Publications of Max Wolfsberg

1. Transient Structures and Kinetics of the Ferrioxalate Redox Reaction Studied by Time-Resolved EXAFS, Optical Spectroscopy, and DFT, J. Chen, H. Zhang, I. V. Tomov, M. Wolfsberg, X. Ding and P. M. Rentzepis, *J. Phys. Chem. A*, 111, 9326 (2007).

2. A Steric Deuterium Isotope Effect in 1,1,3,3-Tetramethylcyclohexane, M. Saunders, M. Wolfsberg, F. A. L. Anet and O. Kronja, *J. Am. Chem. Soc.* 129, 10276 (2007).

3. Isotope Effects on VLE Properties of Fluids and Corresponding States: Critical Point Shifts on Isotopic Substitution, W. A. Van Hook, L. P. N. Rebelo and M. Wolfsberg, *Fluid Phase Equil.* 257, 35 (2007).

4. Isotope Effects in Chemistry and Biology, M. Wolfsberg, A. Kohen and H. H. Limbach, Eds., Taylor Francis (CRC Press) 2006, Comments on Selected Topics in Isotope Theoretical Chemistry; p 89.

5. The Importance of Various Degrees of Freedom in the Theoretical Study of the Diffusion of Methane in Silicalite-1, S. Fritzsche, M. Wolfsberg and R. Haberlandt, *Chem. Phys.* 289, 321 (2003).

6. Isotope Effects on Vapor Phase Second Virial Coefficients, W. A. Van Hook, L. P. N. Rebelo and M. Wolfsberg, *Nukleonika* 47, 547 (2002).

7. An Interpretation of the Vapor Phase Second Virial Coefficient Isotope Effect: Correlation of Virial Coefficient and Vapor Pressure Isotope Effects, W. A. Van Hook, L. P. N. Rebelo and M. Wolfsberg, *J. Phys. Chem. A* 105, 9284 (2001).

8. The Mutual Influence of Dynamic Processes Acting in Different Time Scales, S. Fritzsche, R. Haberlandt, A. Schuring and M. Wolfsberg, *Stud. Surf. Sci. Catal.* 135, 268 (2001).

9. Equilibration of the Kinetic Energy in Small Zeolite Cavities. The Thermalization Effect of Lattice Vibrations and of Mutual Interaction in the Diffusion of Methane in a Cation-Free LTA Zeolite. S. Fritzsch, R. Haberlandt and M. Wolfsberg, *Chem. Phys*. 253, 283 (2000).

10. About the Influence of Lattice Vibrations on the Diffusion of Methane in a Cation-Free LTA Zeolite, S. Fritzsche, M. Wolfsberg, R. Haberlandt, P. Demontis, G. B. Suffrittti and A. Tiloca, *Chem. Phys. Lett.* 296, 253 (1998).

11. $^{12}C/^{13}C$ Kinetic Isotope Effects in the Reactions of CH_4 with OH and Cl. l, M. L. Gupta, P. M. McGrath, R. J. Cicerone, F. S. Rowland and M. Wolfsberg, *Geophys. Res. Lett.* 24, 2761 (1997).

12a. An MD Study on the Diffusion of Methane in a Cation-Free LTA Zeolite. Illustrations and New Results, S. Fritzsche, R. Haberlandt, G. Hofmann, J. Kaerger and M. Wolfsberg, *Chem. Phys. Lett.* 265, 253 (1997).

12b. Methane Diffusion in Zeolites of Structure Type LTA in Dependence on Physical And Chemical Parameters - An MD Study, S. Fritsche, M. Gaub, R. Haberlandt, G. Haberlandt, G. Hofmann, J. Kaerger, and M. Wolfsberg, Progress in Zeolite and Microporous Materials, PTS A-C, Book Series Studies in *Surf. Sci. Catal.* 105, 1859 (1997).

13. Influence of Exchangeable Cations on the Diffusion of Neutral Diffusants in Zeolites of type LTA - An MD Study, S. Fritzsche, R. Haberlandt, J. Karger, H. Pfeifer, K. Heinzinger and M. Wolfsberg, *Chem. Phys. Lett.* 242, 361 (1995).

14. Application of the MUSIC Method for Spectral Estimation to a Model System, D. Kleinhesselink and M. Wolfsberg, *Chem. Phys. Lett.* 205, 461 (1993).

15. Cycloaddition of Acrylonitrile to Allene-Computed Reaction Path (AM1) and Intramolecular and Secondary Isotope Effect, E. A. Halevi and M. Wolfsberg, *J. Chem. Soc., Perkin Trans. 2*, 1493 (1993).

16. Comments on H/D Isotope Effects on Polarizabilities of Small Molecules. Correlation with Virial Coefficient, Molar Volume, and Electronic Second Moment Isotope Effects, A. W. Van hook and M. Wolfsberg, *Z. Naturforsch.* 49a, 5663 (1994).

17. Variational Calculations on Ammonia using Two Symmetrical Normal Modes, M. J. Huang and M. Wolfsberg, *Int. J. Quantum Chem.* 25, 441 (1991).

18. Computer-Simulation Studies of IR Laser Excitation of Water on a Metal-Surface, E. Spohr and M. Wolfsberg, *Surf. Sci.* 253, L395 (1991).

19. Molecular-Dynamics Consideration of the Mutual Thermalization of Guest Molecules in Zeolites, S. Fritzsche, R. Haberlandt, J. Kaerger and M. Wolfsberg, *Chem. Phys. Lett.* 171, 109 (1990).

20. Entropy and Degenerate Rearrangements, E. Spohr and M. Wolfsberg, *J. Phys. Chem.* 94, 6511 (1990).

21. Computer-Simulation Studies of the Adsorption of Water on a Metal-Surface, E. Spohr, P. Bopp and M. Wolfsberg, *Z. Naturforsch.* 46a, 174 (1991).

22. The Evaluation of Power Spectra in Molecular-Dynamics Simulations of Anharmonic Solids and Surfaces, D. Kleinhesselink and M. Wolfsberg, *Surf. Sci.* 262, 189 (1992).

23. Vibrational and Rotational-Excitation in Collisions of Diatomic Molecules with Rigid Surfaces, E. Spohr and M. Wolfsberg, *Chem. Phys. Lett.* 165, 221 (1990).

24. Theoretical Calculation of Equilibrium Isotope Effects using *ab initio* Force-Constants-Application to NMR Isotopic Perturbation Studies, M. Saunders, K. E. Laidig and M. Wolfsberg, *J. Am. Chem. Soc.* 111, 8989 (1989).

25. Evaluation of Isotope Effects on Henry Law Constants by a Molecular-Dynamics Technique, L. X. Dang, P. Bopp and M. Wolfsberg, *Z. Naturforsch.* 44a, 485 (1989).

26. Calculation of Equilibrium Isotope Effects in a Conformationally Mobile Carbocation, M. Saunders, G. W. Cline and M. Wolfsberg, *Z. Naturforsch.* 44a, 480 (1989).

27. A Note on Some Reported C-Isotope and N-Isotope Effects, D. Marx, D. Kleinhesselink and M. Wolfsberg, *J. Am. Chem. Soc.* 111, 1493 (1989).

28. The Accurate Evaluation of an Equilibrium Isotope Effect Involving Diatomic-Molecules. C. L. Chen and M. Wolfsberg, *Isotopenpraxis* 23, 205 (1987).

29. A Numerical Test on the Equivalence of Intramolecular Potential Expansions in Normal and Valence Displacement Coordinates for H_2O, B. Maessen, M. Wolfsberg and L. B. Harding, *J. Phys. Chem.* 89, 3324 (1985).

30. Variational Calculations of Rotational−Vibrational Energy Levels of Formaldehyde-X^1A_1, B. Maessen and M. Wolfsberg, *J. Phys. Chem.* 89, 3876 (1985).

31. Variational Calculations of Rotational−Vibrational Energy-Levels of Water, C. L. Chen, B. Maessen and M. Wolfsberg, *J. Chem. Phys.* 83, 1795 (1985).

10.1021/jp9004373 CCC: $40.75
Published on Web 03/05/2009

32. An Improved Variational Calculation of the Lower Vibrational Energy Levels of the Ammonia Molecule, B. Maessen, P. Bopp, D. R. Mclaughlin and M. Wolfsberg, *Z. Naturforsch.* 39a, 1005 (1984).

33. Vibrational Calculations on Formaldehyde with Improved Force-Fields, B. Maessen and M. Wolfsberg, *J. Phys. Chem.* 88, 6420 (1984).

34. The Dissection of Carbon and Hydrogen Isotope Effects in the Alkanes, M. Wolfsberg, *ZfI Mitt.* 85, 354 (1984).

35. Tunneling in the Automerization of Cyclobutadiene, M. J. Huang and M. Wolfsberg, *J. Am. Chem. Soc.* 106, 4034 (1984).

36.Variational Calculation of Lower Vibrational-Energy Levels of Formaldehyde X^1A_1, B. Maessen and M. Wolfsberg *J. Chem. Phys.* 80, 4651 (1984).

37. The Vibrational-Spectrum of H_2O on Si(100), J. E. Black, P. Bopp and M. Wolfsberg, *Surf. Sci.* 134, 257 (1983).

38. Estimates of Dielectric Shifts in Infrared-Spectra of Pure Liquids for use in the Theoretical Evaluation of Vapor Pressure Isotope Effects, B. Maessen and M. Wolfsberg, *Z. Naturforsch.* 38a, 191 (1983).

39. A Molecular-Model for Dielectric Shifts in Infrared-Spectra of Pure Condensed Liquid Phase and Vapor Pressure Isotope Effects, M. Wolfsberg, *J. Chem. Phys.* 80, 3087 (1984).

40. The Calculation of Vibrational Frequencies of Atoms Adsorbed on Metal Surfaces: H, O and S. on Ni(100) and Ni(111) as Examples, J. E. Black, P. Bopp, K. Lutzenkirchen and M. Wolfsberg, *J. Chem. Phys*. 76, 6431 (1982).

41. Dielectric Effects on the Spectra of Condensed Phases, J. W. Warner and M. Wolfsberg, *J. Chem. Phys.* 78, 1722 (1983).

42. Variational Calculation of the Lower Vibrational-Energy Levels of the Ammonia Melecule, P. Bopp, D. R. Mclaughlin and M. Wolfsberg, *Z. Naturforsch.* 37a, 398 (1982).

43. Evaluation of the Equilibrium-Constant For $H_2O + D_2O = 2HDO$ by Direct Summation over Rotational−Vibrational States, C. L. Chen, P. Bopp and M. Wolfsberg, *J. Chem. Phys*. 77, 579 (1982).

44. The Theoretical Analysis of Isotope Effects "Stable Isotopes", M. Wolfsberg, H. L. Schmidt, H. Forstel and K. Heinzinger, Eds., Elsevier (Amsterdam) 1982; p 3.

45. The Influence on Isotope Effect Calculations of the Method of Obtaining Force-Constants from Vibrational Data, D. Z. Goodson, S. K. Sarpal, P. Bopp and M. Wolfsberg. *J. Phys. Chem.* 86, 659 (1982).

46. Comments on a Model for Isotope Effects on Henry Law Constants in Aqueous-Solution, P. Bopp and M. Wolfsberg, *J. Sol. Chem*. 10, 357 (1981).

47. The Complete Wave Equation of a NonLinear Polyatomic Molecule, F. Webster, M. J. Huang and M. Wolfsberg, *J. Chem. Phys*. 75, 2306 (1981).

48. Direct Calculation of Equilibrium-Constants for Isotopic Exchange-Reactions by *ab initio* Molecular-Orbital Theory, R. F. Hout, M. Wolfsberg and W. J. Hehre, *J. Am. Chem*. 102, 3296 (1980).

49. Convergence of a Perturbation Technique for Evaluating Isotopic Partition-Function Ratios, C. E. Harvie, P. Bopp and M. Wolfsberg, *J. Chem. Phys*. 72, 6349 (1980).

50. Anomalies in the Fractionation by Chemical-Equilibrium of $^{18}O-^{16}O$ Relative to $^{17}O-^{16}O$, S. Skaron and M. Wolfsberg, *J. Chem. Phys*. 72, 6810 (1980).

51. Role of Hyperconjugation in Secondary Beta-Deuterium Isotope Effects, D. J. Defrees, M. Taagepera, B. A. Levi, S. K. Pollack, K. D. Summerhays, R. W. Taft, M. Wolfsberg, and W. J. Hehre, *J. Am. Chem*. 101, 5532 (1979).

52. Calculation of Vibrational Mean-Square Amplitudes of Molecular Internal Coordinates by a Perturbation-Theory Technique, M. Wolfsberg and E. A. Peter, *J. Chem. Phys*. 70, 5722 (1979).

53. Effect of Vibrational Anharmonicity on the Equilibrium $H_2O + D_2O = 2HDO$, M. Wolfsberg, *J. Chem. Phys*. 70, 5322 (1979).

54. Dissection of $^{13}C/^{12}C$ Isotope Effects on the Cyanoacetylene Partition-Function, P. Bopp, K. Heinzinger and M. Wolfsberg, Z. *Naturforsch.* 33a, 1562 (1978).

55. Theoretical Evaluation of the Distribution of ^{13}C in Cyanoacetylene at Thermodynamic-Equilibrium, M. Wolfsberg, P. Bopp and K. Heinzinger, *Astron. Astrophys.* 74, 369 (1979).

56. The Effects of Electron Correlation on Adiabatic Correction and on Equilibrium-Constants for Isotopic Exchange-Reactions, R. D. Bardo, L. I. Kleinman, A. W. Raczkowski and M. Wolfsberg, *J. Chem. Phys*. 69, 1106 (1978).

57. Calculation of one-Electron Properties From Scf-X-α-Sw Functions for H_2O, S. B. Woodruff and M. Wolfsberg, *Chem. Phys. Lett.* 56, 125 (1978).

58. A Priori Calculations on Isotopic Exchange Equilibria, D. J. Defrees, D. Z. Hassner, W. J. Hehre and M. Wolfsberg, *J. Am. Chem. Soc.* 100, 641 (1978).

59. The Adiabatic Correction for Nonlinear Triatomic-Molecules-Techniques and Calculations, R. D. Bardo and M. Wolfsberg, *J. Chem. Phys*. 68, 2686 (1978).

60. Further Empirical Testing of Suitability of a Nonrandom Integration Method for Classical Trajectory Calculations, H. H. Suzukawa and M. Wolfsberg, *J. Chem. Phys*. 68, 1423 (1978).

61. The Wave-Equation of a Nonlinear Triatomic Molecule and Adiabatic Correction to Born−Oppenheimer Approximation, R. D. Bardo and M. Wolfsberg, *J. Chem. Phys*. 67, 593 (1977).

62. Quasiclassical Trajectory Study of Energy-Transfer in CO_2 Rare Gas Systems, H. H. Suzukawa, M. Wolfsberg and D. L. Thompson, *J. Chem. Phys*. 68, 455 (1978).

63. The calculation of Isotopic Partition-Functions Ratios by a Perturbation-Theory Technique. 2. Dissection of Isotope Effect, S. A. Skaron and M. Wolfsberg, *J. Am. Chem. Soc.* 99, 5253 (1977).

64. Numerical-Calculation of One-Electron Properties from SCF-Xα-SW Wave functions for LiH, S. B. Woodruff and M. Wolfsberg, *J. Chem. Phys*. 65, 3687 (1976).

65. Isotope-Effects on Gas-Phase Reaction Processes. I. The Determination of Equilibrium Isotope-Effects by Ion-Cyclotron Resonance Spectroscopy, J. F. Wolf, J. L. Devlin, R. W. Taft, M. Wolfsberg and W. J. Hehre, *J. Am. Chem. Soc.* 98, 287 (1976).

66. Theoretical Calculation of Equilibrium-Constant for Isotopic Exchange-Reaction between H_2O and HD, R. D. Bardo and M. Wolfsberg, *J. Phys. Chem*. 80, 1068 (1976).

67. Nuclear Mass Dependence of Adiabatic Correction to Born−Oppenheimer Approximation, R. D. Bardo and M. Wolfsberg, *J. Chem. Phys*. 62, 4555 (1975).

68. Calculation of Isotopic Partition-Function Ratios by a Perturbation-Theory Technique, G. Singh and M. Wolfsberg, *J. Chem. Phys*. 62, 4165 (1975).

69. Corrections to Born−Oppenheimer Approximation in Calculation of Isotope-Effects on Equilibrium-Constants, M. Wolfsberg and L. I. Kleinman, *ACS Symp. Ser.* 11, 64 (1975).

70. Adiabatic Correction to van der Waals Well Depth of He_2, L. I. Kleinman and M. Wolfsberg, *J. Chem. Phys*. 61, 4366 (1974).

71. Shifts in Vibrational Constants from Corrections to the Born−Oppenheimer Approximation: Effects on Isotopic-Exchange Equilibria, L. I. Kleinman and M. Wolfsberg, *J. Chem. Phys*. 60, 4749 (1974).

72. Corrections to Born−Oppenheimer Approximation and Electronic Effects on Isotopic-Exchange Equilibria. II, L. I. Kleinman and M. Wolfsberg, *J. Chem. Phys*. 60, 4740 (1974).

73. Isotopic Partition-Function Ratios Involving H_2, H_2O, H_2S, H_2Se, and NH_3, J. Bron, C. F. Chang and M. Wolfsbeg, *Z. Naturforsch.* 28a, 129 (1973).

74. Empirical Testing of Suitability of a Nonrandom Integration Method for Classical Trajectory Calculations-Comparisons with Monte-Carlo Techniques, H. H. Suzukawa, D.L. Thompson, V. B. Cheng and M. Wolfsberg, *J. Chem. Phys*. 59, 4000 (1973).

75. Investigations of a Nonrandom Numerical-Method for Multidimensional Integration, V. B. Cheng, H. H. Suzukawa and M. Wolfsberg, *J. Chem. Phys*. 59, 3992 (1973).

76. Corrections to the Born−Oppenheimer Approximation and Electronic Effects on Isotopic-Exchange Equilibria, L. I. Kleinman and M. Wolfsberg, *J. Chem. Phys*. 59, 2043 (1973).

77. Heavy-Atom Kinetic Isotope Effects, M. Stern and M. Wolfsberg, NBS Special Publication 349, June (1972).

78. Effect of Vibrational Anharmonicity on Hydrogen−Deuterium Exchange Equilibria Involving Ammonia Molecules, J. Bron and M. Wolfsberg, *J. Chem. Phys*. 57, 2862 (1972).

79. Theoretical Evaluation of Experimentally Observed Isotope Effects, M. Wolfsberg, *Acc. Chem. Res.* 5, 225 (1972).

80. Gaussian Molecular Orbital Calculations of Hyperconjugation in Ethyl Cation, L. J. Massa, S. Ehrenson and M. Wolfsberg, *Chem. Phys. Lett.* 11, 196 (1971).

81. Effect of Vibrational Anharmonicity on Isotopic Self-Exchange Equilibria $H_2X + D_2X = 2HDX$, M. Wolfsberg, A. A. Massa and J. W. Pyper, *J. Chem. Phys*. 53, 3138 (1970).

82. Exact Classical Calculations on Collisional Energy Transfer to Diatomic Molecules with a Rotational and a Vibrational Degree of Freedom, J. D. Kelley and M. Wolfsberg, *J. Chem. Phys*. 53, 2967 (1970).

83a. Gaussian Molecular Orbital Calculations of the Barrier to Internal Rotation in the Ethyl Cation, L. J. Massa, S. Ehrenson and M. Wolfsberg, *Int. J. Quantum Chem.* 4, 625 (1970).

83b. Gaussian Molecular Orbital Calculations on Hyperconjugation in Ethyl Cation, L. J. Massa, S. Ehrenson, M. Wolfsberg, and C. A. Frishberg, *Chem. Phys. Lett.* 11, 196 (1971).

84. Isotope Effects. M. Wolfsberg, *Annu. Rev. Phys. Chem.* 20, 449 (1969).

85. Simple Expression for Steric Factor in Translational Vibrational Energy Transfer, J. D. Kelley and M. Wolfsberg, *J. Chem. Phys*. 50, 1894 (1969).

86. Solvolytic α-Deuterium Effects for Different Leaving Groups, V. J. Shiner, M. W. Rapp, E. A. Halevi and M. Wolfsberg, *J. Am. Chem. Soc.* 90, 7171 (1968).

87. Correction to Effect of Anharmonicity on Isotopic Exchange Equilibria, M. Wolfsberg, *Adv. Chem. Ser.* 89, 185 (1969).

88. Comment on "Physical Properties of Fluid CH_4 and CD_4: Theory", J. Bigeleis and M. Wolfsberg, *J. Chem. Phys*. 50, 561 (1969).

89. Correction to the Effect of Anharmonicity on Isotopic Exchange Equilibria-Application to Polyatomic Molecules, M. Wolfsberg, *J. Chem. Phys*. 50, 1484 (1969).

90. A Comment on the Steric Factor Approach Translational−Vibrational Energy Transfer, J. D. Kelley and M. Wolfsberg, *J. Phys. Chem.* 71, 2373 (1967).

91. Comment on the Calculation of "Temperature-Independent Factor" in Isotopic Rate-Constant Ratios, M. J. Stern, M. Wolfsberg and C. R. Gatz, *J. Chem. Phys*. 46, 823 (1967).

92. Simplified Procedure for Theoretical Calculation of Isotope Effects Involving Large Molecules, M. J. Stern and M. Wolfsberg, *J. Chem. Phys*. 45, 4105 (1966).

93. Exact Semiclassical Calculations of Translational Vibrational Energy Transfer, J. D. Kelley and M. Wolfsberg, *J. Chem. Phys*. 45, 3881 (1966).

94. Dependence of Vertical Excitation Energy of Benzene on Size and Force Constant of Excited State, S. Ehrenson and M. Wolfsberg, *J. Chem. Phys*. 45, 3879 (1966).

95. On the Absence of Isotope Effects in the Absence of Force Constant Changes, M. J. Stern and M. Wolfsberg, *J. Chem. Phys*. 45, 2618 (1966).

96. Comparison of Approximate Translational-Vibrational Energy-Transfer Formulas with Exact Classical Calculations, J. D. Kelley and M. Wolfsberg, *J. Chem. Phys*. 44, 324 (1966).

97. Isotope Effects as Tools for Elucidation of Reaction Mechanisms-Predictions from Model Calculations, M. J. Stern and M. Wolfsberg, *J. Pharm. Sci.* 54, 849 (1965).

98. Note on Ponderal Effects in Equilibria, M. Wolfsberg, *Tetrahedron Lett.* 46, 3405 (1964).

99. The Influence of Bond Making and Bond Breaking on Hydrogen Isotope Effects in Linear Three Centre Reactions, A. V. Willi and M. Wolfsberg, *Chem. Ind.* 51 2097 (1964). 33.

100. Approximations to Energy-Level Distributions, C. Lifshitz and M. Wolfsberg, *J. Chem. Phys*. 41, 1879 (1964).

101. Validity of Some Approximation Procedures Used in the Theoretical Calculation of Isotope Effects, M. Wolfsberg and M. J. Stern, *Pure Appl. Chem.* 8, 225 (1964).

102. Secondary Isotope Effects as Probe for Force Constant Changes, M. Wolfsberg, *Pure Appl. Chem.* 8, 325 (1964)

103. Theoretical Considerations on Carbon Isotope Effects in Decarboxylation of Malonic Acid, M. J. Stern and M. Wolfsberg, *J. Chem. Phys*. 39, 2776 (1963).

104. Isotope Effects on Internal Frequencies in Condensed Phase Resulting from Interactions with Hindered Translations and Rotations. The Vapor Pressures of the Isotopic Ethylenes. M. J. Stern, W. A. Van Hook and M. Wolfsberg, *J. Chem. Phys.* 39, 3179 (1963).

105. Calculation of Zero-Point Energies of Molecules by Perturbation Methods, M. Wolfsberg, *Z. Naturforsch.* 18a, 216 (1963).

106. Note on the Calculation of Zero-Point Energies and Isotopic Zero Point Energy Differences by a Taylors Series Expansion, J. Bigeleisen, M. Wolfsberg and R. E. Weston, *Z. Naturforsch., A: Astrophys., Phys., Phys. Chem.* 18, 210 (1963).

107. Isotope Effects on Intermolecular Interactions and Isotopic Vapor Pressure Differences, M. Wolfsberg, *J. Chim. Phys. Phys. Chim. Biol.* 60, 15 (1963); Erratum 61, 450 (1964).

108. Temperature Dependence of Carbon Isotope Effect in Dehydration of Formic Acid by Concentrated Sulfuric Acid, J. Bigeleisen, P. E. Yankwich, R. H. Haschemeyer and M Wolfsberg, *J. Am. Chem. Soc.* 84, 1813 (1962).

109. Rate Constants for Unimolecular Decomposition of Excited Molecular Species Near Threshold, M. Wolfsberg, *J. Chem. Phys*. 36, 1072 (1962).

110. Competitive Reaction Rates of Hydrogen Atoms with HCl and Cl_2. Entropy Considerations of HCl_2 Transition State, F. S. Klein and M. Wolfsberg, *J. Chem. Phys*. 34, 1494 (1961).

111. Equilibrium in the Exchange of Tritium Between Ammonia and Hydrogen and the Zero-Point Energy Difference between NH_3 and NH_2T, J. R. Gutman and M. Wolfsberg, *J. Chem. Phys*. 33, 1592 (1960).

112. Isotope Effects on Reaction Rates and the Reaction Coordinate, M. Wolfsberg, *J. Chem. Phys*. 33, 21 (1960).

113. Note on Secondary Isotope Effects in Reaction Rates, M. Wolfsberg, *J. Chem. Phys*. 33, 2 (1960).

114. The Statistical Theory of Mass Spectra: Difficulties in Interpretation of Spectra of the Lower Alkanes, L. Friedman, F. A. Long and M. Wolfsberg, *J. Chem. Phys*. 30, 1605 (1959).

115. Variation of Appearance Potentials of Alkane Fragment Ions with the Repeller Voltage of the Mass Spectrometer Ion Source, L. Friedman, F. A. Long and M. Wolfsberg, *J. Chem. Phys*. 31, 755 (1959).

116. Deuterium Isotope Effect in the Reaction of Hydrogen Molecules with Chlorine Atoms and the Potential Energy of the H_2Cl Transition Complex, J. Bigeleisen, F. S. Klein, R. E. Weston and M. Wolfsberg, *J. Chem. Phys*. 30, 1340 (1959).

117. K-Capture-Positron Ratios for first Forbidden Transitions-Sb^{122}, Rb^{84}, I^{126}, As^{74}, M. L. Perlman, J. P. Welker and M. Wolfsberg, *Phys. Rev.* 110, 381 (1958).

118. Theoretical and Experimental Aspects of Isotope Effects in Chemical Kinetics, J. Bigeleisen and M. Wolfsberg, *Adv. Chem. Phys.* 1, 15 (1958).

119. Study of the Mass Spectra of the Lower Aliphatic Alcohols, L. Friedman, F. A. Long and M. Wolfsberg, *J. Chem. Phys*. 27, 613 (1957).

120. Ionization Efficiency Curves and the Statistical Theory of Mass Spectra, L. Friedman, F. A. Long and M. Wolfsberg, *J. Chem. Phys*. 26, 714 (1957).

121. Multiple Electron Excitation in Auger Processes, M. Wolfsberg and M. L. Perlman, *Phys. Rev.* 99, 1833 (1955).

122. Excitation and Dissociation of Molecules Due to γ-Decay of a Constituent Atom, M. Wolfsberg, *J. Chem. Phys*. 24, 24 (1956).

123. Orbital Electron Excitation Associated with Electron Capture in A^{37}, M. Wolfsberg, *Phys. Rev*. 96, 1712 (1954).

124. Semi-Empirical Study of the H_2Cl Transition Complex through the use of Hydrogen Isotope Effects, J. Bigeleisen and M. Wolfsberg, *J. Chem. Phys*. 23, 1539 (1955).

125. Dipole Velocity and Dipole Length Matrix Elements in π-Electron Systems and Configuration Interaction, M. Wolfsberg, *J. Chem. Phys*. 23, 793 (1955).

126. The Spectra and Electronic Structure of Fluorochromate Ion, Chromyl Chloride, and Some Related Compounds, L. Helmholz, H. Brennan and M. Wolfsberg, *J. Chem. Phys*. 23, 853 (1955).

127. Note on a Nitrogen Molecule Calculation, M. Wolfsberg, *J. Chem. Phys*. 21, 2169 (1953).

128. Fractionation of the Carbon Isotopes in Decarboxylation Reactions. VI. Comparison of the Intermolecular Isotope Effects of a Pair of Isotopic Isomers, J. Bigeleisen and M. Wolfsberg, *J. Chem. Phys.* 21, 2120 (1953).

129. Temperature Independent Factor in the Relative Rates of Isotopic Three-Center Reactions, J. Bigeleisen and M. Wolfsberg, *J. Chem. Phys.* 21, 1972 (1953).

130. Relative Energies of Polar and Nonpolar Valence Bond Functions and Molecular Orbital Method. II, M. Wolfsberg, *J. Chem. Phys.* 21, 943 (1953).

131. Relative Energies of Polar and Nonpolar Valence Bond Functions and Molecular Orbital Method. I, M. Wolfsberg, *J. Chem. Phys.* 21, 943 (1953).

132. The Spectra and Electronic Structure of the Tetrahedral Ions MnO_4^-, CrO_4^{-2}, and ClO_4^-, M. Wolfsberg and L. Helmholz, *J. Chem. Phys.* 20, 837 (1952).

JP9004373