

Publications of Aron Kuppermann[†]

1. The General Formula of Hydrocarbons. A. Kuppermann. *Anais Assoc. Quim. Brasil* **7**, 20 (1948).
2. Study of the Parachor of Rings. A. Kuppermann and F. W. Lima. *Anais Assoc. Quim. Brasil* **8**, 25 (1949).
3. Determination of the Number of Independent Constituents of a System. A. Kuppermann and B. Samú. *Anais Assoc. Quim. Brasil* **10**, 98 (1951).
4. Determination of Masses by Gauss' Double Weighting Method. W. Borzani, A. Kuppermann, and B. Samú. *Anais Assoc. Quim. Brasil* **10**, 117 (1951).
5. Summary of Proceedings of an Informal Discussion on the Radiation Chemistry of Water. A. Kuppermann, S. Lipsky, and L. Monchick, Eds. Radiation Project, Department of Chemistry, University of Notre Dame, April 1955 (33 pages).
6. Decomposition of *n*-Butane in an Electric Discharge. A. Kuppermann, Ph.D. Dissertation, University of Notre Dame, August 1955 (102 pages).
7. Quantum-Mechanical Calculation of One-Electron Properties. I. General Formulation. M. Karplus, A. Kuppermann, and L. M. Isaacson. *J. Chem. Phys.* **29**, 1240 (1958).
8. The Quantum-Mechanical Calculation of One-Electron Properties. II. One- and Two-Center Moment Integrals. A. Kuppermann, M. Karplus, and L. M. Isaacson. *Z. Naturforsch.* **14a**, 311 (1959).
9. Decomposition of *n*-Butane in an Electric Discharge. A. Kuppermann and M. Burton. *Radiat. Res.* **10**, 636 (1959).
10. Theoretical Foundations of Radiation Chemistry. A. Kuppermann. *J. Chem. Educ.* **36**, 279 (1959).
11. Ferrous and Ceric Sulfate Dosimeters. Interpretation of the Effect of Radiation Quality. A. Kuppermann. *Publ. Inst. Energia Atomica (Brasil)* No. 40 (1960).
12. Nonmolecular Nature of the Nitric-Oxide-Inhibited Thermal Decomposition of *n*-Butane. A. Kuppermann and J. G. Larson. *J. Chem. Phys.* **33**, 1264 (1960).
13. Diffusion Kinetics in Radiation Chemistry. A. Kuppermann. In *Actions Chimiques et Biologiques des Radiations*; M. Haissinsky, Ed.; Masson et Cie: Paris 1961; V^eme Serie, Chapter 3, pp 85–166.
14. Diffusion Kinetics. A. Kuppermann. *Nucleonics* **19**, 38 (1961).
15. Ion–Molecule Reactions in the Nitrogen–Deuterium System. D. A. Hutchinson, A. Kuppermann, and L. G. Pobo. In *Proceedings of ASTM Committee E14 on Mass Spectrometry*, Chicago, June 1961; pp 75–88.
16. Diffusion Kinetics in Radiation Chemistry. I. Generalized Formulation and Criticism of Diffusion Model. A. Kuppermann and G. G. Belford. *J. Chem. Phys.* **36**, 1412 (1962).
17. Diffusion Kinetics in Radiation Chemistry. II. One-Radical-One-Solute Model; Calculations. A. Kuppermann and G. G. Belford. *J. Chem. Phys.* **36**, 1427 (1962).
18. Application of Numerical Methods to the Theory of the Periodic Deviations in the Schottky Effect. G. G. Belford, A. Kuppermann, and T. E. Phipps. *Phys. Rev.* **128**, 524 (1962).
19. Determination of Electronic Energy Levels of Molecules by Low-Energy Electron Impact Spectroscopy. A. Kuppermann and L. M. Raff. *J. Chem. Phys.* **37**, 2497 (1962).
20. Differences Between Low-Energy Electron-Impact Spectra at 0° and at Large Scattering Angle. A. Kuppermann and L. M. Raff. *J. Chem. Phys.* **39**, 1607 (1963).
21. Electron-Impact Spectroscopy. A. Kuppermann and L. M. Raff. *Discuss. Faraday Soc.* **35**, 30 (1963).
22. Excited States Produced by Low-Energy Electrons. A. Kuppermann and L. M. Raff. In *Physical Processes in Radiation Biology*; Academic Press: New York 1964; pp 161–181.
23. Radiation Chemistry. A. Kuppermann. In *The Science of Ionizing Radiation*; L. E. Etter, Ed.; Charles C. Thomas: Springfield, IL, 1965; Chapter 10, pp 210–228.
24. Energy Threshold for the D + H₂ → DH + H Reaction. A. Kuppermann and J. M. White. *J. Chem. Phys.* **44**, 4352 (1966).
25. Diffusion Model of the Radiation Chemistry of Aqueous Solutions. A. Kuppermann. In *Radiation Research* 1966; G. Silini, Ed.; North-Holland: Amsterdam, 1967; pp 212–234.
26. Electron-Impact Excitation Cross Section for the Two Lowest Triplet States of Molecular Hydrogen. D. C. Cartwright and A. Kuppermann. *Phys. Rev.* **163**, 86 (1967).
27. Dynamics of Reaction of Monoenergetic Atoms in a Thermal Gas. A. Kuppermann, J. Stevenson, and P. O'Keefe. *Discuss. Faraday Soc.* **44**, 46 (1967).
28. Reaction of Monoenergetic Deuterium Atoms with Hydrogen Molecules. A. Kuppermann. In *Proceedings of the Nobel Symposium 5 on Fast Reactions in Primary Processes in Chemical Kinetics*; Stig Claesson, Ed.; Interscience: New York, 1967; pp 131–140.
29. Argon Resonance Line Lamp for Vacuum Ultraviolet Photochemistry. A. L. Lane and A. Kuppermann. *Rev. Sci. Instrum.* **39**, 126 (1968).
30. Differences in the Angular Dependencies of Spin- and Symmetry-Forbidden Excitation Cross Sections by Low-Energy Electron Impact Spectroscopy. J. K. Rice, A. Kuppermann, and S. Trajmar. *J. Chem. Phys.* **48**, 945 (1968).
31. Chemical Reaction Cross Sections and Rate Constants. E. F. Greene and A. Kuppermann. *J. Chem. Educ.* **45**, 361 (1968).
32. Vibrational Energy Transfer in Collisions Between Diatomic Molecules. M. E. Riley and A. Kuppermann. *Chem. Phys. Lett.* **1**, 537 (1968).
33. Formation of Positive and Negative Ions on Rhenium, Oxygenated Tungsten, Hafnium, Lanthanum Hexaboride, and Thoriated Tungsten Surfaces. A. Persky, E. F. Greene, and A. Kuppermann. *J. Chem. Phys.* **49**, 2347 (1968).
34. Triplet States of Acetylene by Electron Impact. S. Trajmar, J. K. Rice, P. S. P. Wei, and A. Kuppermann. *Chem. Phys. Lett.* **1**, 703 (1968).
35. Rearrangement Collisions: Effect of Core Terms, Non-orthogonality and Conservation of Particle Flux on Approximate Theories. D. G. Truhlar, D. C. Cartwright, and A. Kuppermann. *Phys. Rev.* **175**, 113 (1968).
36. A Low-Energy, High-Resolution Electron Impact Spectrometer. S. Trajmar, J. K. Rice, and A. Kuppermann. NASA-JPL Publication, Technical Memorandum 33-373, 1 March 1968.
37. Angular Dependence of Low-Energy Electron-Impact Excitation Cross Section of the Lowest Triplet States of H₂. S.

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- Trajmar, D. C. Cartwright, J. K. Rice, R. T. Brinkmann, and A. Kuppermann. *J. Phys. Chem.* **73**, 1722 (1969).
38. Low-Energy, High-Angle Electron-Impact Spectrometry. A. Kuppermann, J. K. Rice, and S. Trajmar. *J. Phys. Chem.* **72**, 3894 (1968).
 39. Applications of the Statistical Phase Space Theory to Reactions of Atomic Hydrogen with Deuterium Halides. D. G. Truhlar and A. Kuppermann. *J. Phys. Chem.* **73**, 1722 (1969).
 40. Instrumental Effects in a Retarding Field Energy Analyzer. P. S. P. Wei and A. Kuppermann. *Rev. Sci. Instrum.* **40**, 783 (1969).
 41. Reactive Collisions. A. Kuppermann. *Isr. J. Chem.* b, 303 (1969).
 42. Differential and Integral Cross Sections for Excitation of the 2^1P State of Helium by Electron Impact. D. G. Truhlar, J. K. Rice, A. Kuppermann, S. Trajmar, and D. C. Cartwright. *Phys. Rev. A* **1**, 778 (1970).
 43. Electron Impact Spectrometry. S. Trajmar, J. K. Rice, and A. Kuppermann. In *Advances in Chemical Physics*; I. Prigogine and S. A. Rice, Eds.; John Wiley and Sons: New York, 1970; pp 15–90.
 44. Differential Elastic Scattering of D_2 by N_2 in Crossed Molecular Beams. D. H. Winicur, A. L. Moursund, W. R. Devereaux, L. R. Martin, and A. Kuppermann. *J. Chem. Phys.* **52**, 3299 (1970).
 45. Quantum Mechanics of the $H + H_2$ Reaction: Exact Scattering Probabilities for Collinear Collisions. D. G. Truhlar and A. Kuppermann. *J. Chem. Phys.* **52**, 3841 (1970).
 46. Electron Scattering by H_2 With and Without Vibrational Excitation. III. Experimental and Theoretical Study of Inelastic Scattering. S. Trajmar, D. G. Truhlar, J. K. Rice, and A. Kuppermann. *J. Chem. Phys.* **52**, 4516 (1970).
 47. Puzzles in the Diffusion Kinetics of the Radiation Chemistry of Aqueous Solutions. A. Kuppermann. In *Proceedings of the International Meeting on Primary Effects in Chemistry and Biology*; National Atomic Energy Commission, Buenos Aires, Argentina, 1970; pp 104–122.
 48. Linear $H + H_2$: Exact and Approximate Reaction Probabilities. A. Kuppermann. In *Proceedings of the Conference on Potential Energy Surfaces in Chemistry*, University of California at Santa Cruz, 10–13 August 1970; W. A. Lester, Ed.; IBM Research Laboratory: San Jose, CA, 1971; pp 121–134.
 49. Exact Tunneling Calculations. D. G. Truhlar and A. Kuppermann. *J. Am. Chem. Soc.* **93**, 1840 (1971).
 50. Detection and Identification of Triplet States of H_2O by Electron Impact. S. Trajmar, W. Williams, and A. Kuppermann. *J. Chem. Phys.* **54**, 2274 (1971).
 51. A Test of Transition State Theory Against Exact Quantum Mechanical Calculations. D. G. Truhlar and A. Kuppermann. *Chem. Phys. Lett.* **9**, 269 (1971).
 52. Classical and Quantum Reaction Probabilities and Thermal Rate Constants for the Collinear $H + H_2$ Exchange Reaction with Vibrational Excitation. J. M. Bowman and A. Kuppermann. *Chem. Phys. Lett.* **12**, 1 (1971).
 53. Exact and Approximate Quantum Mechanical Reaction Probabilities and Rate Constants for the Collinear $H + H_2$ Reaction. D. G. Truhlar and A. Kuppermann. *J. Chem. Phys.* **56**, 2332 (1972).
 54. Angular Dependence of Electron Impact Excitation Cross Sections of O_2 . S. Trajmar, W. Williams, and A. Kuppermann. *J. Chem. Phys.* **56**, 3759 (1972).
 55. Comparison of Boundary-Value and Initial-Value Methods for the Accurate Quantum-Mechanical Solution of the Collinear Reactive Scattering Problem. D. J. Diestler, D. G. Truhlar, and A. Kuppermann. *Chem. Phys. Lett.* **13**, 1 (1972).
 56. Angular Distribution of Electrons from the Photoionization of Ethylene. D. C. Mason, A. Kuppermann, and D. M. Mintz. In *Electron Spectroscopy*; D. A. Shirley, Ed.; North-Holland: Amsterdam, 1972; pp 269–275.
 57. New Gas Lasers Committee Report on “Electronic Transition Chemically and Electrically Excited Lasers” (Report on Meeting held at The Aerospace Corporation, Los Angeles, California, 20–22 September 1972). Leroy E. Wilson et al. Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico, Technical Report No. AFWL-TR-73-60, May 1973.
 58. Interaction of Low-Energy Electrons with Molecules. A. A. Kuppermann. In *Advances in Radiation Research, Physics and Chemistry*; J. F. Duplan and A. Chapiro, Eds.; Gordon and Breach: London, 1973; pp 133–143.
 59. Electron Impact Excitation of H_2O . S. Trajmar, W. Williams, and A. Kuppermann. *J. Chem. Phys.* **58**, 2521 (1973).
 60. Large Quantum Effects in the Collinear $F + H_2 \rightarrow FH + H$ Reaction. G. C. Schatz, J. M. Bowman, and A. Kuppermann. *J. Chem. Phys.* **58**, 4023 (1973).
 61. String-Plucking Model for Vibrational Excitation of Molecules. R. J. Gordon and A. Kuppermann. *J. Chem. Phys.* **58**, 5776 (1973).
 62. Exact Quantum Mechanical Reaction Probabilities and Rate Constants for the Isotopic Collinear $H + H_2$ Reactions. D. G. Truhlar, A. Kuppermann, and J. T. Adams. *J. Chem. Phys.* **59**, 395 (1973).
 63. Role of Direct and Resonant (Compound State) Processes and Their Interference in the Quantum Dynamics of the Collinear $H + H_2$ Exchange Reaction. G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **59**, 964 (1973).
 64. Quantum Initial Conditions in Quasi-Classical Trajectory Calculations. J. M. Bowman, A. Kuppermann and G. C. Schatz. *Chem. Phys. Lett.* **19**, 21 (1973).
 65. Comparison of Semiclassical, Exact Quantum, and Quasi-Classical Reactive Transition Probabilities for the Collinear $H + H_2$ Reaction. J. M. Bowman and A. Kuppermann. *Chem. Phys. Lett.* **19**, 166 (1973).
 66. Triplet States in 1,3-Butadiene. O. A. Mosher, W. M. Flicker, and A. Kuppermann. *Chem. Phys. Lett.* **19**, 332 (1973).
 67. A Direct Test of the vibrationally Adiabatic Theory of Chemical Reactions. J. M. Bowman, A. Kuppermann, J. T. Adams, and D. G. Truhlar. *Chem. Phys. Lett.* **20**, 229 (1973).
 68. Use of Central-Field Potentials for Describing $H_2(D_2)$ Elastic Scattering by Other Molecules. R. J. Gordon, M. J. Coggiola, and A. Kuppermann. *Chem. Phys. Lett.* **20**, 493 (1973).
 69. Electronic Spectroscopy of s-trans 1,3-Butadiene by Electron Impact. O. A. Mosher, W. M. Flicker, and A. Kuppermann. *J. Chem. Phys.* **59**, 6502 (1973).
 70. Central-Field Intermolecular Potentials from the Differential Elastic Scattering of $H_2(D_2)$ by Other Molecules. A. Kuppermann, R. J. Gordon, and M. J. Coggiola. *Faraday Discuss. Chem. Soc.* **55**, 145 (1973).
 71. Semiclassical S Matrix Theory of Reactive and Nonreactive Atom-Molecule Collisions. J. M. Bowman and A. Kuppermann. *Chem. Phys.* **2**, 158 (1973).
 72. Comparison of Semiclassical, Quasiclassical and Exact Quantum Transition Probabilities for the Collinear $H + H_2$ Exchange Reaction. J. M. Bowman and A. Kuppermann. *J. Chem. Phys.* **59**, 6524 (1973).
 73. Violation of Microscopic Reversibility and the Use of Reverse Quasi-Classical Trajectories for Calculating Reaction

Cross Sections. J. M. Bowman, G. C. Schatz, and A. Kuppermann. *Chem. Phys. Lett.* **24**, 378 (1974).

74. Diffusion Kinetics in Radiation Chemistry: An Assessment. A. Kuppermann. In *Physical Mechanisms in Radiation Chemistry*; R. D. Cooper and R. W. Woods, Eds.; Technical Information Center, Office of Information Services, U.S. Atomic Energy Commission, 1974; pp 155–176.

75. An Apparatus for the Production of High Isotopic Purity Deuterium. A. Persky and A. Kuppermann. *J. Phys. E* **7**, 889 (1974).

76. Coplanar and Collinear Quantum Mechanical Reactive Scattering: The Importance of Virtual Vibrational Channels in the H + H₂ Exchange Reaction. A. Kuppermann, G. C. Schatz, and M. Baer. *J. Chem. Phys.* **61**, 4362 (1974).

77. Abstraction Fraction in the Reaction of Deuterium Atoms with HBr and HI. A. Persky and A. Kuppermann. *J. Chem. Phys.* **61**, 5035 (1974).

78. Electronic Spectroscopy of the Fluoroethylenes by Electron Impact. M. J. Coggiola, O. A. Mosher, W. M. Flicker, and A. Kuppermann. *Chem. Phys. Lett.* **27**, 14 (1974).

79. Electron Impact Spectroscopy of *trans*-Azomethane. O. A. Mosher, M. S. Foster, W. M. Flicker, A. Kuppermann, and J. Beauchamp. *Chem. Phys. Lett.* **29**, 236 (1974).

80. Automatic Mass-Spectrometric Analysis: Preliminary Report on Development of a Novel Mass-Spectrometric System for Biomedical Applications. W. J. Dreyer, A. Kuppermann, H. G. Boettger, C. E. Giffin, D. D. Norris, S. L. Grotch, and L. P. Theard. *Clin. Chem.* **20**, 998 (1974).

81. Quantum Mechanical Reactive Scattering: An Accurate Three-Dimensional Calculation. A. Kuppermann and G. C. Schatz. *J. Chem. Phys.* **62**, 2502 (1975).

82. Electronic Spectroscopy of Propadiene (Allene) by Electron Impact. O. A. Mosher, W. M. Flicker, and A. Kuppermann. *J. Chem. Phys.* **62**, 2600 (1975).

83. Angular Distributions in the Electron Impact Excitation of Xe at 20 eV. W. Williams, S. Trajmar, and A. Kuppermann. *J. Chem. Phys.* **62**, 3031 (1975).

84. Electronic Spectroscopy of *trans*-Azomethane by Electron Impact. O. A. Mosher, M. S. Foster, W. M. Flicker, J. L. Beauchamp, and A. Kuppermann. *J. Chem. Phys.* **62**, 3424 (1975).

85. Exact Quantum, Quasiclassical, and Semiclassical Reaction Probabilities for the Collinear F + H₂ → FH + H Reaction. G. C. Schatz, J. M. Bowman, and A. Kuppermann. *J. Chem. Phys.* **63**, 674 (1975).

86. Exact Quantum, Quasiclassical, and Semiclassical Reaction Probabilities for the Collinear F + D₂ → FD + D Reaction. G. C. Schatz, J. M. Bowman, and A. Kuppermann. *J. Chem. Phys.* **63**, 685 (1975).

87. A Useful Mapping of Triatomic Potential Energy Surfaces. A. Kuppermann. *Chem. Phys. Lett.* **32**, 374 (1975).

88. The Scattering of Excited by Ground-State Atoms. Application to He₂^{*}. B. Andresen and A. Kuppermann. *Mol. Phys.* **32**, 997 (1975).

89. A Semi-Numerical Approach to the Construction and Fitting of Triatomic Potential Energy Surfaces. J. M. Bowman and A. Kuppermann. *Chem. Phys. Lett.* **34**, 5213 (1975).

90. Dynamical Resonances in Collinear, Coplanar, and Three-Dimensional Quantum Mechanical Reactive Scattering. G. C. Schatz and A. Kuppermann. *Phys. Rev. Lett.* **35**, 1266 (1975).

91. Singlet → Triplet Transitions in Methyl-Substituted Ethylenes. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys. Lett.* **36**, 56 (1975).

92. Electron Impact Investigation of Electronic Excitation in Furan, Thiophene, and Pyrrole. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **64**, 1315 (1976).

93. Electron Impact Spectroscopy of the Fluoroethylenes. M. J. Coggiola, W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **65**, 2655 (1976).

94. Excited Electronic States of Ketene. R. P. Frueholz, W. M. Flicker, and A. Kuppermann. *Chem. Phys. Lett.* **38**, 57 (1976).

95. Progress in the Quantum Dynamics of Reactive Molecular Collisions. A. Kuppermann. In *The Physics of Electronic and Atomic Collisions* (Invited Lectures, Review Papers, and Progress Reports of the IXth International Conference on the Physics of Electronic and Atomic Collisions, Seattle, 24–30 July 1975); J. S. Ridley and R. Geballe, Eds.; University of Washington, Seattle, WA, 1976; pp 259–274.

96. Surface Functions for Three-Dimensional Reactive Scattering. R. T. Ling and A. Kuppermann. In *The Physics of Electronic and Atomic Collisions* (Abstracts of papers of the IXth International Conference on The Physics of Electronic and Atomic Collisions, Seattle, Washington, 24–30 July 1975); J. S. Ridley and R. Geballe, Eds.; University of Washington Press: Seattle, WA, 1976; pp 353–354.

97. Triplet States of Furan, Thiophene and Pyrrole. W. M. Flicker, O. A. Mosher and A. Kuppermann. *Chem. Phys. Lett.* **38**, 489 (1976).

98. Quantum Mechanical Reactive Scattering for Planar Atom Plus Diatom Systems. I. Theory. A. Kuppermann, G. C. Schatz, and M. Baer. *J. Chem. Phys.* **65**, 4596 (1976).

99. Quantum Mechanical Reactive Scattering for Planar Atom Plus Diatom Systems. II. Accurate Cross Sections for H + H₂. G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **65**, 4624 (1976).

100. Quantum Mechanical Reactive Scattering for Three-Dimensional Atom Plus Diatom Systems. I. Theory. G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **65**, 4642 (1976).

101. Quantum Mechanical Reactive Scattering for Three-Dimensional Atom Plus Diatom Systems. II. Accurate Cross Sections for H + H₂. G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **65**, 4668 (1976).

102. An Exact Quantum Study of Vibrational Deactivation by Reactive and Nonreactive Collisions in the Collinear Isotopic H + HF Systems. G. C. Schatz and A. Kuppermann. In *Proceedings of the Army Symposium on High Energy Transfer Lasers: Current Problems in High Energy Transfer Lasers*, Redstone Arsenal, Alabama, 3–4 November 1975; U. S. Army Missile Command, Redstone Arsenal, Alabama, August 1976, Special Report RF-7T-1, 132-142.

103. Large Quantum Effects in a Model Electronically Nonadiabatic Reaction: Ba + N₂O → BaO* + N₂. J. M. Bowman, S. C. Leisure, and A. Kuppermann. *Chem. Phys. Lett.* **43**, 374 (1976).

104. Validity of the Adiabatic Approximation for Vibrational Energy Transfer in Collisions Between Diatomic Molecules. J. P. Dwyer and A. Kuppermann. *Chem. Phys. Lett.* **44**, 499 (1976).

105. Variable Angle Photoelectron Spectrometer. D. C. Mason, D. M. Mintz, and A. Kuppermann. *Rev. Sci. Instrum.* **48**, 926 (1977).

106. The Importance of Isotope-Dependent Transmission Coefficients in Calculating Low-Temperature Isotope Effects. D. G. Truhlar, A. Kuppermann, and J. P. Dwyer. *Mol. Phys.* **33**, 683 (1977).

107. Classical Dynamics of Triatomic Systems: Energized Harmonic Molecules. C. A. Parr, A. Kuppermann, and R. N. Porter. *J. Chem. Phys.* **66**, 2914 (1977).
108. Angular Momentum Decoupling Approximations in the Quantum Dynamics of Reactive Systems. A. Kuppermann, G. C. Schatz, and J. P. Dwyer. *Chem. Phys. Lett.* **45**, 71 (1977).
109. Low Energy, Variable Angle Electron-Impact Excitation of 1,3,4-Hexatriene. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys. Lett.* **45**, 492 (1977).
110. Excited Electronic States of the Fluorobenzenes by Variable-Angle Electron Impact Spectroscopy. R. P. Frueholz, W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys. Lett.* **52**, 86 (1977).
111. Chemi-Ionization in K-I Collisions. I. Integral Cross Sections. B. Andresen, A. Kuppermann, and A. E. de Vries. *Z. Physik A* **289**, 1 (1978).
112. Chemi-Ionization in K-I Collisions. II. Differential Cross Sections. B. Andresen and A. Kuppermann. *Z. Phys. A* **289**, 11 (1978).
113. Doublet → Quartet Transitions in Nitric Oxide as Detected by Electron Impact Spectroscopy. R. P. Frueholz, R. Rianda, and A. Kuppermann. *J. Chem. Phys.* **68**, 775 (1978).
114. Electron-Impact Investigation of Excited Singlet States in 1,3-Butadiene. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys.* **30**, 307 (1978).
115. Doublet → Quartet Transitions in Nitric Oxide by Low-Energy, Variable-Angle Electron Scattering. R. P. Frueholz, R. Rianda, and A. Kuppermann. *Chem. Phys.* **30**, 315 (1978).
116. Excited Electronic States of 1,3,5-Cycloheptatriene. R. P. Frueholz, R. Rianda, and A. Kuppermann. *Chem. Phys. Lett.* **57**, 183 (1978).
117. Detection of a Second Triplet State in Thiophosgene by Electron-Impact Spectroscopy. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys. Lett.* **57**, 183 (1978).
118. Photoelectron Angular Distributions of Carbon–Carbon Pi Electrons in Ethylene, Benzene, and Their Fluorinated Derivatives. J. A. Sell, D. M. Mintz, and A. Kuppermann. *Chem. Phys. Lett.* **58**, 601 (1978).
119. An Accurate Determination of the He–Ar van der Waals Potential. M. Keil, A. Kuppermann, and J. T. Slankas. *Chem. Phys. Lett.* **59**, 339 (1978).
120. An Empirical Anisotropic Intermolecular Potential for He + CO₂. M. Keil, G. A. Parker, and A. Kuppermann. *Chem. Phys. Lett.* **59**, 443 (1978).
121. Electron-Impact Spectroscopy of the Alkynes: A Comparison of Propyne and 1-Butyne with Acetylene. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **69**, 3311 (1978).
122. Vibronic Structure of the Second Triplet State of 1,3,5-Hexatriene. R. P. Frueholz and A. Kuppermann. *J. Chem. Phys.* **69**, 3443 (1978).
123. Electronic Spectroscopy of 1,3,5,7-Cyclooctatetraene by Low-Energy, Variable-Angle Electron Impact. R. P. Frueholz and A. Kuppermann. *J. Chem. Phys.* **69**, 3614 (1978).
124. Electron-Impact Excitation of Low-Lying Electronic States in CS₂, OCS and SO₂. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **69**, 3910 (1978).
125. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. I. Sensitivity of the Elastic Differential Cross Section to the Interatomic Potential. M. Keil and A. Kuppermann. *J. Chem. Phys.* **69**, 3917 (1978).
126. Energy Dependence of the Differential Photoelectron Cross Sections of Molecular Nitrogen. D. M. Mintz and A. Kuppermann. *J. Chem. Phys.* **69**, 3953 (1978).
127. Angular Distributions in the Photoelectron Spectra of Benzene and Its Monohalogenated Derivatives. J. A. Sell and A. Kuppermann. *Chem. Phys.* **33**, 367 (1978).
128. Angular Distributions in the Photoelectron Spectroscopy of SF₆. J. A. Sell and A. Kuppermann. *Chem. Phys.* **33**, 379 (1978).
129. Electronic Spectroscopy of Polyatomic Molecules by Low-Energy, Variable-Angle Electron Impact. A. Kuppermann, W. M. Flicker, and O. A. Mosher. *Chem. Rev.* **79**, 77 (1979).
130. An Exact Quantum Mechanical Transition State Theory. I. An Overview. Aron Kuppermann. *J. Phys. Chem.* **83**, 171 (1979).
131. Angular Distributions in the Photoelectron Spectroscopy of Carbon Monoxide. J. A. Sell, A. Kuppermann, and D. M. Mintz. *J. Electron Spectrosc.* **16**, 127 (1979).
132. Investigation of Low-Lying Electronic States in Nitromethane by Electron-Impact Spectroscopy. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *Chem. Phys. Lett.* **60**, 518 (1979).
133. Angular Distributions in the Photoelectron Spectroscopy of Furan, Thiophene, and Pyrrole. J. A. Sell and A. Kuppermann. *Chem. Phys. Lett.* **61**, 355 (1979).
134. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. II. The He–Ar van der Waals Potential. M. Keil, J. T. Slankas, and A. Kuppermann. *J. Chem. Phys.* **70**, 482 (1979).
135. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. III. Anisotropic Intermolecular Potentials for He + N₂, O₂, CO, and NO. M. Keil, J. T. Slankas, and A. Kuppermann. *J. Chem. Phys.* **70**, 541 (1979).
136. Electronic Spectroscopy of UF₆ and WF₆ by Electron Impact. R. Rianda, R. P. Frueholz, and A. Kuppermann. *J. Chem. Phys.* **70**, 1056 (1979).
137. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. IV. Spherically Symmetric Intermolecular Potentials for He + CH₄, NH₃, H₂O, SF₆. J. T. Slankas, M. Keil, and A. Kuppermann. *J. Chem. Phys.* **70**, 1482 (1979).
138. Electronic Spectroscopy of Benzene and the Fluorobenzenes by Variable Angle Electron Impact. R. P. Frueholz, W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **70**, 3057 (1979).
139. Electron Spectroscopy of 1,3-Cyclopentadiene, 1,3-Cyclohexadiene, and 1,3-Cycloheptadiene by Electron Impact. R. P. Frueholz, W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **70**, 2003 (1979).
140. Excited Electronic States of Cyclohexene, 1,4-Cyclohexadiene, Norbornene, and Norbornadiene as Studied by Electron-Impact Spectroscopy. R. P. Frueholz, W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **70**, 1986 (1979).
141. Comment on “Theory of Collisions Between an Atom and a Diatomic Molecule in the Body-Fixed Coordinate System.” G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **70**, 3151 (1979).
142. Photoelectron Spectroscopy of Ethylene, Isobutylene, Trimethylethylene and Tetramethylethylene at Variable Angle. D. M. Mintz and A. Kuppermann. *J. Chem. Phys.* **71**, 3499 (1979).
143. Variable Angle Photoelectron Spectroscopy of the Fluoroethylenes. J. A. Sell and A. Kuppermann. *J. Chem. Phys.* **71**, 4703 (1979). 144.
144. Theoretical Aspects of the Mechanism of Simple Chemical Reactions. A. Kuppermann. In *Proceedings of the Summer School on Chemical Photophysics*, “Dynamique Re-

actionnelle des Etats Excités"; P. Glorieux, D. Lecler, and R. Vetter, Eds.; Les Houches, France, 18–20 June 1979; Editions du Centre National de la Recherche Scientifique: Paris, 1979; pp 298–384.

145. A Simple Model of Dynamic Resonances in Collinear Reactive Scattering. A. Kuppermann and J. P. Dwyer. In *Electronic and Atomic Collisions* (Abstracts of papers of the XIth International Conference on the Physics of Electronic and Atomic Collisions, Kyoto, August 1979); K. Takayanagi and N. Oda, Eds.; The Society for Atomic Collision Research, Japan, 1979; pp 888–889.

146. Vibrational Deactivation on Chemically Reactive Potential Surfaces: An Exact Quantum Study of a Low Barrier Collinear Model of $H + FH$, $D + FD$, $H + FD$, and $D + FH$. G. C. Schatz and A. Kuppermann. *J. Chem. Phys.* **72**, 2737 (1980).

147. Variable Angle Electron-Impact Excitation of Nitromethane. W. M. Flicker, O. A. Mosher, and A. Kuppermann. *J. Chem. Phys.* **72**, 2788 (1980).

148. Detection of the 3A_2 State of CS_2 by Multiphoton Ionization. R. Rianda, D. J. Moll, and A. Kuppermann. *Chem. Phys. Lett.* **73**, 469 (1980).

149. Hyperspherical Coordinates in Quantum Mechanical Collinear Reactive Scattering. A. Kuppermann, J. A. Kaye, and J. P. Dwyer. *Chem. Phys. Lett.* **74**, 257 (1980).

150. Collinear Quantum Mechanical Probabilities for the $I + HI \rightarrow IH + I$ Reaction Using Hyperspherical Coordinates. J. A. Kaye and A. Kuppermann. *Chem. Phys. Lett.* **77**, 573 (1981).

151. Accurate Quantum Calculations of Reactive Systems. A. Kuppermann. In *Theoretical Chemistry—Theory of Scattering: Papers in Honor of Henry Eyring*; D. Henderson, Ed.; Academic Press: New York, 1981; Vol. 6, Part A, Chapter 2, pp 79–164.

152. Few-Body Molecular Collisions: Theoretical. A. Kuppermann. *Nucl. Phys. A* **353**, 287c (1981).

153. Quantum Mechanical Coupled-Channel Collision-Induced Dissociation Calculations with Hyperspherical Coordinates. J. A. Kaye and A. Kuppermann. *Chem. Phys. Lett.* **78**, 546 (1981).

154. Reactive Scattering Resonances and Their Physical Interpretation: The Vibrational Structure of the Transition State. A. Kuppermann. In *Potential Energy Surfaces and Dynamics Calculations*; D. G. Truhlar, Ed.; Plenum Press: New York, 1981; pp 375–420.

155. Collision Lifetime Matrix Analysis of the First Resonance in the Collinear $F + H_2$ Reaction and its Isotopically Substituted Analogues. A. Kuppermann and J. A. Kaye. *J. Phys. Chem.* **85**, 1969 (1981).

156. A Physical Interpretation of the Collinear Reactive Scattering Resonances in the $F + HD$, H_2 , and D_2 Systems. V. K. Babamov and A. Kuppermann. *J. Chem. Phys.* **77**, 1891 (1982).

157. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. V. Anisotropic Intermolecular Potentials for $He + CO_2$, N_2O , C_2N_2 . G. A. Parker, M. Keil, and A. Kuppermann. *J. Chem. Phys.* **78**, 1145 (1983).

158. Collinear Quantum Mechanical Probabilities and Rate Constants for the $Br + HCl$ ($v = 2,3,4$) Reaction Using Hyperspherical Coordinates. J. A. Kaye and A. Kuppermann. *Chem. Phys. Lett.* **92**, 574 (1982).

159. Doublet → Quartet and Doublet → Doublet Electronic Transitions in NO_2 by Electron Impact. R. Rianda, R. P. Frueholz, and A. Kuppermann. *J. Chem. Phys.* **79**, 5914 (1983).

160. Singlet → Triplet Transitions in $C\equiv N$ Containing Molecules by Electron Impact. R. Rianda, R. P. Frueholz, and A. Kuppermann. *J. Chem. Phys.* **80**, 4035 (1984).

161. Photoacoustic Detection of Stimulated Emission Pumping in *p*-Difluorobenzene. D. J. Moll, G. R. Parker, Jr., and A. Kuppermann. *J. Chem. Phys.* **80**, 4800 (1984).

162. Time-Resolved Two-Color Photoacoustic and Multiphoton Ionization Spectroscopy of Aniline. D. J. Moll, G. R. Parker, Jr., and A. Kuppermann. *J. Chem. Phys.* **80**, 4808 (1984).

163. High-Energy Overtone Spectroscopy of Some Deuterated Methanes. J. W. Perry, D. J. Moll, A. Kuppermann, and A. H. Zewail. *J. Chem. Phys.* **82**, 1195 (1985).

164. An Electron-Impact Investigation of the Singlet → Triplet Transitions in the Chloro-Substituted Ethylenes. C. F. Koerting, K. N. Walzl, and A. Kuppermann. *Chem. Phys. Lett.* **109**, 140 (1984).

165. An Intense Beam of Metastable H_3 Molecules. J. F. Garvey and A. Kuppermann. *Chem. Phys. Lett.* **107**, 491 (1984).

166. Test of Variational Transition State Theory Against Accurate Quantal Results for a Reaction With a Very Large Reaction-Path Curvature and a Low Barrier. D. G. Truhlar, B. C. Garrett, P. G. Hipes, and A. Kuppermann. *J. Chem. Phys.* **81**, 3542 (1984).

167. Quantum Mechanical Partitioning of Kinetic Energy in Collision-Induced Dissociation. J. A. Kaye and A. Kuppermann. *Chem. Phys. Lett.* **115**, 158 (1985).

168. Quantum Mechanical Study of the Reaction $Be + FH$ ($v = 0,1$) → $BeF(v') + H$. J. F. Garvey, J. A. Kaye, and A. Kuppermann. *Chem. Phys. Lett.* **118**, 384 (1985).

169. Toward a State-To-State Transition State Theory. A. Kuppermann and R. D. Levine. *J. Chem. Phys.* **83**, 4 (1985).

170. Collinear Quasi-Classical Trajectory Study of Collision-Induced Dissociation on a Model Potential Energy Surface. J. A. Kaye and A. Kuppermann. *J. Chem. Phys.* **84**, 1463 (1986).

171. Hyperspherical Coordinate Formulation of the Electron-Hydrogen Atom Scattering Problem. D. M. Hood and A. Kuppermann. In *Theory of Chemical Reaction Dynamics*; D. C. Clary, Ed.; D. Reidel: Boston, 1986; pp 193–214.

172. A Test of the Babamov-Marcus vibrationally Adiabatic Theory of Hydrogen Atom Transfer Reactions. P. G. Hipes and A. Kuppermann. *J. Phys. Chem.* **90**, 3630 (1986).

173. Three-Dimensional Quantum Mechanical Reactive Scattering Using Symmetrized Hyperspherical Coordinates. A. Kuppermann and P. G. Hipes. *J. Chem. Phys.* **84**, 5962 (1986).

174. Design and Operation of a Stable Intense High-Temperature Arc-Discharge Source of Hydrogen Atoms and Metastable Trihydrogen Molecules. J. F. Garvey and A. Kuppermann. *Rev. Sci. Instrum.* **57**, 1061 (1986).

175. An Electron-Impact Spectroscopy Investigation of CH_3 and Some of Its Pyrolytic Precursors. K. N. Walzl, C. F. Koerting, I. M. Xavier, Jr., and A. Kuppermann. *J. Chem. Phys.* **86**, 88 (1987).

176. Total Scattering, Surface Ionization and Photoionization of a Beam of H_3 Metastable Molecules. J. Garvey and A. Kuppermann. *J. Chem. Phys.* **86**, 6766 (1987).

177. Lifetime Analysis of High Energy Resonances in Three-Dimensional Reactive Scattering. P. G. Hipes and A. Kuppermann. *Chem. Phys. Lett.* **133**, 1 (1987).

178. The Spectroscopy of the Group VIIb Transition Metal Hexacarbonyls Using the Electron Impact Method. C. F. Koerting, K. N. Walzl, and A. Kuppermann. *J. Chem. Phys.* **86**, 6646 (1987).

179. Electron-Impact Spectroscopy of Various Diketone Compounds. K. N. Walzl, I. M. Xavier, Jr., and A. Kuppermann. *J. Chem. Phys.* **86**, 6701 (1987).
180. Electron-Impact Spectroscopy of Acetaldehyde. K. N. Walzl, C. F. Koerting, and A. Kuppermann. *J. Chem. Phys.* **87**, 3796 (1987).
181. Quantum Mechanical Calculation of the Reactions $D + HF(v=0,1,2) \rightarrow DF(v') + H$ and $H + FD(v=0,1,2,3) \rightarrow HF(v') + D$ on a Realistic Potential Energy Surface. J. A. Kaye, A. Kuppermann, and J. P. Dwyer. *Chem. Phys.* **118**, 153 (1987).
182. Reply to Comment on "Total scattering, surface ionization and photoionization of a beam of H_3 metastable molecules." J. F. Garvey and A. Kuppermann. *J. Chem. Phys.* **88**, 5985 (1988).
183. Chemical Reaction Dynamics: Integration of Coupled Sets of Ordinary Differential Equations on the Caltech Hypercube. P. G. Hipes, T. Mattson, Y.-S. M. Wu, and A. Kuppermann. In *Proceedings of the Third Conference on Hypercube Concurrent Computers and Application*; G. C. Fox, Ed.; ACM Press: New York, 1988; pp 1051–1061.
184. Gauss-Jordan Inversion with Pivoting on the Caltech Mark II Hypercube. P. G. Hipes and A. Kuppermann. In *Proceedings of the Third Conference on Hypercube Concurrent Computers and Applications*; G. C. Fox, Ed.; ACM Press: New York, 1988; pp 1621–1634.
185. Observation and Analysis of Emission Spectra of Tungsten Hydride. J. F. Garvey and A. Kuppermann. *J. Phys. Chem.* **92**, 4583 (1988).
186. Mass Effect in Quantum Mechanical Collision-Induced Dissociation in Collinear Reactive Atom–Diatomic Molecule Collisions. J. A. Kaye and A. Kuppermann. *Chem. Phys.* **125**, 279 (1988).
187. Barrier Height Dependence of the Dynamics in the Collinear $HF(v) + H$ and $HF(v) + D$ Systems. J. A. Kaye, A. Kuppermann, and J. P. Dwyer. *J. Phys. Chem.* **92**, 6602 (1988).
188. Quantum Mechanical Calculations on the Systems $HF(v) + H$ and $HF(v) + D$ on a Realistic Potential Energy Surface. J. A. Kaye, A. Kuppermann, and J. P. Dwyer. *J. Phys. Chem.* **92**, 6595 (1988).
189. Collision Lifetime Matrix Analysis of the Two Lowest Energy Resonances in the Collinear $H + H_2$ System. J. A. Kaye and A. Kuppermann. *Chem. Phys.* **127**, 97 (1988).
190. The Use of Local Hyperspherical Surface Functions in Scattering Theory. A. Kuppermann. In *Microscopic Methods in Few Body Systems Theory*; A. M. Gorbatov, Ed.; Kalinin State University, Kalinin, USSR, 1988; Vol. 2, pp 128–134.
191. Hyperspherical Coordinate Reactive Scattering using Variational Surface Functions. S. A. Cuccaro, P. G. Hipes, and A. Kuppermann. *Chem. Phys. Letters* **154**, 155 (1989).
192. Symmetry Analysis of Accurate $H + H_2$ Resonances For Low Partial Waves. S. A. Cuccaro, P. G. Hipes, and A. Kuppermann. *Chem. Phys. Lett.* **157**, 440 (1989).
193. Calculation of Bound Rovibrational States on the First Electronically Excited State of the H_3 System. B. Lepetit, Z. Peng, and A. Kuppermann. *Chem. Phys. Lett.* **166**, 572 (1990).
194. Numerical Study of the Geometric Phase in the $H + H_2$ Reaction. B. Lepetit and A. Kuppermann. *Chem. Phys. Lett.* **166**, 581 (1990).
195. Quantum Mechanical Reactive Scattering Using a High-Performance Distributed-Memory Parallel Computer. M. Y.-S. Wu, S. A. Cuccaro, P. G. Hipes, and A. Kuppermann. *Chem. Phys. Lett.* **168**, 429 (1990).
196. Excited Electronic Potential Energy Surfaces and Transition Moments for the H_3 System. Z. Peng, J. S. Wright, and A. Kuppermann. *Chem. Phys. Lett.* **175**, 242 (1990).
197. Quantum Chemical Reaction Dynamics on a Highly Parallel Supercomputer. Y.-S. M. Wu, S. A. Cuccaro, P. G. Hipes, and A. Kuppermann. *Theor. Chim. Acta* **79**, 225 (1991).
198. Theoretical Calculation of Experimentally Observable Consequences of the Geometric Phase on Chemical Reaction Cross Sections. Y.-S. M. Wu, A. Kuppermann, and B. Lepetit. *Chem. Phys. Lett.* **186**, 319 (1991).
199. Prediction of the Effect of the Geometric Phase on Product Rotational State Distributions and Integral Cross Sections. Y.-S. M. Wu and A. Kuppermann. *Chem. Phys. Lett.* **201**, 178 (1993).
200. The Geometric Phase Effect Shows Up in Chemical Reactions. A. Kuppermann and Y.-S. M. Wu. *Chem. Phys. Lett.* **205**, 577 (1993); erratum, **213**, 636 (1993).
201. A New Look at Symmetrized Hyperspherical Coordinates. A. Kuppermann. In *Advances in Molecular Vibrations and Collision Dynamics*. J. Bowman, Ed.; JAI: Greenwich, CT, 1994; Vol. 2B, pp 117–186.
202. The Importance of the Geometric Phase Effect for the $H + D_2 \rightarrow HD + D$ Reaction. Y.-S. M. Wu and A. Kuppermann. *Chem. Phys. Lett.* **235**, 105 (1995).
203. The Quantitative Prediction and Lifetime of a Pronounced Reactive Scattering Resonance. A. Kuppermann and Y.-S. M. Wu. *Chem. Phys. Lett.* **241**, 229 (1995); erratum, **243**, 586 (1995).
204. Excited Electronic Potential-Energy Surfaces and Transition Moments for the H_3 System. Z. W. Peng, S. Kristyan, A. Kuppermann, and J. S. Wright. *Phys. Rev. A* **52**, 1005 (1995).
205. Reactive Scattering with Row-Orthonormal Hyperspherical Coordinates. I. Transformation Properties and Hamiltonian for Triatomic Systems. A. Kuppermann. *J. Phys. Chem.* **100**, 2621 (1996).
206. Hyperspherical Coordinates in Reactive Scattering Theory. A. Kuppermann. *New Methods in Quantum Theory*; C. A. Tsipis, V. S. Popov, D. R. Herschbach, and J. S. Avery, Eds.; Kluwer: Dordrecht, The Netherlands, 1996; pp 501–529.
207. The Geometric Phase in Reaction Dynamics. A. Kuppermann. *Dynamics of Molecules and Chemical Reactions*; R. E. Wyatt and J. Z. H. Zhang, Eds.; Marcel Dekker: New York, 1996; pp 411–472.
208. Reactive Scattering with Row-Orthonormal Hyperspherical Coordinates. 2. Transformation Properties and Hamiltonian for Tetraatomic Systems. A. Kuppermann. *J. Phys. Chem.* **101**, 6368 (1997).
209. On the Geometric Phase Effect on Tetra-Atomic Reactions: The $OH + H_2 \rightarrow H_2O + H$ Reaction. G. D. Billing and A. Kuppermann. *Chem. Phys. Lett.* **294**, 26 (1998).
210. A Very High Accuracy Potential Energy Surface for H_3 . Y.-S. M. Wu, A. Kuppermann, and J. B. Anderson. *Phys. Chem. Chem. Phys.* **1**, 929 (1999).
211. Chemically Accurate ab Initio Potential Energy Surfaces for the Lowest $^3A'$ and $^3A''$ Electronically Adiabatic States of $O(^3P) + H_2$. Stephanie Rogers, Desheng Wang, Aron Kuppermann, and Stephen Walch. *J. Phys. Chem. A* **104**, 2308 (2000).
212. A Quantum and Semiclassical Study of Dynamical Resonances in the $CNO \rightarrow CN + O$ Reaction. R. Abrol, L. Wiesenfeld, B. Lambert, and A. Kuppermann. *J. Chem. Phys.*, in press.