Reaction of Singlet Methylenes Radicals with Trimethylsilane. *J. Chem. Phys.* **1970**, *52*, 4004–4010.
4. Hase, W. L. Relative Rates of Singlet Methylenes Insertion Reactions. Decomposition Kinetics of Several Chemically Activated Alkanes and Alkylsilanes. Ph.D. Dissertation, New Mexico State University, 1970.
5. Hase, W. L.; Simons, J. W. Excitation Energies of Chemically Activated Isobutane and Neopentane and the Correlation of Their Decomposition Rates with Radical Recombination Rates. *J. Chem. Phys.* **1971**, *54*, 1277–1283.
6. Hase, W. L.; Simons, J. W. Calculation of the Thermal A-factors for Methyl and Ethyl Rupture from Chemically Activated Ethyltrimethylsilane. An Application of RRKM Theory. *J. Organomet. Chem.* **1971**, *32*, 47–59.
7. Hase, W. L.; Phillips, R. J.; Simons, J. W. Vibrational Deactivation of Singlet Methylenes. *Chem. Phys. Lett.* **1971**, *12*, 161–165.
8. Hase, W. L.; Johnson, R. L.; Simons, J. W. The Decomposition of Chemically Activated *n*-Butane, Isopentane, Neohexane and *n*-Pentane and the Correlation of Their Decomposition Rates with Radical Recombination Rates. *Int. J. Chem. Kinet.* **1972**, *4*, 1–35.
9. Hase, W. L.; Brieland, W. G.; McGrath, P. W.; Simons, J. W. Kinetic Study of the Reaction of Methylenes Radicals with Dimethylsilane. The Decomposition of Chemically Activated Trimethylsilane and Methylethylsilane. *J. Phys. Chem.* **1972**, *76*, 459–486.
10. Growcock, F. B.; Hase, W. L.; Simons, J. W. Kinetics of vibrationally hot Propane Produced by Methylenes Insertion into Ethane. *J. Phys. Chem.* **1972**, *76*, 607–614.
11. Hase, W. L. Theoretical Critical Configuration for Ethane Decomposition and Methyl Radical Recombination. *J. Chem. Phys.* **1972**, *57*, 730–733.
12. Growcock, F. B.; Hase, W. L.; Simons, J. W. Kinetics of Chemically Activated Ethane. *Int. J. Chem. Kinet.* **1973**, *5*, 77–92.
13. Growcock, F. B.; Hase, W. L.; Simons, J. W. Decomposition Kinetics of Chemically Activated Dimethylsilane and Ethylsilane. *J. Am. Chem. Soc.* **1973**, *95*, 3454–3459.
14. Bunker, D. L.; Hase, W. L. On Non-RRKM Unimolecular Kinetics: Molecules in General and CH₃NC in Particular. *J. Chem. Phys.* **1973**, *59*, 4621–4632.; **1978**, *69*, 4711 (erratum).
15. Chou, C. C.; Hase, W. L. RRKM Theory Applied to Decomposition of Hot Atom Substitution Products c-C₄H₇T and c-C₄D₇T. *J. Phys. Chem.* **1974**, *78*, 2309–2315.
16. Hase, W. L.; Feng, D.-F. Classical Trajectory Study of the Unimolecular Decomposition of H—C≡C—Cl, H—C≡C—H and Cl—C≡Cl—Cl. *J. Chem. Phys.* **1974**, *61*, 4690–4699.
17. Scott, R. L.; Richardson, A. E.; Simons, J. W.; Hase, W. L. Decomposition of Chemically Activated Ethyltrimethylgermane. The Arrhenius A-factors for Rupture of Group IVA-Methyl Bonds. *Int. J. Chem. Kinet.* **1975**, *7*, 547–555.
18. Kelley, P. M.; Hase, W. L.; Simons, J. W. Absence of an Energy Dependence for CH₂(¹A₁) Reaction with the C–H and Si–H Bonds of Dimethylsilane. *J. Phys. Chem.* **1975**, *79*, 1043–1044.
19. Kelley, P. M.; Hase, W. L. Ketene Photochemistry. Relative CH₂(¹A₁) Quantum Yields at 3130, 3340 and 3660 Å. *Chem. Phys. Lett.* **1975**, *35*, 57–62.
20. Simons, J. W.; Hase, W. L.; Phillips, R. J.; Porter, E. J.; Growcock, F. B. Chemically Activated Methylcyclobutane. Exothermicity of Singlet Methylenes Reactions and the Heat of Formation of Singlet Methylenes. *Int. J. Chem. Kinet.* **1975**, *7*, 879–894.
21. Hase, W. L.; Feng, D.-F. Trajectory Studies of Unimolecular Processes. II. Dynamics of Chloroacetylene Dissociation. *J. Chem. Phys.* **1976**, *64*, 651–655.
22. Hase, W. L.; Sloane, C. S. Predissociation of Chloroacetylene. *J. Chem. Phys.* **1976**, *64*, 2256–2257.
23. Hase, W. L. Dynamics of Unimolecular Reactions. In *Modern Theoretical Chemistry*, Vol. 2; Miller, W. H., Ed.; Plenum Publishing Co: New York, 1976; pp 121–170.
24. Hase, W. L. The Criterion of Minimum State Density in Unimolecular Rate Theory. An Application to Ethane Dissociation. *J. Chem. Phys.* **1976**, *64*, 2442–2449.
25. Sloane, C. S.; Hase, W. L. Ethyl Radical Potential Energy Surface. *Faraday Discuss. Chem. Soc.* **1977**, *62*, 210–221.
26. Hase, W. L. Efficiency of Intramolecular Vibrational Energy Redistribution in Model Systems: Chloroacetylene. *Ber. Bunsen-Ges. Phys. Chem.* **1977**, *81*, 207–209.
27. Sloane, C. S.; Hase, W. L. On the Dynamics of State Selected Unimolecular Reactions: Chloroacetylene Dissociation and Predissociation. *J. Chem. Phys.* **1977**, *66*, 1523–1533.
28. Hase, W. L.; Kelley, P. M. A Bimolecular Mechanism for Ketene Photodissociation in the Near Ultraviolet. *J. Chem. Phys.* **1977**, *66*, 5093–5099.
29. Nagy, P. J.; Hase, W. L. Intramolecular Vibrational Energy Relaxation in Benzene. *Chem. Phys. Lett.* **1978**, *54*, 73–76; **1978**, *58*, 482 (erratum).
30. Hase, W. L. Reply to Carr's Comments. *J. Chem. Phys.* **1978**, *68*, 4329–4331.
31. Wolf, R. J.; Hase, W. L. Energetics of Methylenes Radicals Formed by the 214 nm Photolysis of Diazomethane. *J. Phys. Chem.* **1978**, *82*, 1850–1855.

32. Hase, W. L.; Mrowka, G.; Brudzynski, R. J.; Sloane, C. S. An Analytic Function Describing the $\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_5$ Potential Energy Surface. *J. Chem. Phys.* **1978**, *69*, 3548–3562; **1981**, *72*, 6321 (erratum).
33. Bunker, D. L.; Wright, K. R.; Hase, W. L.; Houle, F. A. Exit-Channel Coupling Effects in the Unimolecular Decomposition of Triatomics. *J. Phys. Chem.* **1979**, *83*, 933–936 (Don Bunker Festschrift).
34. Hase, W. L.; Wolf, R. J.; Sloane, C. S. Trajectory Studies of the Molecular Dynamics of Ethyl Radical Decomposition. *J. Chem. Phys.* **1979**, *71*, 2911–2928; **1982**, *76*, 2771 (erratum).
35. Thomas, D. W.; Brudzynski, R. J.; Robin, M. L.; Hase, W. L. Photochemistry of Phenylcyclopropane. *J. Photochem.* **1979**, *11*, 227–239.
36. Hase, W. L. On the Relationship Between Unimolecular Lifetimes and Relative Translational Energy Distributions. *Chem. Phys. Lett.* **1979**, *67*, 263–266.
37. Wolf, R. J.; Hase, W. L. Trajectory Studies of Model $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$ Dissociation. I. Random Vibrational Excitation. *J. Chem. Phys.* **1980**, *72*, 316–331.
38. Wolf, R. J.; Hase, W. L. Importance of Angular Momentum Constraints in the Product Energy Partitioning of Model $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$ Dissociation. *J. Chem. Phys.* **1980**, *73*, 3010–3011.
39. Wolf, R. J.; Hase, W. L. Quasiperiodic Trajectories for a Multidimensional Anharmonic Classical Hamiltonian Excited Above the Unimolecular Threshold. *J. Chem. Phys.* **1980**, *73*, 3779–3790.
40. Hase, W. L.; Buckowski, D. G. Monte Carlo Sampling of a Microcanonical Ensemble of Classical Harmonic Oscillators. *Chem. Phys. Lett.* **1980**, *74*, 284–286.
41. Hase, W. L.; Ludlow, D. M.; Wolf, R. J.; Schlick, T. Translational and Vibrational Energy Dependence of the Cross Section for $\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_5^*$. *J. Phys. Chem.* **1981**, *85*, 958–968.
42. Hase, W. L.; Feng, D.-F. Dynamics of Ion Solvation. $\text{Li}^+ + \text{H}_2\text{O} \rightarrow \text{Li}^+(\text{H}_2\text{O})^*$. *J. Chem. Phys.* **1981**, *75*, 738–744.
43. Hase, W. L.; Bhalla, K. C. A Classical Trajectory Study of the $\text{F} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_4\text{F} \rightarrow \text{H} + \text{C}_2\text{H}_3\text{F}$ Reaction Dynamics. *J. Chem. Phys.* **1981**, *75*, 2807–2819.
44. Hase, W. L.; Wolf, R. J. Trajectory Studies of Model $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$ Dissociation. II. Angular Momenta and Energy Partitioning and Their Relation to non-RRKM Dynamics. *J. Chem. Phys.* **1981**, *75*, 3809–3820.
45. Hase, W. L. Overview of Unimolecular Dynamics. In *Potential Energy Surfaces and Dynamics Calculations*; Truhlar, D. G., Ed.; Plenum: New York, 1981; pp 1–36.
46. Hase, W. L.; Wolf, R. J. Effect of Potential Energy Surface Properties on Unimolecular Dynamics for a Model Alkyl Radical Dissociation Reaction: $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$. In *Potential Energy Surfaces and Dynamics Calculations*; Truhlar, D. G., Ed.; Plenum: New York, 1981; pp 37–74.
47. Duchovic, R. J.; Hase, W. L.; Schlegel, H. B.; Frisch, M. J.; Raghavachari, K. Ab Initio Potential Energy Curve for CH Bond Dissociation in Methane. *Chem. Phys. Lett.* **1982**, *89*, 120–125.
48. Hase, W. L. Semiclassical Vibrational Energy Levels for a Model $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$ Hamiltonian. *J. Phys. Chem.* **1982**, *86*, 2873–2879.
49. Hase, W. L.; Buckowski, D. G. Dynamics of Ethyl Radical Decomposition. II. Applicability of Classical Mechanics to Large Molecule Unimolecular Reaction Dynamics. *J. Comput. Chem.* **1982**, *3*, 335–343.
50. Swamy, K. N.; Hase, W. L. Dynamics of Ion-Molecule Recombination. II. An Alkali Ion and a Water Molecule. *J. Chem. Phys.* **1982**, *77*, 3011–3021.
51. Hase, W. L.; Schlegel, H. B. Resolution of a Paradox Concerning the Forward and Reverse Rate Constants for $\text{C}_2\text{H}_5 \rightarrow \text{H} + \text{C}_2\text{H}_4$. *J. Phys. Chem.* **1982**, *86*, 3901–3904.
52. Swamy, K. N.; Hase, W. L. Search for Quasiperiodic Motion in vibrationally excited Formaldehyde Formed by $\text{S}_1 \rightarrow \text{S}_0$ Internal Conversion. *Chem. Phys. Lett.* **1982**, *92*, 371–378.
53. Schlegel, H. B.; Bhalla, K. C.; Hase, W. L. *Ab Initio* Molecular Orbital Studies of $\text{H} + \text{C}_2\text{H}_4$ and $\text{F} + \text{C}_2\text{H}_4$. 2. Comparison of the Energetics. *J. Phys. Chem.* **1982**, *86*, 4883–4888.
54. Bhuiyan, L. B.; Hase, W. L. Sum and Density of States for Anharmonic Polyatomic Molecules. Effect of Bend-Stretch Coupling. *J. Chem. Phys.* **1983**, *78*, 5052–5058.
55. Hase, W. L. Classical Number and Density of States. *J. Chem. Educ.* **1983**, *60*, 379–381.
56. Hase, W. L.; Buckowski, D. G.; Swamy, K. N. Dynamics of Ethyl Radical Decomposition. III. Effect of Chemical Activation Versus Microcanonical Sampling. *J. Phys. Chem.* **1983**, *87*, 2754–2763 (Henry Eyring Festschrift).
57. Swamy, K. N.; Hase, W. L. A Quasiclassical Trajectory Calculation of the $\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_5$ Bimolecular Rate Constant. *J. Phys. Chem.* **1983**, *87*, 4715–4720.
58. Hase, W. L. Variational Unimolecular Rate Theory. *Acc. Chem. Res.* **1983**, *16*, 258–264.
59. Truhlar, D. G.; Hase, W. L.; Hynes, J. T. The Current Status of Transition State Theory. *J. Phys. Chem.* **1983**, *87*, 2664–2682.
60. Duchovic, R. J.; Hase, W. L.; Schlegel, H. B. An Analytic Function for the $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Potential Energy Surface. *J. Phys. Chem.* **1984**, *88*, 1339–1347.
61. Hase, W. L.; Duchovic, R. J.; Swamy, K. N.; Wolf, R. J. Trajectory Studies of Model $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$ Dissociation. III. Details of the Lifetime Distribution Following Chemical Activation. *J. Chem. Phys.* **1984**, *80*, 714–719.
62. Duchovic, R. J.; Swamy, K. N.; Hase, W. L. Semiclassical Vibrational Eigenvalues of a Three-Dimensional Hamiltonian. *J. Chem. Phys.* **1984**, *80*, 1462–1468.
63. Swamy, K. N.; Hase, W. L. Dynamics of Ion-Molecule Recombination. III. Trends in the Recombination Efficiency. *J. Am. Chem. Soc.* **1984**, *106*, 4071–4077.
64. Duchovic, R. J.; Hase, W. L. Sensitivity of the $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination Rate Constant to the Shape of the C–H Stretching Potential. *Chem. Phys. Lett.* **1984**, *110*, 474–477.
65. Date, N.; Hase, W. L.; Gilbert, R. G. Collisional Deactivation of Highly vibrationally Excited Molecules. Dynamics of the Collision Event. *J. Phys. Chem.* **1984**, *88*, 5135–5138.
66. Marcus, R. A.; Hase, W. L.; Swamy, K. N. RRKM and Non-RRKM Behavior in Chemical Activation Studies. *J. Phys. Chem.* **1984**, *88*, 6717–6720 (Peter Debye Festschrift).

67. Swamy, K. N.; Hase, W. L. The Heavy-Atom Effect in Intramolecular Vibrational Energy Transfer. *J. Chem. Phys.* **1985**, *82*, 123–133.
68. Duchovic, R. J.; Hase, W. L. A Dynamical Study of the $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination Reaction. *J. Chem. Phys.* **1985**, *82*, 3599–3606.
69. Hase, W. L.; Date, N.; Bhuiyan, L. B.; Buckowski, D. G. Energy Transfer in Collisions of Ar with Highly Excited Water and Methane. *J. Phys. Chem.* **1985**, *89*, 2502–2507.
70. Swamy, K. N.; Hase, W. L. Semiclassical Eigenvalues of a Three-Dimensional Hamiltonian with One Arbitrary Trajectory. *Chem. Phys. Lett.* **1985**, *114*, 248–252.
71. Hase, W. L. On Nonexponential Unimolecular Dissociation of Molecules Prepared by Vibrational Overtone Excitation. *Chem. Phys. Lett.* **1985**, *116*, 312–316.
72. Hase, W. L.; Duchovic, R. J. Thermal Rate Constant for $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination. Comparison of Quasiclassical Trajectory and Variational Transition State Theory. *J. Chem. Phys.* **1985**, *83*, 3448–3453.
73. Swamy, K. N.; Hase, W. L. Quantum and Semiclassical Vibrational Transition Frequencies for a Hamiltonian with Stretch Bend Potential Energy Coupling. *J. Chem. Phys.* **1986**, *84*, 361–368.
74. Mondro, S. L.; Vande Linde, S.; Hase, W. L. Reaction Path and Variational Transition State Theory Rate Constant for $\text{Li}^+ + \text{H}_2\text{O} \rightarrow \text{Li}^+(\text{H}_2\text{O})$ Association. *J. Chem. Phys.* **1986**, *84*, 3783–3787.
75. Nyman, G.; Rynefors, K.; Hase, W. L. Trajectory Study of Energy Partitioning in $\text{CF}_3\text{CN} \rightarrow \text{CF}_3 + \text{CN}$ Dissociation Dynamics. *J. Chem. Phys.* **1986**, *110*, 27–39.
76. Swamy, K. N.; Hase, W. L.; Garrett, B. C.; McCurdy, C. W.; McNutt, J. F. Mode Specificity in the Model Unimolecular Reaction $\text{H}-\text{C}-\text{C} \rightarrow \text{H} + \text{C}=\text{C}$. *J. Phys. Chem.* **1986**, *90*, 3517–3524 (Rudy Marcus Festschrift).
77. Lu, D.-h.; Hase, W. L.; Wolf, R. J. The Sensitivity of IVR in Benzene to Bend-Stretch Potential Energy Coupling. *J. Chem. Phys.* **1986**, *85*, 4422–4426.
78. Wolf, R. J.; Bhatia, D. S.; Hase, W. L. Effect of Bond Stretch Excitation on the Attenuation of Bending Forces. *Chem. Phys. Lett.* **1986**, *132*, 493–497.
79. Hase, W. L. Unimolecular and Intramolecular Dynamics: Relationship to Potential Energy Surface Properties. *J. Phys. Chem.* **1986**, *90*, 365–374.
80. Lemon, W. J.; Hase, W. L. A Potential Energy Function for The Hydroperoxyl Radical. *J. Phys. Chem.* **1987**, *91*, 1596–1602.
81. Vande Linde, S. R.; Mondro, S. L.; Hase, W. L. Transition States and Rate Constants for Ion-Molecule Association. II. $\text{Li}^+ + (\text{CH}_3)_2\text{O} \rightarrow \text{Li}^+[(\text{CH}_3)_2\text{O}]$. *J. Chem. Phys.* **1987**, *86*, 1348–1355.
82. Hase, W. L.; Mondro, S. L.; Duchovic, R. J.; Hirst, D. M. Thermal Rate Constant for $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination. III. Comparison of Experiment and Canonical Variational Transition State Theory. *J. Am. Chem. Soc.* **1987**, *109*, 2916–2922.
83. Hase, W. L. Properties of Variational Transition States for Association Reactions. *Chem. Phys. Lett.* **1987**, *139*, 389–394.
84. Lu, D.-h.; Hase, W. L. Quasiclassical Trajectory Study of the $n = 3$ Overtone State of Benzene. *Chem. Phys. Lett.* **1987**, *142*, 187–190.
85. Lu, D.-h.; Hase, W. L. Classical Trajectory Calculation of the Benzene Overtone Spectra. *J. Phys. Chem.* **1988**, *92*, 3217–3225.
86. Vande Linde, S. R.; Hase, W. L. Dynamics of Ion-Molecule Recombination. IV. $\text{Li}^+ + (\text{CH}_3)_2\text{O}$ Association. *Comput. Phys. Commun.* **1988**, *51*, 17–34.
87. Hu, X.; Hase, W. L. Effect of Anharmonicity on Inter-molecular Energy Transfer from Highly vibrationally Excited Molecules. *J. Phys. Chem.* **1988**, *92*, 4040–4046.
88. Lu, D.-h.; Hase, W. L. Classical Mechanics of Intramolecular Vibrational Energy Flow in Benzene. IV. Models with Reduced Dimensionality. *J. Chem. Phys.* **1988**, *89*, 6723–6736.
89. Whyte, A. R.; Lim, K. M.; Gilbert, R. G.; Hase, W. L. The Calculation and Interpretation of Average Collisional Energy Transfer Parameters. *Chem. Phys. Lett.* **1988**, *152*, 377–381.
90. Hase, W. L.; Hu, X. Semiempirical Canonical Variational Transition State Theory Model for Association Reactions. *Chem. Phys. Lett.* **1988**, *156*, 115–118.
91. Hase, W. L.; Richou, M.-C.; Mondro, S. L. Reaction Path and Kinetics for Na^+ Complexation with 18-Crown-6. *J. Phys. Chem.* **1989**, *93*, 539–545.
92. Lu, D.-h.; Hase, W. L. Sensitivity of Unimolecular Lifetime Distributions and Energy Dependent Rate Constants to Fluctuations in State Specific Rate Constants. *J. Chem. Phys.* **1989**, *90*, 1557–1563.
93. Vande Linde, S. R.; Hase, W. L. A Direct Mechanism for $\text{S}_{\text{N}}2$ Nucleophilic Substitution Enhanced by Mode Selective Vibrational Excitation. *J. Am. Chem. Soc.* **1989**, *111*, 2349–2351.
94. Lu, D.-h.; Hase, W. L. Monoenergetic Unimolecular Rate Constants and Their Dependence on Pressure and Fluctuations in State Specific Unimolecular Rate Constants. *J. Phys. Chem.* **1989**, *93*, 1681–1683.
95. Hu, X.; Hase, W. L. Properties of Canonical Variational Transition State Theory for Association Reactions without Potential Energy Barriers. *J. Phys. Chem.* **1989**, *93*, 6029–6038.
96. Hase, W. L.; Cho, S.-W.; Lu, D.-h.; Swamy, K. N. The Role of State Specificity in Unimolecular Rate Theory. *Chem. Phys.* **1989**, *139*, 1–13.
97. Lu, D.-h.; Hase, W. L. Classical Mechanics of Intramolecular Vibrational Energy Flow in Benzene. V. Effect of Zero Point Energy Motion. *J. Chem. Phys.* **1989**, *91*, 7490–7497.
98. Steinfeld, J. I.; Francisco, J. S.; Hase, W. L. *Chemical Kinetics and Dynamics*; Prentice Hall: New York, 1989.
99. Miller, W. H.; Hase, W. L.; Darling, C. L. A Simple Model for Correcting the Zero Point Energy Problem in Classical Trajectory Simulations of Polyatomic Molecules. *J. Chem. Phys.* **1989**, *91*, 2863–2868.
100. Hase, W. L.; Wardlaw, D. M. Transition-State Theory for Association Reactions without Potential Energy Barriers. In *Bimolecular Collisions*; Baggott, J. E., Ashfold, M. N., Eds.; Burlington House: London, 1989; pp 171–208.
101. Vande Linde, S. R.; Hase, W. L. A Complete Multi-Dimensional Analytic Potential Energy Surface For $\text{Cl}^- + \text{CH}_3\text{Cl}$ $\text{S}_{\text{N}}2$ Nucleophilic Substitution. *J. Phys. Chem.* **1990**, *94*, 2778–2788.

102. Vande Linde, S. R.; Hase, W. L. Trajectory Studies of SN₂ Nucleophilic Substitution. I. Dynamics of Cl⁻ + CH₃Cl Reactive Collisions. *J. Chem. Phys.* **1990**, *93*, 7962–7980.
103. Cho, S.-W.; Hase, W. L.; Swamy, K. N. A Model Analytic Potential Energy Function for Formyl Radical Decomposition. *J. Phys. Chem.* **1990**, *94*, 7371–7377.
104. Zhu, L.; Hase, W. L. Comparison of Models for Calculating the RRKM Unimolecular Rate Constant k(E,J). *Chem. Phys. Lett.* **1990**, *175*, 117–124.
105. Vande Linde, S. R.; Hase, W. L. Non-RRKM Kinetics in Gas-Phase S_N2 Nucleophilic Substitution. *J. Phys. Chem.* **1990**, *94*, 6148–6150.
106. Tardiff, J.; Deal, R. M.; Hase, W. L.; Lu, D.-h. Dissociation and IVR Pathways for the CF₃H(H₂O)₃ Cluster. *J. Cluster Sci.* **1990**, *1*, 337–356.
107. Gonzalez, C.; Thiesen, J.; Zhu, L.; Schlegel, H. B.; Hase, W. L.; Kaiser, E. W. Kinetics of the Reaction between OH and HO₂ on the Singlet Potential Energy Surface. *J. Phys. Chem.* **1991**, *95*, 6784–6792.
108. Hu, X.; Hase, W. L.; Pirraglia, T. Vectorization of the General Monte Carlo Classical Trajectory Program VENUS. *J. Comput. Chem.* **1991**, *12*, 1014–1024.
109. Hu, X.; Hase, W. L. Modification of the DHS Analytic Potential Energy Function for H + CH₃ → CH₄. Comparison of CVTST, Trajectory and Experimental Association Rate Constants. *J. Chem. Phys.* **1991**, *95*, 8073–8082.
110. Aubanel, E. E.; Wardlaw, D. M.; Zhu, L.; Hase, W. L. Role of Angular Momentum in Statistical Unimolecular Rate Theory. *Int. Rev. Phys. Chem.* **1991**, *10*, 249–286.
111. Cho, Y. J.; Vande Linde, S. J.; Zhu, L.; Hase, W. L. Trajectory Studies of S_N2 Nucleophilic Substitution. II. Nonstatistical Central Barrier Recrossing in the Cl⁻ + CH₃Cl System. *J. Chem. Phys.* **1992**, *96*, 8275–8287.
112. Gonzalez, C.; Thiesen, J.; Schlegel, H. B.; Hase, W. L.; Kaiser, E. W. Kinetics of the Reaction between OH and HO₂ on the Triplet Potential Energy Surface. *J. Phys. Chem.* **1992**, *96*, 1767–1774.
113. Hase, W. L.; Darling, C. L.; Zhu, L. Dynamics of Ion-Molecule Recombination. V. A Study of Energy Transfer Pathways. *J. Chem. Phys.* **1992**, *96*, 8295–8306.
114. Hu, X.; Hase, W. L. Use of Microclusters to Simulate Cage, Trapping and Chaperon Effects in Association Reactions. *J. Phys. Chem.* **1992**, *96*, 7535–7546.
115. Besler, B. H.; Hase, W. L.; Hass, K. C. A Theoretical Study of Growth Mechanisms of the {110} Surface of Diamond from Acetylene and Hydrogen Mixtures. *J. Phys. Chem.* **1992**, *96*, 9369–9376.
116. Hu, X.; Hase, W. L. Effect of Solvation on the Dynamics of H + CH₃ Association. *Z. Phys. D* **1992**, *25*, 57–65.
117. Chen, W.; Hase, W. L.; Schlegel, H. B. Ab Initio MO Calculations of the Thermochemistry of BX, AlX, OBX and OAIX (X = O, F, Cl). In *Gas-Phase Metal Reactions*; Fontijn, A., Ed.; Elsevier Science Publishers B.V.: New York, 1992; pp 179–187.
118. Zhu, L.; Chen, W.; Hase, W. L.; Kaiser, E. W. Comparison of Models for Treating Angular Momentum in RRKM Calculations with Vibrator Transition States. Pressure and Temperature Dependence of Cl + C₂H₂ Association. *J. Phys. Chem.* **1993**, *97*, 311–322.
119. Hu, X.; Hase, W. L. Dependence of the Chemical Dynamics of Intercluster Association Reactions on the Strength of the Solute-Solvent Intermolecular Potential. *J. Chem. Phys.* **1993**, *98*, 7826–7837.
120. Hase, W. L.; Cho, Y. J. Trajectory Studies of S_N2 Nucleophilic Substitution. III. Dynamical Stereochemistry and Energy Transfer Pathways for the Cl⁻ + CH₃Cl Association and Direct Substitution Reactions. *J. Chem. Phys.* **1993**, *98*, 8626–8639.
121. Accary, C.; Barbarat, P.; Hase, W. L.; Hass, K. C. Dynamics of H-Atom Association with the {111} Surface of Diamond. In *Diamond Materials*; Dismukes, J. P., Ravi, K. V., Eds.; Electrochemical Society: Pennington, NJ, 1993; pp 178–185.
122. Accary, C.; Barbarat, C.; Hase, W. L.; Hass, K. C. Importance of Energy Transfer and Lattice Properties in H-Atom Association with the {111} Surface of Diamond. *J. Phys. Chem.* **1993**, *97*, 9934–9941.
123. Barbarat, P.; Accary, C.; Hase, W. L. Comparison of Canonical Variational Transition State Theory (CVTST) Rate Constants for H-Atom Association with Alkyl Radicals and with the {111} Surface of Diamond. *J. Phys. Chem.* **1993**, *97*, 11706–11711.
124. Hase, W. L.; Zhu, L. An Analytic Hindered Rotor Model for Calculating Microcanonical Variational Unimolecular Rate Constants from Reaction Path Properties. *Int. J. Chem. Kinet.* **1994**, *26*, 407–419.
125. Peslherbe, G. H.; Hase, W. L. Analysis and Extension of a Model for Constraining Zero-Point Energy Flow in Classical Trajectory Simulations. *J. Chem. Phys.* **1994**, *100*, 1179–1189.
126. Wang, H.; Zhu, L.; Hase, W. L. A Model Multidimensional Analytic Potential Energy Function for the Cl⁻ + CH₃Br → ClCH₃ + Br⁻ Reaction. *J. Phys. Chem.* **1994**, *98*, 1608–1619.
127. de Sainte Claire, P.; Barbarat, P.; Hase, W. L. Ab Initio Potential and Variational Transition State Theory Rate Constant for H-Atom Association with the Diamond-{111} Surface. *J. Chem. Phys.* **1994**, *101*, 2476–2488.
128. Peslherbe, G. H.; Hase, W. L. A Comparison of Classical Trajectory and Statistical Unimolecular Rate Theory Calculations of Al₃ Decomposition. *J. Chem. Phys.* **1994**, *101*, 8535–8553.
129. Wang, H.; Peslherbe, G. H.; Hase, W. L. Trajectory Studies of S_N2 Nucleophilic Substitution. IV. Intramolecular and Unimolecular Dynamics of the Cl⁻ - -CH₃-Br and ClCH₃- - -Br⁻ Complexes. *J. Am. Chem. Soc.* **1994**, *116*, 9644–9651.
130. Chen, W.; Hase, W. L.; Schlegel, H. B. Ab Initio Classical Trajectory Study of H₂CO → H₂ + CO Dissociation. *Chem. Phys. Lett.* **1994**, *228*, 436–442.
131. Hase, W. L. Computer Simulation of Gas-Phase Chemical Reactions: Applications to S_N2 Nucleophilic Substitution. *Science* **1994**, *266*, 998–1002.
132. Peslherbe, G. H.; Wang, G.; Hase, W. L. Unimolecular Dynamics of Cl⁻ - -CH₃Cl Intermolecular Complexes Formed by Cl⁻ + CH₃Cl Association. *J. Chem. Phys.* **1995**, *102*, 5626–5635.
133. de Sainte Claire, P.; Peslherbe, G. H.; Hase, W. L. Energy Transfer Dynamics in the Collision-Induced Dissociation of Al₆ and Al₁₃ Clusters. *J. Phys. Chem.* **1995**, *99*, 8147–8161.

134. Stumpf, M.; Dobbyn, A. J.; Keller, H.-M.; Hase, W. L.; Schinke, R. Quantum Mechanical Study of the Unimolecular Dissociation of HO₂: A Rigorous Test of RRKM Theory. *J. Chem. Phys.* **1995**, *102*, 5867–5870.
135. Song, K.; de Sainte Claire, P.; Hase, W. L.; Hass, K. C. Comparison of Molecular Dynamics and Variational Transition State Theory Calculations of the Rate Constant for H-Atom Association with the Diamond{111} Surface. *Phys. Rev. B* **1995**, *52*, 2949–2958.
136. Wang, H.; Hase, W. L. Statistical Rate Theory Calculations of the Cl⁻ + CH₃Br → ClCH₃ + Br⁻ Rate Constant Versus Temperature, Kinetic Energy, and H(D) Isotopic Substitution. *J. Am. Chem. Soc.* **1995**, *117*, 9347–9356.
137. Song, K.; Peslherbe, G. H.; Hase, W. L.; Dobbyn, A. J.; Stumpf, M.; Schinke, R. Comparison of Quantum and Semiclassical Variational Transition State Models for the HO₂ → H + O₂ Microcanonical Rate Constant. *J. Chem. Phys.* **1995**, *103*, 8891–8900.
138. Oudejans, L.; Miller, R. E.; Hase, W. L. Unimolecular Processes in Weakly Bound Complexes: Correlated Product State Distributions. *Faraday Discuss. Chem. Soc.* **1995**, *102*, 323–338.
139. de Sainte Claire, P.; Song, K.; Hase, W. L.; Brenner, D. W. Comparison of *Ab Initio* and Empirical Potentials for H-Atom Association with Diamond Surfaces. *J. Phys. Chem.* **1996**, *100*, 1761–1766.
140. de Sainte Claire, P.; Hase, W. L. Thresholds for the Collision-Induced Dissociation of Clusters by Rare Gas Impact. *J. Phys. Chem.* **1996**, *100*, 8190–8196.
141. Peslherbe, G. H.; Hase, W. L. Semiempirical MNDO, AM1, and PM3 Direct Dynamics Trajectory Studies of Formaldehyde Unimolecular Dissociation. *J. Chem. Phys.* **1996**, *104*, 7882–7894.
142. Peslherbe, G. H.; Wang, H.; Hase, W. L. Trajectory Studies of S_N2 Nucleophilic Substitution. V. Semiempirical Direct Dynamics of Cl⁻ - CH₃Br Unimolecular Decomposition. *J. Am. Chem. Soc.* **1996**, *118*, 2257–2266.
143. Hase, W. L.; Schlegel, H. B.; Balbyshev, V.; Page, M. An Ab Initio Study of the Transition State and Forward and Reverse Rate Constants for C₂H₅ → H + C₂H₄. *J. Phys. Chem.* **1996**, *100*, 5354–5361.
144. Peslherbe, G. H.; Hase, W. L. Comparison of Zero-Point Energy Constrained and Quantum Anharmonic RRKM and Phase Space Theory Rate Constants for Al₃ Dissociation. *J. Chem. Phys.* **1996**, *104*, 9445–9460.
145. Wang, H.; Hase, W. L. Reaction Path Hamiltonian Analysis of the Dynamics for Cl⁻ + CH₃Br → ClCH₃ + Br⁻ S_N2 Nucleophilic Substitution. *Chem. Phys.* **1996**, *212*, 247–258.
146. Nisamov, B.; Setser, D. W.; Wang, H.; Peslherbe, G. H.; Hase, W. L. Quasiclassical Trajectory Calculations for the OH(X²π) and OD(X²π) + HBr Reactions: Energy Partitioning and Rate Constants. *J. Chem. Phys.* **1996**, *105*, 9897–9911.
147. Peslherbe, G. H.; Hase, W. L. Statistical Anharmonic Unimolecular Rate Constants for the Dissociation of Fluxional Molecules. Application to Aluminum Clusters. *J. Chem. Phys.* **1996**, *105*, 7432–7447.
148. Doubleday, C., Jr.; Bolton, K.; Peslherbe, G. H.; Hase, W. L. A Direct Dynamics Simulation of the Lifetime of Trimethylene. *J. Am. Chem. Soc.* **1996**, *118*, 9922–9931.
149. Baer, T.; Hase, W. L. *Unimolecular Reaction Dynamics—Theory and Experiments*; Oxford University Press: New York, 1996.
150. Seeley, J. V.; Morris, R. A.; Viggiano, A. A.; Wang, H.; Hase, W. L. Temperature Dependencies of the Rate Constants and Branching Ratios for the Reactions of Cl⁻(H₂O)_{0–3} with CH₃Br and Thermal Dissociation Rates for Cl⁻(CH₃Br). *J. Am. Chem. Soc.* **1997**, *119*, 577–584.
151. de Sainte Claire, P.; Hase, W. L.; Peslherbe, G. H.; Wang, H. Linear Free of Activation Relationship for Association Reactions. *J. Am. Chem. Soc.* **1997**, *119*, 5007–5012.
152. de Sainte Claire, P.; Hase, W. L. Empirical Potential for Methyl Radical Association with Diamond Surfaces. *Phys. Rev. B* **1997**, *56*, 13543–13555.
153. Wang, H.; Hase, W. L. Kinetics of F⁻ + CH₃Cl S_N2 Nucleophilic Substitution. *J. Am. Chem. Soc.* **1997**, *119*, 3093–3102.
154. Wang, H.; Goldfield, E. M.; Hase, W. L. Quantum Dynamical Study of the Cl⁻ + CH₃Br S_N2 Reaction. *J. Chem. Soc., Faraday Trans.* **1997**, *93*, 737–746.
155. Hanley, L.; Lim, H.; Schultz, D. G.; Wainhaus, S. B.; de Sainte Claire, P.; Hase, W. L. Surface Energy Transfer by Low Energy Polyatomic Ion Collisions. *Nucl. Instrum. Methods Phys. Res., Sect. B* **1997**, *125*, 218–222.
156. de Sainte Claire, P.; Hass, K. C.; Schneider, W. F.; Hase, W. L. Simulations of Hydrocarbon Adsorption and Subsequent Water Penetration on an Aluminum Oxide Surface. *J. Chem. Phys.* **1997**, *106*, 7331–7342.
157. Doubleday, C., Jr.; Bolton, K.; Hase, W. L. Direct Dynamics Study of the Stereomutation of Cyclopropane. *J. Am. Chem. Soc.* **1997**, *119*, 5251–5252.
158. Bolton, K.; Hase, W. L.; Doubleday, C., Jr. Isomerization of Deuterated Cyclopropanes—The Possibility for Stereochemical Control. *Ber. Bunsen-Ges. Phys. Chem.* **1997**, *101*, 414–422.
159. Wang, H.; Hase, W. L. Lyapunov Exponents for the Intramolecular Motion of the Cl⁻ - CH₃Br Complex. *Int. J. Mass Spectrom. Ion Processes* **1997**, *167/168*, 573–585.
160. Schultz, D. G.; Weinhaus, S. B.; Hanley, L.; de Sainte Claire, P.; Hase, W. L. Classical Dynamics Simulations of SiMe₃⁺ Ion-Surface Scattering. *J. Chem. Phys.* **1997**, *106*, 10337–10348.
161. Bosio, S. B. M.; Hase, W. L. Energy Transfer in Rare Gas Collisions with Self-Assembled Monolayers. *J. Chem. Phys.* **1997**, *107*, 9677–9686.
162. Hase, W. L.; de Sainte Claire, P. Simulations of Energy Transfer in the Collision-Induced Dissociation of Al₆(O_h) Clusters by Rare Gas Impact. In *Highly Excited States: Relaxation, Reaction, and Structure*; Mullin, A., Schatz, G. C., Eds.; ACS Symposium Series; American Chemical Society: Washington, DC, 1997; pp 276–290.
163. de Sainte Claire, P.; Hase, W. L.; Song, K. Role of the Surface Site in the Kinetics of H-Atom Association with Diamond Surfaces. *J. Phys. Chem. B* **1998**, *102*, 382–386.
164. Bosio, S. B. M.; Hase, W. L. Simulations of Energy Transfer in Cr⁺(CO)₆ Surface Induced Dissociation. *Int. J. Mass Spectrom. Ion Processes* **1998**, *174*, 1–9.

165. Song, K.; Hase, W. L. The Role of State Specificity in Temperature and Pressure Dependent Unimolecular Rate Constants for $\text{HO}_2 \rightarrow \text{H} + \text{O}_2$ Dissociation. *J. Phys. Chem. A* **1998**, *102*, 1292–1296.
166. Doubleday, C., Jr.; Bolton, K.; Hase, W. L. Direct Dynamics Quasiclassical Trajectory Study of the Thermal Stereomutation of Cyclopropane. *J. Phys. Chem. A* **1998**, *102*, 3648–3658.
167. Wittbrodt, J. M.; Hase, W. L.; Schlegel, H. B. An *Ab Initio* Study of the Interaction of Water with Cluster Models of the Aluminum Terminated (0001) α -Aluminum Oxide Surface. *J. Phys. Chem. B* **1998**, *102*, 6539–6548.
168. Bolton, K.; Hase, W. L.; Schlegel, H. B.; Song, K. A Direct Dynamics Study of $\text{F} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_3\text{F} + \text{H}$ Product Energy Distributions. *Chem. Phys. Lett.* **1998**, *288*, 621–627.
169. Mann, D. J.; Hase, W. L. Trajectory Studies of $\text{S}_{\text{N}}2$ Nucleophilic Substitution. 6. Translational Activation of the $\text{Cl}^- + \text{CH}_3\text{Cl}$ Reaction. *J. Phys. Chem. A* **1998**, *102*, 6208–6214.
170. Su, T.; Wang, H.; Hase, W. L. Trajectory Studies of $\text{S}_{\text{N}}2$ Nucleophilic Substitution. 7. $\text{F}^- + \text{CH}_3\text{Cl} \rightarrow \text{FCH}_3 + \text{Cl}^-$. *J. Phys. Chem. A* **1998**, *102*, 9819–9828.
171. Hase, W. L. Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory. *Acc. Chem. Res.* **1998**, *31*, 659–665.
172. Hase, W. L. Classical Trajectory Simulations: Final Conditions. In *Encyclopedia of Computational Chemistry*, Vol. 1; Allinger, N. L., Ed.; Wiley: New York, 1998; pp 399–402.
173. Hase, W. L. Classical Trajectory Simulations: Initial Conditions. In *Encyclopedia of Computational Chemistry*, Vol. 1; Allinger, N. L., Ed.; Wiley: New York, 1998; pp 402–407.
174. Hase, W. L.; Wang, H.; Peslherbe, G. H. Dynamics of Gas-Phase $\text{S}_{\text{N}}2$ Nucleophilic Substitution Reactions. In *Advances in Gas Phase Ion Chemistry*, Vol. 3; Babcock, L. M., Adams, N. G., Eds.; JAI Press: Greenwich, CT, 1998; pp 125–156.
175. Bolton, K.; Hase, W. L.; Peslherbe, G. H. Direct Dynamics Simulations of Reactive Systems. In *Multidimensional Molecular Dynamics Methods*; Thompson, D. L., Ed.; World Scientific Publishing: London, 1998; pp 143–189.
176. Bolton, K.; Hase, W. L. Integrating the Classical Equations of Motion. In *Encyclopedia of Computational Chemistry*, Vol. 2; Allinger, N. L., Ed.; Wiley: New York, 1998; pp 1347–1360.
177. Bolton, K.; Hase, W. L.; Doubleday, C., Jr. A QM/MM Direct Dynamics Trajectory Investigation of Trimethylene Decomposition in an Argon Bath. *J. Phys. Chem. B* **1998**, *103*, 3691–3687.
178. Song, K.; Hase, W. L. Fitting Classical Microcanonical Unimolecular Rate Constants to a Modified RRK Expression. Anharmonic and Variational Effects. *J. Chem. Phys.* **1999**, *110*, 6198–6207.
179. Bolton, K.; Bosio, S. B. M.; Hase, W. L.; Schneider, W. F.; Hass, K. C. Comparison Between United and Explicit Atom Models for Simulating Alkane Chains Physisorbed on an Aluminum Terminated (0001) α -Aluminum Oxide Surface. *J. Phys. Chem. B* **1999**, *103*, 3885–3895.
180. Bolton, K.; Schlegel, H. B.; Hase, W. L.; Song, K. A Quasiclassical *Ab Initio* Direct Dynamics Investigation of the $\text{F} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_3\text{F} + \text{H}$ Product Energy Distributions. *Phys. Chem. Chem. Phys.* **1999**, *1*, 999–1011.
181. Meroueh, O.; Hase, W. L. Collisional Activation of Small Peptides. *J. Phys. Chem. A* **1999**, *103*, 3981–3990.
182. Li, G.; Hase, W. L. Ab Initio Direct Dynamics Trajectory Study of the $\text{Cl}^- + \text{CH}_3\text{Cl}$ $\text{S}_{\text{N}}2$ Reaction at High Reagent Translational Energy. *J. Am. Chem. Soc.* **1999**, *121*, 7124–7129.
183. Millam, J. M.; Bakken, V.; Chen, W.; Hase, W. L.; Schlegel, H. B. *Ab Initio* Classical Trajectories on the Born-Oppenheimer Surface: Hessian-Based Integrators Using Fifth Order Polynomial and Rational Function Fits. *J. Chem. Phys.* **1999**, *111*, 3800–3805.
184. Steinfeld, J. I.; Francisco, J. S.; Hase, W. L. *Chemical Kinetics and Dynamics*, 2nd ed.; Prentice Hall: New York, 1999.
185. Peslherbe, G. H.; Hase, W. L. Accurate Phase Space Theory and Molecular Dynamics Calculations of Aluminum Cluster Dissociation. In *Theory of Atomic and Molecular Clusters*; Jellinek, J., Ed.; Springer: New York, 1999; pp 228–254.
186. Peslherbe, G. H.; Wang, H.; Hase, W. L. Monte Carlo Sampling for Classical Trajectory Simulations. In *Monte Carlo Methods in Chemical Physics, Advances in Chemical Physics*, Vol. 105; Ferguson, D. M., Siepman, J. I., Truhlar, D. G., Eds.; Wiley: New York, 1999; pp 171–201.
187. Hase, W. L.; de Sainte Claire, P.; Song, K. Hydrogen-Atom and Methyl-Radical Association with the Diamond {111} Surface. In *Advances in Classical Trajectory Methods*, Vol. 4; Hase, W. L., Ed.; JAI Press: Greenwich, CT, 1999; pp 189–233.
188. Mann, D. J.; Hase, W. L. Computer Simulation of Sliding Hydroxylated Alumina Surfaces. *Tribol. Lett.* **2000**, *7*, 153–159.
189. Jin, R. Y.; Song, K.; Hase, W. L. Molecular Dynamics Simulations of the Structures of Alkane/Hydroxylated α - Al_2O_3 (0001) Interfaces. *J. Phys. Chem. B* **2000**, *104*, 2692–2701.
190. Sawilowsky, E. F.; Schlegel, H. B.; Hase, W. L. Structures and Energies for Methane Complexed with Alumina Clusters. *J. Phys. Chem. A* **2000**, *104*, 4920–4927.
191. Roy, S.; Jin, R. Y.; Chaudhary, V.; Hase, W. L. Parallel Molecular Dynamics Simulations of Alkane/Hydroxylated α -Aluminum Oxide Interfaces. *Comput. Phys. Commun.* **2000**, *128*, 210–218.
192. Yan, T.-Y.; Hase, W. L. Origin of the Boltzmann Translational Energy Distribution in the Scattering of Hyperthermal Ne Atoms off a Self-Assembled Monolayer. *Phys. Chem. Chem. Phys.* **2000**, *2*, 901–910.
193. Meroueh, O.; Hase, W. L. Energy Transfer Pathways in the Collisional Activation of Peptides. *Int. J. Mass Spectrom.* **2000**, *201*, 233–244.
194. Li, G.; Bosio, S. B. M.; Hase, W. L. A QM/MM Model for $\text{O}(\text{P}^3)$ Reaction with an Alkyl Thiolate Self-Assembled Monolayer. *J. Mol. Struct.* **2000**, *556*, 43–57 (Lou Allinger Special Issue).
195. Peslherbe, G. H.; Hase, W. L. Product Energy and Angular Momentum Partitioning in Aluminum Cluster Dissociation. *J. Phys. Chem. A* **2000**, *104*, 10556–10564 (Bradley Moore Festschrift).

196. Yan, T.-Y.; Hase, W. L.; Barker, J. R. Identifying Trapping Desorption in Gas-Surface Scattering *Chem. Phys. Lett.* **2000**, *329*, 84–91.
197. Hase, W. L.; Koch, W. Gas-Phase Ion Chemistry: A Fruitful Playground for the Interplay Between Experiment and Theory. *Int. J. Mass Spectrom.* **2000**, *201*, ix–x.
198. Sun, L.; de Sainte Claire, P.; Meroueh, O.; Hase, W. L. Dynamics of Ar + CH₄/Ni{111} Collision-Induced Desorption. *J. Chem. Phys.* **2001**, *114*, 535–544.
199. Mann, D. J.; Zhong, L.; Hase, W. L. Effect of Surface Stiffness on the Friction of Sliding Model α -Hydroxylated Alumina Surfaces. *J. Phys. Chem. B* **2001**, *105*, 12032–12045.
200. Yan, T.-Y.; Hase, W. L. A Hamiltonian with a Subset of Normal Modes for Studying Mode Specific Energy Transfer in Intermolecular Collisions. *J. Phys. Chem. A* **2001**, *105*, 2617–2625 (Bill Miller Festschrift).
201. Meroueh, O.; Hase, W. L. Effect of Surface Stiffness on the Efficiency of Surface-Induced Dissociation. *Phys. Chem. Chem. Phys.* **2001**, *3*, 2306–2314.
202. Song, K.; Hase, W. L. Anharmonic Semiclassical VTST Rate Constant Model for H-Atom Association with Different Sites on the Diamond {111} Surface. *J. Phys. Chem. A* **2001**, *105*, 2453–2457.
203. Song, K.; Sun, L.; Hase, W. L. Trajectory Studies of S_N2 Nucleophilic Substitution. 8. Central Barrier Dynamics for Gas Phase Cl[−] + CH₃Cl. *J. Am. Chem. Soc.* **2001**, *123*, 5753–5756.
204. Mann, D. J.; Hase, W. L. Direct Dynamics Simulations of the Oxidation of a Single Wall Carbon Nanotube. *Phys. Chem. Chem. Phys.* **2001**, *3*, 4376–4383.
205. Hase, W. L. Statistical Mechanical Description of Chemical Kinetics: RRKM. In *Encyclopedia of Chemical Physics and Physical Chemistry, Vol. 1, Fundamentals*; Moore, J. H., Spencer, N. D., Eds.; Institute of Physics: Philadelphia, 2001; pp 865–896.
206. Li, G.; Hase, W. L.; Doubleday, C., Jr. Dynamics of the Biradical Mediating Vinylcyclopropane–Cyclopentene Rearrangement. *Phys. Chem. Chem. Phys.* **2002**, *4*, 304–312.
207. Meroueh, O.; Hase, W. L. Dynamics of Energy Transfer in Peptide–Surface Collisions. *J. Am. Chem. Soc.* **2002**, *124*, 1524–1531.
208. Mann, D. J.; Hase, W. L. Ab Initio Direct Dynamics of Cyclopropyl Radical Ring Opening. *J. Am. Chem. Soc.* **2002**, *124*, 3208–3209.
209. Sun, L.; Song, K.; Hase, W. L. A S_N2 Reaction that Avoids its Deep Potential Energy Minimum. *Science* **2002**, *296*, 875–878.
210. Xie, H.; Song, K.; Mann, D. J.; Hase, W. L. Temperature Gradients and Frictional Energy Dissipation in the Sliding of Hydroxylated α -Alumina Surfaces. *Phys. Chem. Chem. Phys.* **2002**, *4*, 5377–5385.
211. Song, K.; Sun, L.; Hase, W. L.; Grebenschchikov, S. Y.; Schinke, R. Relationships between Mode Specific and Thermal Unimolecular Rate Constants for HOCl → OH + Cl Dissociation. *J. Phys. Chem. A* **2002**, *106*, 8339–8344 (Don Setser Festschrift).
212. Mann, D. J.; Halls, M. D.; Hase, W. L. Direct Dynamics Studies of CO Assisted Carbon Nanotube Growth. *J. Phys. Chem. B* **2002**, *106*, 12418–12425.
213. Meroueh, O.; Wang, Y.; Hase, W. L. Direct Dynamics Simulations of Collision- and Surface-Induced Dissociation of N-Protonated Glycine. Shattering Fragmentation. *J. Phys. Chem. A* **2002**, *106*, 9983–9992 (Jack Beauchamp Festschrift).
214. Yan, T.-Y.; Hase, W. L. Comparisons of Models for Simulating Energy Transfer in Ne-Atom Collisions with an Alkyl Thiolate Self-Assembled Monolayer. *J. Phys. Chem. B* **2002**, *106*, 8029–8037 (John Tully Festschrift).
215. Wang, Y.; Hase, W. L.; Wang, H. Trajectory Studies of S_N2 Nucleophilic Substitution. 9. Microscopic Reaction Pathways and Chemical Kinetics for Cl[−] + CH₃Br. *J. Chem. Phys.* **2003**, *118*, 2688–2695.
216. Meroueh, O.; Song, K.; Hase, W. L. Dynamics of High Energy Cr⁺(CO)₆ Collisions with Hydrogenated Surfaces. *J. Chem. Phys.* **2003**, *118*, 2893–2902.
217. Sun, L.; Song, K.; Hase, W. L.; Riveros, J. Stationary Points for the OH[−] + CH₃F → CH₃OH + F[−] Potential Energy Surface. *Int. J. Mass Spectrom.* **2003**, *227*, 315–325.
218. Liu, J.; Song, K.; Hase, W. L.; Anderson, S. L. Direct Dynamics Study of Energy Transfer and Collision-Induced Dissociation: Effect of Impact Energy, Geometry, and Reactant Vibrational Modes in H₂CO⁺–Ne Collisions. *J. Chem. Phys.* **2003**, *119*, 3040–3050.
219. Yan, T.-Y.; Isa, N.; Gibson, K. D.; Sibener, S. J.; Hase, W. L. Role of Surface Intramolecular Dynamics in the Efficiency of Energy Transfer in Ne-Atom Collisions with a n-Hexylthiolate Self-Assembled Monolayer. *J. Phys. Chem. A* **2003**, *107*, 10600–10607 (Charles Parmenter Festschrift).
220. Wang, J.; Wang, Y.; Meroueh, O.; Hase, W. L. Efficiency of Energy Transfer in Protonated Diglycine and Dialanine SID. Effects of Collision Angle, Peptide Ion Size, and Intramolecular Potential. *Int. J. Mass Spectrom.* **2003**, *230*, 57–64.
221. Hase, W. L.; Scuseria, G. E. Guest Editors' Introduction: Computational Chemistry. *Comput. Sci. Eng.* **2003**, *5*, 12–13.
222. Wang, Y.; Song, K.; Hase, W. L. Direct Dynamics Study of N-Protonated Diglycine Surface-Induced Dissociation. Influence of Collision Energy. *J. Am. Soc. Mass Spectrom.* **2003**, *14*, 1402–1412.
223. Hase, W. L.; Song, K.; Gordon, M. Direct Dynamics Simulations. *Comput. Sci. Eng.* **2003**, *5*, 36–44.
224. Hase, W. L. Classical Trajectory Simulations. In *Encyclopedia of Mass Spectrometry, Vol. 1, Theory and Ion Chemistry*; Gross, M., Caprioli, R., Armentrout, P. B., Eds.; Elsevier Science: New York, 2003; pp 40–46.
225. Grebenschchikov, S. Y.; Schinke, R.; Hase, W. L. State-Specific Dynamics of Unimolecular Dissociation. In *Comprehensive Chemical Kinetics, Vol. 39, Unimolecular Kinetics Part 1. The Reaction Step*; Green, N. J. B., Ed.; Elsevier Science: Amsterdam, The Netherlands, 2003; pp 105–242.
226. Sun, L.; Hase, W. L. Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations. In *Reviews in Computational Chemistry, Vol. 19*; Lipkowitz, K. B., Larter, R., Cundari, T. R., Eds.; Wiley: New York, 2003; pp 79–146.
227. Sun, L.; Chang, E.; Song, K.; Hase, W. L. Transition State Dynamics and a QM/MM Model for the Cl[−] + C₂H₅Cl S_N2 Reaction. *Can. J. Chem.* **2004**, *82*, 891–899 (Gerhard Herzberg Special Issue).

228. Chaudhary, V.; Hase, W. L.; Jiang, H.; Sun, L.; Thaker, D. Experiments with Parallelizing Tribology Simulations. *J. Supercomputing* **2004**, *28*, 323–343.
229. Isa, N.; Gibson, K. D.; Yan, T.-Y.; Hase, W. L.; Sibener, S. J. Experimental and Simulation Study of Neon Collision Dynamics with a 1-Decanethiol Monolayer. *J. Chem. Phys.* **2004**, *120*, 2417–2433.
230. Yan, T.-Y.; Hase, W. L.; Tully, J. C. A Washboard with Moment of Inertia Model of Gas-Surface Scattering. *J. Chem. Phys.* **2004**, *120*, 1031–1043.
231. Yan, T.-Y.; Hase, W. L.; Doubleday, C. Energetics, Transition States, and Intrinsic Reaction Coordinates for Reactions Associated with O(³P) Processing of Hydrocarbon Materials. *J. Chem. Phys.* **2004**, *120*, 9253–9265.
232. Yan, T.-Y.; Doubleday, D.; Hase, W. L. A PM3-SRP + Analytic Function Potential Energy Surface Model for O(³P) Reactions with Alkanes. Application to O(³P) + Ethane. *J. Phys. Chem. A* **2004**, *108*, 9863–9875 (Tom Baer Festschrift).
233. Liu, J.; Song, K.; Hase, W. L.; Anderson, S. L. Direct Dynamics Trajectory Study of Vibrational Effects: Can Polanyi Rules be Generalized to a Polyatomic System? *J. Am. Chem. Soc.* **2004**, *126*, 8602–8603.
234. Sun, L.; Hase, W. L. Ab Initio Direct Dynamics Simulation of C₂H₅F → C₂H₄ + HF Product Energy Partitioning. *J. Chem. Phys.* **2004**, *121*, 8831–8845.
235. Hase, W. L.; Miller, R. E. Personal and Professional History of Tomas Baer. *J. Phys. Chem. A* **2004**, *108*, 9625–9626.
236. Hase, W. L. S_N2 Reactions and Their Double-Well Potentials. In *Encyclopedia of Mass Spectrometry*, Vol. 5, *Fundamentals of and Applications to Organic (and Organometallic) Compounds*; Gross, M., Capriolli, R., Nibbering, N. M. M., Eds.; Elsevier Science: New York, 2004; pp 504–515.
237. Chaudhary, V.; Hase, W. L.; Jiang, H.; Sun, L.; Thaker, D. Comparing Various Parallelizing Approaches for Tribology Simulations. In *High Performance Scientific and Engineering Computing: Hardware/Software Support*; Yang, L. T., Pan, Y., Eds.; Kluwer Academic: Boston, 2004; pp 231–252.
238. Sun, L.; Petersen, K.; Alexeev, Y.; Windus, T.; Kindt, J. T.; Hase, W. L. Effect of the Ar–Ni(s) Potential on the Cross Section for Ar + CH₄/Ni{111} Collision Induced Desorption and the Need for a More Accurate CH₄/Ni{111} Potential. *J. Chem. Phys.* **2005**, *122*, 044704/1–6.
239. Wang, J.; Hase, W. L. An Intermolecular Potential to Represent Collisions of Protonated Peptide Ions with Fluorinated Alkane Surfaces. *J. Phys. Chem. B* **2005**, *109*, 8320–8324 (George Flynn Festschrift).
240. Mazyar, O. A.; Xie, H.; Hase, W. L. Non-Equilibrium Energy Dissipation at the Interface of Sliding Model Hydroxylated α -Alumina Surfaces. *J. Chem. Phys.* **2005**, *122*, 0947131/1–12.
241. Liu, J.; Song, K.; Hase, W. L.; Anderson, S. L. Direct Dynamics Trajectory study of the Reaction of Formaldehyde Cation with D₂: Vibrational and Zero-Point Effects on Quasiclassical Trajectories. *J. Phys. Chem. A* **2005**, *109*, 11376–11384 (Jack Simons Festschrift).
242. Hase, W. L.; Schinke, R. Role of Computational Chemistry in the Development of Unimolecular Rate Theory. In *Theory and Applications of Computational Chemistry: The First 40 Years*; Dykstra, C. E., Frenking, G., Kim, K. S., Scuseria, G., Eds.; Elsevier: New York, 2005; pp 397–423.
243. Martínez-Núñez, E.; Fernández-Ramos, A.; Vázquez, S. A.; Xue, M.; Hase, W. L. Quasiclassical Dynamics Simulation of the Collision-Induced Dissociation of Cr(CO)₆⁺. *J. Chem. Phys.* **2005**, *123*, 154311/1–9.
244. Vayner, G.; Alexeev, Y.; Wang, J.; Windus, T. L.; Hase, W. L. Ab Initio and Analytic Intermolecular Potentials for Ar–CF₄. *J. Phys. Chem. A*, published online Nov 18, <http://dx.doi.org/10.1021/jp054592p> (Jürgen Troe Festschrift).
245. Mazyar, O. A.; Hase, W. L. Dynamics and Kinetics of Heat Transfer at the Interface of Model Diamond {111} Nanosurfaces. *J. Phys. Chem. A* **2006**, *110*, 526–536 (Donald G. Truhlar Festschrift).