

## List of Publications of Fritz Schaefer

1. H. F. Schaefer and F. E. Harris, "Configuration Interaction Using Open-Shell Spin-Projected Functions", *Chem. Phys. Lett.* **1**, 407 (1967).
2. H. F. Schaefer and F. E. Harris, "Electronic Structure of Atomic Boron", *Phys. Rev.* **167**, 67 (1968).
3. H. F. Schaefer and F. E. Harris, "Calculation of the Electronic Affinity of Boron", *Phys. Rev.* **170**, 108 (1968).
4. H. F. Schaefer, R. A. Klemm, and F. E. Harris, "Atomic Hyperfine Structure. I. Polarization Wave Functions for the Ground States of B, C, N, O, and F", *Phys. Rev.* **176**, 49 (1968).
5. H. F. Schaefer and F. E. Harris, "Ab Initio Calculations on 62 Low-Lying States of the O<sub>2</sub> Molecule", *J. Chem. Phys.* **48**, 4946 (1968).
6. H. F. Schaefer and U. Kaldor, "Calculation of Spin Densities for Light Atoms", *J. Chem. Phys.* **49**, 469 (1968).
7. U. Kaldor, H. F. Schaefer, and F. E. Harris, "Spin-Extended and Configuration-Interaction Studies of First Row Atoms", *Int. J. Quantum Chem.* **IIS**, 13 (1968).
8. H. F. Schaefer and F. E. Harris, "Construction and Use of Atomic L–S Eigenfunctions", *J. Comput. Phys.* **3**, 217 (1968).
9. H. F. Schaefer and F. E. Harris, "Metastability of the <sup>1</sup>D State of the Nitrogen Negative Ion", *Phys. Rev. Lett.* **21**, 1561 (1968).
10. H. F. Schaefer, R. A. Klemm, and F. E. Harris, "Atomic Hyperfine Structure. II. First-Order Wave Functions for the Ground States of B, C, N, O, and F", *Phys. Rev.* **181**, 152 (1969).
11. H. F. Schaefer and R. A. Klemm, "Atomic Hyperfine Structure. III. Excited States of C, N, and O", *Phys. Rev.* **188**, 152 (1969).
12. H. F. Schaefer, R. A. Klemm, and F. E. Harris, "First-Order Wave Functions, Orbital Correlation Energies, and Electron Affinities of First Row Atoms", *J. Chem. Phys.* **51**, 4643 (1969).
13. H. F. Schaefer, "Diatomic Molecule Symmetry Eigenfunctions by Direct Diagonalization", *J. Comput. Phys.* **6**, 142 (1970).
14. H. F. Schaefer, D. R. McLaughlin, F. E. Harris, and B. J. Alder, "Calculation of the Attractive He Pair Potential", *Phys. Rev. Lett.* **25**, 988 (1970).
15. J. W. Viers, F. E. Harris, and H. F. Schaefer, "Pair Correlations and the Electronic Structure of Neon", *Phys. Rev. A* **1**, 24 (1970).
16. H. F. Schaefer and R. A. Klemm, "Atomic Hyperfine Structure. IV. Positive and Negative First Row Ions", *Phys. Rev. A* **1**, 1063 (1970).
17. P. S. Bagus, B. Liu, and H. F. Schaefer, "Study of the Contact-Term Contribution to the Hyperfine Structure Obtained from Spin-Unrestricted Hartree–Fock Wave Functions", *Phys. Rev. A* **2**, 555 (1970).
18. T. G. Heil, S. V. O'Neil, and H. F. Schaefer, "High Precision Valence Bond Potential Curve for the Cl<sub>2</sub> Molecule", *Chem. Phys. Lett.* **5**, 253 (1970).
19. S. Rothenberg, R. H. Young, and H. F. Schaefer, "Ground-State Self-Consistent-Field Wave Functions and Molecular Properties for the Isoelectric Series SiH<sub>4</sub>, PH<sub>3</sub>, H<sub>2</sub>S, and HCl", *J. Am. Chem. Soc.* **92**, 3243 (1970).
20. C. F. Bender and H. F. Schaefer, "New Theoretical Evidence for the Nonlinearity of the Triplet Ground State of Methylene", *J. Am. Chem. Soc.* **92**, 4984 (1970).
21. H. F. Schaefer, "New Approach to Electronic Structure Calculations for Diatomic Molecules: Application to F<sub>2</sub> and Cl<sub>2</sub>", *J. Chem. Phys.* **52**, 6241 (1970).
22. W. H. Miller and H. F. Schaefer, "Theoretical Treatment of Penning Ionization-He(1s2s<sup>1</sup>S, <sup>3</sup>S)", *J. Chem. Phys.* **53**, 1421 (1970).
23. S. V. O'Neil and H. F. Schaefer, "Valence-Excited States of Carbon Monoxide", *J. Chem. Phys.* **53**, 3994 (1970).
24. S. Rothenberg and H. F. Schaefer, "Theoretical Study of SO<sub>2</sub> Molecular Properties", *J. Chem. Phys.* **53**, 3014 (1970).
25. O. R. Platas and H. F. Schaefer, "Symmetry-Adapted Pair Correlations for Open-Shell Systems: Correlation Energy and Hyperfine Structure of the Nitrogen Atom", *Phys. Rev. A* **4**, 33 (1971).
26. S. V. O'Neil, P. K. Pearson, and H. F. Schaefer, "Repulsive <sup>3</sup>Σ<sup>-</sup> and Low-Lying (1.9 eV) <sup>3</sup>Σ<sup>+</sup> States of BeO", *Chem. Phys. Lett.* **10**, 404 (1971).
27. S. Rothenberg and H. F. Schaefer, "Self-Consistent-Field Potential Energy Surface in Three Dimensions for the Cl + H<sub>2</sub> → ClH + H Chemical Reaction", *Chem. Phys. Lett.* **10**, 565 (1971).
28. D. R. McLaughlin and H. F. Schaefer, "Interatomic Correlation Energy and the van der Waals Attraction Between Two Helium Atoms", *Chem. Phys. Lett.* **12**, 244 (1971).
29. C. F. Bender and H. F. Schaefer, "Ground (<sup>2</sup>A<sub>1</sub>) and First Excited (<sup>2</sup>B<sub>1</sub>(Π)) States of CH<sub>2</sub><sup>+</sup> and BH<sub>2</sub>", *J. Mol. Spectrosc.* **37**, 423 (1971).
30. S. Rothenberg and H. F. Schaefer, "Self-Consistent-Field Wave Functions, Energies, Multipole Moments, Diamagnetic Susceptibility and Shielding Tensors, and Electric Field Gradient Tensors for Nitrogen Dioxide and Ozone", *Mol. Phys.* **21**, 317 (1971).
31. T. G. Heil and H. F. Schaefer, "Four New Bound, Low-Lying States of Cyanogen: <sup>4</sup>Σ<sup>+</sup>, <sup>4</sup>Σ<sup>-</sup>, <sup>4</sup>Π, <sup>4</sup>Δ", *Astrophys. J.* **163**, 425 (1971).
32. D. H. Liskow, H. F. Schaefer, and C. F. Bender, "Geometry and Electronic Structure of the Hydroperoxyl Radical", *J. Am. Chem. Soc.* **93**, 6734 (1971).
33. H. F. Schaefer and S. Rothenberg, "Magnetic Hyperfine Structure of NO<sub>2</sub>", *J. Chem. Phys.* **54**, 1423 (1971).
34. H. F. Schaefer, "Ab Initio Potential Curve for the X <sup>3</sup>Σ<sub>g</sub><sup>-</sup> State of O<sub>2</sub>", *J. Chem. Phys.* **54**, 2207 (1971).
35. H. F. Schaefer and T. G. Heil, "Electronic Structures and Potential Energy Curves for the Low-Lying States of the CN Radical", *J. Chem. Phys.* **54**, 2573 (1971).
36. S. Rothenberg and H. F. Schaefer, "Methane as a Numerical Experiment for Polarization Basis Function Selection", *J. Chem. Phys.* **54**, 2764 (1971).

37. S. V. O'Neil, H. F. Schaefer, and C. F. Bender, "C<sub>2v</sub> Potential Energy Surfaces for Seven Low-Lying States of CH<sub>2</sub>", *J. Chem. Phys.* **55**, 162 (1971).
38. H. F. Schaefer, "Electron Correlation in the Lowest <sup>1</sup>Σ<sup>+</sup> State of Beryllium Oxide", *J. Chem. Phys.* **55**, 176 (1971).
39. S. V. O'Neil and H. F. Schaefer, "Configuration Interaction Study of the X <sup>3</sup>Σ<sup>-</sup>, a <sup>1</sup>Δ, and b <sup>1</sup>Σ<sup>+</sup> States of NH", *J. Chem. Phys.* **55**, 394 (1971).
40. C. A. Slocumb, W. H. Miller, and H. F. Schaefer, "Collisional Quenching of Metastable Hydrogen Atoms", *J. Chem. Phys.* **55**, 926 (1971).
41. P. S. Bagus and H. F. Schaefer, "Direct Near-Hartree-Fock Calculations on the 1s Hole State of NO<sup>+</sup>", *J. Chem. Phys.* **55**, 1474 (1971).
42. H. F. Schaefer and C. F. Bender, "Multiconfiguration Wave Functions for the Water Molecule", *J. Chem. Phys.* **55**, 1720 (1971).
43. B. Liu and H. F. Schaefer, "Krypton Monofluoride and Its Positive Ion", *J. Chem. Phys.* **55**, 2369 (1971).
44. H. F. Schaefer and W. H. Miller, "Curve Crossing of the B <sup>3</sup>Σ<sup>-</sup><sub>u</sub> and <sup>3</sup>Π<sub>u</sub> States of O<sub>2</sub> and Its Relation to Predissociation in the Schumann-Runge Bands", *J. Chem. Phys.* **55**, 4107 (1971).
45. C. F. Bender and H. F. Schaefer, "Electronic Splitting Between the <sup>2</sup>B<sub>1</sub> and <sup>2</sup>A<sub>1</sub> States of the NH<sub>2</sub> Radical", *J. Chem. Phys.* **55**, 4798 (1971).
46. P. K. Pearson, C. F. Bender, and H. F. Schaefer, "Theoretical Description of Molecular Rydberg States: B <sup>1</sup>Σ<sup>+</sup> Lowest <sup>3</sup>Σ<sup>+</sup> States of BH", *J. Chem. Phys.* **55**, 5235 (1971).
47. D. R. McLaughlin, C. F. Bender, and H. F. Schaefer, "Geometry and Force Constant Determination from Correlated Wave Functions for Polyatomic Molecules: Ground States of H<sub>2</sub>O and CH<sub>2</sub>", *Theor. Chim. Acta* **25**, 352 (1972).
48. C. F. Bender, T. H. Dunning, Jr., H. F. Schaefer, W. A. Goddard, and W. J. Hunt, "Multiconfiguration Wavefunctions for the lowest (ππ\*) Excited States of Ethylene", *Chem. Phys. Lett.* **15**, 171 (1972).
49. D. R. Yarkony and H. F. Schaefer, "Walsh Diagram for Zinc Difluoride", *Chem. Phys. Lett.* **15**, 514 (1972).
50. C. F. Bender, H. F. Schaefer, and P. A. Kollman, "The Long-Range Intermolecular Potential of H<sub>2</sub> - H<sub>2</sub>", *Mol. Phys.* **24**, 235 (1972).
51. D. H. Liskow, C. F. Bender, and H. F. Schaefer, "Theoretical Reaction Coordinate for the Methyl Iso-cyanide Isomerization", *J. Am. Chem. Soc.* **94**, 5178 (1972).
52. P. S. Bagus, B. Liu, and H. F. Schaefer, "Electronic Structure and Properties of Krypton Difluoride", *J. Am. Chem. Soc.* **94**, 6635 (1972).
53. D. H. Liskow and H. F. Schaefer, "Sign of the Dipole Moment and Other Properties of Methylsilane", *J. Am. Chem. Soc.* **94**, 6641 (1972).
54. C. F. Bender, H. F. Schaefer, D. R. Franceschetti, and L. C. Allen, "Singlet-Triplet Energy Separation, Walsh-Mulliken Diagrams, and Single d-Polarization Effects in Methylene", *J. Am. Chem. Soc.* **94**, 6888 (1972).
55. P. S. Bagus and H. F. Schaefer, "Localized and Delocalized 1s Hole States of the O<sub>2</sub><sup>+</sup> Molecular Ion", *J. Chem. Phys.* **56**, 224 (1972).
56. T. G. Heil and H. F. Schaefer, "Potential Curves for the Valence-Excited States of Silicon Monoxide. A Theoretical Study", *J. Chem. Phys.* **56**, 958 (1972).
57. H. F. Schaefer, D. Wallach, and C. F. Bender, "Interaction Potential Between Ground-State Helium Atom and the B <sup>1</sup>Σ<sub>u</sub><sup>+</sup> State of the Hydrogen Molecule", *J. Chem. Phys.* **56**, 1219 (1972).
58. W. H. Miller, C. A. Slocumb, and H. F. Schaefer, "Molecular Autoionization Lifetimes and Cross Sections for Penning Ionization: Numerical Results for He\*(1s 2s <sup>3</sup>S) + H(1s <sup>2</sup>S)", *J. Chem. Phys.* **56**, 1347 (1972).
59. P. K. Pearson, S. V. O'Neil, and H. F. Schaefer, "Role of Electron Correlation in *A Priori* Predictions of the Electronic Ground State of BeO", *J. Chem. Phys.* **56**, 3938 (1972).
60. P. K. Pearson, S. V. O'Neil, and H. F. Schaefer, "Potential Energy Surface Including Electron correlation for the Chemical Reaction F + H<sub>2</sub> → FH + H. I. Preliminary Surface", *J. Chem. Phys.* **56**, 4626 (1972).
61. D. H. Liskow, C. F. Bender, and H. F. Schaefer, "Bending Frequency of the C<sub>3</sub> Molecule", *J. Chem. Phys.* **56**, 5075 (1972).
62. C. F. Bender and H. F. Schaefer, "Linear Symmetric H<sub>4</sub>", *J. Chem. Phys.* **57**, 217 (1972).
63. V. Bondybey, P. K. Pearson, and H. F. Schaefer, "Theoretical Potential Energy Curves for OH, HF<sup>+</sup>, HF, HF<sup>-</sup>, NEH<sup>+</sup>, and NeH", *J. Chem. Phys.* **57**, 1123.
64. D. H. Liskow, C. F. Bender, and H. F. Schaefer, "Some Features of the CH<sub>3</sub>NC → CH<sub>3</sub>CN Potential Surface", *J. Chem. Phys.* **47**, 4509 (1972).
65. C. F. Bender, S. V. O'Neil, P. K. Pearson, and H. F. Schaefer, "Potential Energy Surface Including Electron Correlation for F + H<sub>2</sub> → FH + H: Refined Linear Surface", *Science* **176**, 1412 (1972).
66. H. F. Schaefer, *The Electronic Structure of Atoms and Molecules: A Survey of Rigorous Quantum Mechanical Results* (Addison-Wesley, Reading, MA, 1972). 437 pages.
67. S. Rothenberg and H. F. Schaefer, "Molecular Properties of the Triatomic Difluorides BeF<sub>2</sub>, BF<sub>2</sub>, CF<sub>2</sub>, NF<sub>2</sub>, and OF<sub>2</sub>", *J. Am. Chem. Soc.* **95**, 2095 (1973).
68. D. H. Liskow, H. F. Schaefer, P. S. Bagus, and B. Liu, "Probable Nonexistence of Xenon Monofluoride as a Chemically Bound Species in the Gas Phase", *J. Am. Chem. Soc.* **95**, 4056 (1973).
69. R. W. Hand, W. J. Hunt, and H. F. Schaefer, "Electronic Structure of Iron Trifluoride", *J. Am. Chem. Soc.* **95**, 4517 (1973).
70. S. V. O'Neil, P. K. Pearson, H. F. Schaefer, and C. F. Bender, "On the H + F<sub>2</sub> → HF + F Reaction. An *Ab Initio* Potential Energy Surface", *J. Chem. Phys.* **58**, 1126 (1973).
71. P. S. Bagus and H. F. Schaefer, "<sup>7</sup>Σ<sup>+</sup> and <sup>7</sup>Π States of Manganese Hydride", *J. Chem. Phys.* **58**, 1844 (1973).
72. S. D. Augustin, W. H. Miller, P. K. Pearson, and H. F. Schaefer, "Potential Curves and Inelastic Cross Sections for Low Energy Collisions of O<sup>+</sup> and He", *J. Chem. Phys.* **58**, 2845 (1973).
73. G. M. Schwenzler, D. H. Liskow, H. F. Schaefer, P. S. Bagus, B. Liu, A. D. McLean, and M. Yoshimine, "Use of Nonrelativistic Wavefunctions for the Prediction of Properties of Molecules Containing Atoms of High Z. PbO as a Test Case", *J. Chem. Phys.* **58**, 3181 (1973).

74. P. K. Pearson, W. J. Hunt, C. F. Bender, and H. F. Schaefer, "Simplest Halogen Atom Plus Alkali Dimer Potential Surface;  $F + Li_2 \rightarrow LiF + Li$ ", *J. Chem. Phys.* **58**, 5358 (1973).
75. H. F. Schaefer, "Electron Correlation in Molecules", in *Energy, Structure, and Reactivity*, editors D. W. Smith and W. B. McRae (John Wiley, New York, 1973). Pages 148–163.
76. D. R. Yarkony, W. J. Hunt, and H. F. Schaefer, "Relation Between Electronic Structure and the Chemiluminescence Arising from Collisions Between Alkaline Earth Atoms and Halogen Molecules", *Mol. Phys.* **26**, 941 (1973).
77. S. V. O'Neil, H. F. Schaefer, and C. F. Bender, "Barrier Height for the Exchange Reaction  $F + HF \rightarrow FH + F$ ", *Proc. Natl. Acad. Sci. U.S.A.* **71**, 104 (1974).
78. P. K. Pearson, G. L. Blackman, H. F. Schaefer, B. Roos, and U. Wahlgren, "HNC Molecule in Interstellar Space? Some Pertinent Theoretical Calculations", *Astrophys. J. Lett.* **184**, L19 (1973).
79. C. W. Bauschlicher, S. V. O'Neil, R. K. Preston, H. F. Schaefer, and C. F. Bender, "Avoided Intersection of Potential Energy Surfaces: The ( $H^+ + H_2$ ,  $H + H^+_2$ ) System", *J. Chem. Phys.* **59**, 1286 (1973).
80. B. J. Garrison, W. H. Miller, and H. F. Schaefer, "Penning and Associative Ionization of Triplet Metastable Helium Atoms", *J. Chem. Phys.* **59**, 3193 (1973).
81. S. V. O'Neil, H. F. Schaefer, and C. F. Bender, "Geometry of the  $LiO_2$  Radical", *J. Chem. Phys.* **59**, 3608 (1973).
82. H. F. Schaefer, "Status of *Ab Initio* Molecular Structure Predictions", in *Critical Evaluation of Chemical and Physical Structural Information*, editors D. R. Lide and M. A. Paul (National Academy of Sciences, Washington, DC, 1974). Pages 591–602.
83. D. R. Yarkony, H. F. Schaefer, and S. Rothenberg, "Geometries of the Methoxy Radical ( $X^2E$  and  $A^2A_1$  States) and the Methoxide Ion", *J. Am. Chem. Soc.* **96**, 656 (1974).
84. D. R. Yarkony, S. V. O'Neil, H. F. Schaefer, C. P. Baskin, and C. F. Bender, "Interaction Potential Between Two Rigid HF Molecules", *J. Chem. Phys.* **60**, 855 (1974).
85. P. K. Pearson and H. F. Schaefer, "Some Properties of  $H_2CN^+$ : A Potentially Important Interstellar Species", *Astrophys. J.* **192**, 33 (1974).
86. U. Wahlgren, B. Liu, P. K. Pearson, and H. F. Schaefer, "Theoretical Support for the Assignment of X-ogen to the  $HCO^+$  Molecular Ion", *Nature* **246**, 4 (1973).
87. C. W. Bauschlicher, and H. F. Schaefer, "Distortion of Atomic Orbitals within Molecules", *Chem. Phys. Lett.* **24**, 412 (1974).
88. D. H. Liskow, C. F. Bender, and H. F. Schaefer, "Potential Energy Surfaces Related to the Ion–Molecule Reaction  $C^+ + H_2$ ", *J. Chem. Phys.* **61**, 2507 (1974).
89. G. M. Schwenzer, S. V. O'Neil, H. F. Schaefer, C. P. Baskin, and C. F. Bender, "Geometries of the Excited Electronic States of HCN", *J. Chem. Phys.* **60**, 2787 (1974).
90. C. P. Baskin, C. F. Bender, C. W. Bauschlicher, and H. F. Schaefer, "Reaction Pathways for the Triplet Methylene Abstraction  $CH_2(^3B_1) + H_2 \rightarrow CH_3 + H$ ", *J. Am. Chem. Soc.* **96**, 2709 (1974). Also in *Quantum Chemistry: The State of the Art* (Science Research Council, London, 1975). Pages 57–63.
91. C. F. Bender, C. W. Bauschlicher, and H. F. Schaefer, "Saddle Point Geometry and Barrier Height for  $H + F_2 \rightarrow HF + F$ ", *J. Chem. Phys.* **60**, 3707 (1974).
92. D. R. Yarkony and H. F. Schaefer, "Triplet Electronic Ground State of Trimethylenemethane", *J. Am. Chem. Soc.* **96**, 3754 (1974).
93. D. H. Liskow, J. M. McKelvey, C. F. Bender, and H. F. Schaefer, "A *Priori* Prediction of the Cohesive Energy of One-Dimensional Metallic Hydrogen", *Phys. Rev. Lett.* **32**, 933 (1974).
94. H. F. Schaefer and W. H. Miller, "Large Scale Scientific Computation via Minicomputer", *Comput. Chem.* **1**, 85 (1976).
95. D. R. Yarkony, H. F. Schaefer, and S. Rothenberg, " $X^3A_2$ ,  $^1E$ , and  $b^1A_1$  Electronic States of Methylnitrene", *J. Am. Chem. Soc.* **96**, 5974 (1974).
96. B. J. Garrison and H. F. Schaefer, "Molecular Properties of Excited Electronic States: The  $\tilde{a}^3A''$  and  $\tilde{A}^1A''$  States of Formaldehyde", *J. Chem. Phys.* **61**, 3039 (1974).
97. D. R. Yarkony and H. F. Schaefer, "Correlation Diagram for  $He + He \rightarrow Be$ ", *J. Chem. Phys.* **61**, 4921 (1974).
98. P. K. Pearson, H. F. Schaefer, J. H. Richardson, L. M. Stephenson, and J. I. Brauman, "Three Isomers of the  $NO_2^-$  Ion", *J. Am. Chem. Soc.* **96**, 6778 (1974).
99. S. R. Ungemach and H. F. Schaefer, "The Weak Attraction Between Water and Methane", *J. Am. Chem. Soc.* **96**, 7898 (1974).
100. H. F. Schaefer, "Potential Beneath the Surface", *Chem. Br.* **11**, 227 (1975).
101. C. E. Dykstra, P. K. Pearson, and H. F. Schaefer, "Electronic Structure of Nitrenes:  $LiN$ , The Simplest Ionic Species", *J. Am. Chem. Soc.* **97**, 2321 (1975).
102. G. M. Schwenzer, H. F. Schaefer, and C. F. Bender, "Excited Electronic States of HNC, Hydrogen Isocyanide", *J. Chem. Phys.* **63**, 569 (1975).
103. G. M. Schwenzer, H. F. Schaefer, and C. F. Bender, "Excited Electronic States of HNC, Hydrogen Isocyanide", *J. Am. Chem. Soc.* **97**, 1393 (1975).
104. P. K. Pearson and H. F. Schaefer, "Potential Energy Surface for the Model Unimolecular Reaction  $HNC \rightarrow HCN$ ", *J. Chem. Phys.* **62**, 350 (1975).
105. P. Siegbahn and H. F. Schaefer, "Potential Energy Surfaces for  $H + Li_2 \rightarrow LiH + Li$ . Ground-State Surface from Large Scale Configuration Interaction", *J. Chem. Phys.* **62**, 3488 (1975).
106. C. F. Bender, B. J. Garrison, and H. F. Schaefer, "A Critical Test of Semi-Empirical  $FH_2$  Potential Energy Surfaces: The Barrier Height for  $H + FH \rightarrow HF + H$ ", *J. Chem. Phys.* **62**, 1188 (1975).
107. C. W. Bauschlicher, D. H. Liskow, C. F. Bender, and H. F. Schaefer, "Model Studies of Chemisorption. Interaction Between Atomic Hydrogen and Beryllium Clusters", *J. Chem. Phys.* **62**, 4815 (1975).
108. C. E. Dykstra and H. F. Schaefer, "Electronic Structure of Dicarboxyls: The Ground State of Glyoxal", *J. Am. Chem. Soc.* **97**, 7210 (1975).
109. R. R. Lucchese and H. F. Schaefer, "Charge-Transfer Complexes.  $NH_3-F_2$ ,  $NH_3-Cl_2$ ,  $HN_3-CIF$ ,  $N(CH_3)_3-F_2$ ,  $N(CH_3)_3-CIF$ ", *J. Am. Chem. Soc.* **97**, 7205 (1975).
110. P. S. Bagus, B. Liu, D. H. Liskow, and H. F. Schaefer, "Electron Correlation and the Reality of  $XeF_2^+$ ", *J. Am. Chem. Soc.* **97**, 7216 (1975).

111. G. M. Schwenzer, C. F. Bender, and H. F. Schaefer, "Confirmation of the Discrepancy Between Theory and Experiment for the  $\tilde{B}^1 A'$  State of HCN", *Chem. Phys. Lett.* **36**, 179 (1975).
112. B. J. Garrison, W. A. Lester, and H. F. Schaefer, "Hartree-Fock Interaction Potential Between a Rigid Asymmetric Top and a Spherical Atom: (H<sub>2</sub>CO, He)", *J. Chem. Phys.* **63**, 1449 (1975).
113. L. Radom and H. F. Schaefer, "Theoretical Predictions of the Molecular Structure of Sulfur Tetrafluoride", *Austr. J. Chem.* **28**, 2069 (1975).
114. D. R. Yarkony and H. F. Schaefer, "The Acetyl Cation and its Geometrical Isomers", *J. Chem. Phys.* **63**, 4317 (1975).
115. D. R. Yarkony and H. F. Schaefer, "Multiplet Splittings in the Photoelectron Spectra of Organic Radicals: Trimethylenemethane", *Chem. Phys. Lett.* **35**, 291 (1975).
116. J. W. Birks, H. S. Johnston, and H. F. Schaefer, "NeH<sub>2</sub> Potential Energy Surface Including Electron Correlation", *J. Chem. Phys.* **63**, 1741 (1975).
117. D. S. Marynick and H. F. Schaefer, "Theoretical Studies of Metal-Phosphosphate Interactions. The Interaction of Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Be<sup>2+</sup>, Mg<sup>2+</sup>, and Ca<sup>2+</sup> with H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and (CH<sub>3</sub>O)<sub>2</sub>PO<sub>2</sub><sup>-</sup>: Implications for Nucleic Acid Solvation", *Proc. Natl. Acad. Sci. U.S.A.* **72**, 3794 (1975).
118. B. J. Garrison, W. A. Lester, P. Siegbahn, and H. F. Schaefer, "Effect of Electron Correlation on the H<sub>2</sub>CO-He Interaction Potential", *J. Chem. Phys.* **63**, 4167 (1975).
119. H. F. Schaefer, "Are Minicomputers Suitable for Large Scale Scientific Computation?" *Proceedings of the Eleventh Annual IEEE Computer Society Conference*, September, 1975, Washington, DC (IEEE, Piscataway, NJ, 1975). Pages 61-64.
120. C. E. Dykstra and H. F. Schaefer, "Electronic Structure of Dicarboxyls: Glyoxal Excited States", *J. Am. Chem. Soc.* **98**, 401 (1976).
121. C. W. Bauschlicher, H. F. Schaefer, and C. F. Bender, "The Least-Motion Insertion Reaction CH<sub>2</sub>(<sup>1</sup>A<sub>1</sub>) + H<sub>2</sub> → CH<sub>4</sub>: Theoretical Study of a Process Forbidden by Orbital Symmetry", *J. Am. Chem. Soc.* **98**, 1653 (1976).
122. C. P. Baskin, C. F. Bender, R. R. Lucchese, C. W. Bauschlicher, and H. F. Schaefer, "Molecular Structure and Properties of CH<sub>3</sub>BeF and CH<sub>3</sub>MgF", *J. Mol. Struct.* **32**, 125 (1976).
123. S. R. Ungemach and H. F. Schaefer, "Molecular Structure of the ClF<sub>2</sub> and ClF<sub>4</sub> Radicals. A Theoretical Study", *J. Am. Chem. Soc.* **98**, 1658 (1976).
124. D. R. Yarkony, H. F. Schaefer, and C. F. Bender, "Self-Consistent-Field Wavefunctions Using a Symmetry-Restricted Annihilation of Single-Excitations Procedure", *J. Chem. Phys.* **64**, 981 (1976).
125. C. E. Dykstra and H. F. Schaefer, "Excited Electronic States of Ketene", *J. Am. Chem. Soc.* **98**, 2689 (1976).
126. C. W. Bauschlicher, C. F. Bender, H. F. Schaefer, and P. S. Bagus, "Chemisorption and the Properties of Metal Clusters", *Chem. Phys.* **15**, 227 (1976).
127. C. W. Bauschlicher, C. F. Bender, and H. F. Schaefer, "Transition States for the Abstraction Reactions of Triplet Methylene with Hydrogen and Methane", *J. Am. Chem. Soc.* **98**, 3072 (1976).
128. R. B. Brewington, C. F. Bender, and H. F. Schaefer, "Tetrahedral Be<sub>4</sub>", *J. Chem. Phys.* **64**, 905 (1976).
129. J. H. Meadows and H. F. Schaefer, "One- and Two-Configuration Hartree-Fock Limit Predictions for the Singlet-Triplet Separation in Methylene and Silylene", *J. Am. Chem. Soc.* **98**, 4383 (1976).
130. S. R. Ungemach and H. F. Schaefer, "Basis Set Dependence of *Ab Initio* Predictions for AB<sub>4</sub> Molecules", *Chem. Phys. Lett.* **38**, 407 (1976).
131. H. F. Schaefer, "Molecular Electronic Structure Theory: 1972-1975", *Annu. Rev. Phys. Chem.* **27**, 261 (1976).
132. W. C. Swope and H. F. Schaefer, "Model Organometallic Systems. The Interaction of <sup>2</sup>S Be<sup>+</sup>, <sup>1</sup>S Be, and <sup>3</sup>P Be with Acetylene and Ethylene", *J. Am. Chem. Soc.* **98**, 7962 (1976).
133. C. W. Bauschlicher, H. F. Schaefer and P. S. Bagus, "Structure and Energetics of Simple Carbenes. CH<sub>2</sub>, CHF, CHCl, CHBr, CF<sub>2</sub>, CCl<sub>2</sub>", *J. Am. Chem. Soc.* **99**, 7106 (1977).
134. C. F. Bender, J. H. Meadows, and H. F. Schaefer, "Potential Energy Surfaces for Ion-Molecule Reactions. Intersection of the <sup>3</sup>A<sub>2</sub> and <sup>3</sup>B<sub>1</sub> Surfaces of NH<sub>2</sub><sup>+</sup>", *Faraday Discuss. Chem. Soc.* **62**, 59 (1977).
135. R. R. Lucchese, K. Haber, and H. F. Schaefer, "Charge-Transfer Complexes. NH<sub>3</sub>-O<sub>3</sub>, NH<sub>3</sub>-SO<sub>2</sub>, and N(CH<sub>3</sub>)<sub>3</sub>-SO<sub>2</sub>", *J. Am. Chem. Soc.* **98**, 7617 (1976).
136. C. E. Dykstra and H. F. Schaefer, "Instructional Approach to Molecular Electronic Structure Theory", *J. Chem. Educ.* **54**, 310 (1977).
137. S. Alexandratos, A. Steitwieser, and H. F. Schaefer, "The Simplest Metallocene: Cyclopentadienyllithium", *J. Am. Chem. Soc.* **98**, 7959 (1976).
138. C. E. Dykstra, H. F. Schaefer, and W. Meyer, "A Theory of Self-Consistent Electron Pairs. Computational Methods and Preliminary Applications", *J. Chem. Phys.* **65**, 2740 (1976).
139. H. F. Schaefer, C. F. Bender, and J. H. Richardson, "A Peroxy Isomer of Nitrogen Dioxide", *J. Phys. Chem.* **80**, 2035 (1976).
140. R. R. Lucchese and H. F. Schaefer, "Dicyanocarbene: Triplet and Singlet Structures and Energetics", *J. Am. Chem. Soc.* **99**, 13 (1977).
141. C. E. Dykstra, H. F. Schaefer, and W. Meyer, "Electron Correlation in Small Metal Clusters. Application of a Theory of Self-Consistent Electron Pairs to the Be<sub>4</sub> System", *J. Chem. Phys.* **65**, 5141 (1976).
142. C. W. Bauschlicher, K. Haber, H. F. Schaefer, and C. F. Bender, "Concerted Non-Least-Motion Pathway for the Singlet Methylene Insertion Reaction CH<sub>2</sub>(<sup>1</sup>A<sub>1</sub>) + H<sub>2</sub> → CH<sub>4</sub>", *J. Am. Chem. Soc.* **99**, 3610 (1977).
143. B. R. Brooks and H. F. Schaefer, "A Model Transition-Metal Carbene System. MnCH<sub>2</sub>", *Mol. Phys.* **34**, 193 (1977).
144. W. C. Swope and H. F. Schaefer, "Model Studies of  $\pi$ -Bonded Organometallic Systems. Mn-C<sub>2</sub>H<sub>2</sub> and Mn-C<sub>2</sub>H<sub>4</sub>", *Mol. Phys.* **34**, 1037 (1977).
145. S. R. Ungemach, H. F. Schaefer, and B. Liu, "Concerning *Ab Initio* Potential Energy Surfaces for F + H<sub>2</sub>", *Faraday Discuss. Chem. Soc.* **62**, 330 (1977).
146. R. R. Lucchese, B. R. Brooks, J. H. Meadows, W. C. Swope and H. F. Schaefer, BERKELEY: An "Open Ended" Configuration Interaction (CI) Program Designed for Minicomputers", *J. Comput. Phys.* **26**, 243 (1978).

147. C. F. Bender and H. F. Schaefer, "Potential Energy Surfaces for Fluorine Hydrogen Systems", in *Fluorine-Containing Free Radicals: Kinetics and Dynamics of Reactions*, American Chemical Society, Symposium Series, Vol. 66, editor John Root (American Chemical Society, Washington, DC, 1978). Pages 283–295.
148. M. Trenary, H. F. Schaefer, and P. Kollman, "A Novel Class of Molecular Complexes. Li–NH<sub>3</sub>, Li–H<sub>2</sub>O, Li–HF, Li–H<sub>2</sub>S, Na–H<sub>2</sub>O, and Na–HF", *J. Am. Chem. Soc.* **99**, 3885 (1977).
149. S. R. Ungemach, H. F. Schaefer, and B. Liu, "Theoretical Dipole Moment Function of the X <sup>1</sup>Σ<sup>+</sup> State of HI", *J. Mol. Spectrosc.* **66**, 99 (1977).
150. R. R. Lucchese and H. F. Schaefer, "Energy Separation Between the Open (C<sub>2v</sub>) and Closed (D<sub>3h</sub>) Forms of Ozone", *J. Chem. Phys.* **67**, 848 (1977).
151. N. R. Carlsen and H. F. Schaefer, "Open (C<sub>2v</sub>) and Closed (D<sub>3h</sub>) Forms of the S<sub>3</sub> Molecule, Thiozone", *Chem. Phys. Lett.* **48**, 390 (1977).
152. H. F. Schaefer, "The Fuzzy Interface Between Surface Chemistry, Heterogeneous Catalysis, and Organometallic Chemistry", *Acc. Chem. Res.* **10**, 287 (1977).
153. P. K. Pearson, R. R. Lucchese, W. H. Miller, and H. F. Schaefer, "Theoretical Chemistry via Minicomputer", American Chemical Society, Symposium Series, Vol. 57, editor Peter Lykos (American Chemical Society, Washington, DC, 1977). Pages 171–190.
154. C. E. Dykstra, R. R. Lucchese, and H. F. Schaefer, "Electron Correlation Effects on the Excitation Energies of the Lowest Triplet States of Glyoxal", *J. Chem. Phys.* **67**, 2422 (1977).
155. C. E. Dykstra, M. Hereld, R. R. Lucchese, H. F. Schaefer, and W. Meyer, "Molecular Structure of the Methyl Anion CH<sub>3</sub><sup>-</sup>. An Investigation of the Effects of Electron Correlation Using the Theory of Self-Consistent Electron Pairs (SCEP)", *J. Chem. Phys.* **67**, 4071 (1977).
156. R. R. Lucchese, H. F. Schaefer, and C. E. Dykstra, "Excitation Energies of the n → π\* <sup>3</sup>A' and π → π\* <sup>3</sup>A' States of Acrolein", *Chem. Phys. Lett.* **51**, 600 (1977).
157. L. Radom and H. F. Schaefer, "On the Limits of Stability of Multiply Charged Monocyclic Aromatic Cations: C<sub>3</sub>H<sub>3</sub><sup>+</sup>, C<sub>4</sub>H<sub>4</sub><sup>2+</sup>, C<sub>5</sub>H<sub>5</sub><sup>3+</sup>, C<sub>6</sub>H<sub>6</sub><sup>4+</sup>, C<sub>7</sub>H<sub>7</sub><sup>+</sup>, C<sub>8</sub>H<sub>8</sub><sup>2+</sup>, C<sub>9</sub>H<sub>9</sub><sup>3+</sup>", *J. Am. Chem. Soc.* **99**, 7522 (1977).
158. R. R. Lucchese and H. F. Schaefer, "Extensive Configuration Interaction (CI) Studies of the Methylene Single-Triplet Separation", *J. Am. Chem. Soc.* **99**, 6765 (1977).
159. B. R. Brooks and H. F. Schaefer, "Reactions of Carbynes. Potential Energy Surfaces for the Doublet and Quartet Methylidyne (CH) Reactions with Molecular Hydrogen", *J. Chem. Phys.* **67**, 5146 (1977).
160. H. F. Schaefer, editor, *Methods of Electronic Structure Theory*, Modern Theoretical Chemistry Vol. 3 (Plenum Press, New York, 1977). 462 pages.
161. H. F. Schaefer, editor, *Applications of Electronic Structure Theory*, Modern Theoretical Chemistry Vol. 4 (Plenum Press, New York, 1977). 461 pages.
162. S. Bell and H. F. Schaefer, "Ab Initio SCF and CI Studies of Three States of NH<sub>2</sub>", *J. Chem. Phys.* **67**, 5173 (1977).
163. C. F. Bender and H. F. Schaefer, "Ionic Excited States of Ne<sub>2</sub>F<sup>+</sup>", *Chem. Phys. Lett.* **53**, 27 (1978).
164. R. R. Lucchese and H. F. Schaefer, "Formulation of the Direct Configuration Interaction Method for Triplet Spin States. Applications to Glyoxal", *J. Chem. Phys.* **68**, 769 (1978).
165. B. H. Mahan, H. F. Schaefer, and S. R. Ungemach, "Some Features of the Potential Energy Surface for the F<sup>+</sup> + H<sub>2</sub> Ion–Molecule Reaction", *J. Chem. Phys.* **68**, 781 (1978).
166. H. F. Schaefer, "Atom-Molecule Potentials", Chapter 2a in *Atom-Molecule Collision Theory: A Guide for the Experimentalist*, editor R. B. Bernstein (Plenum, New York, 1979). Pages 45–77.
167. R. R. Lucchese and H. F. Schaefer, "Metal Carbene Complexes and the Possible Role of Hydroxycarbene in Formaldehyde Laser Photochemistry", *J. Am. Chem. Soc.* **100**, 298 (1978).
168. C. E. Dykstra and H. F. Schaefer, "The Vinylidene-Acetylene Rearrangement. An SCEP Study of Model Unimolecular Reaction", *J. Am. Chem. Soc.* **100**, 1378 (1978).
169. C. E. Dykstra, A. S. Gaylord, W. D. Gwinn, W. C. Swope, and H. F. Schaefer, "The Uncoupled Symmetric Stretching Frequency of H<sub>3</sub><sup>+</sup>", *J. Chem. Phys.* **68**, 3951 (1978).
170. D. P. Craig, L. Radom, and H. F. Schaefer, "Multiply Charged Aromatic Cations: The Heptalenium Dication", *Austr. J. Chem.* **31**, 261 (1978).
171. M. Trenary, H. F. Schaefer, and P. A. Kollman, "Electronic Structure of Li–H<sub>2</sub>O and Related Neutral Molecular Complexes, Including Al–H<sub>2</sub>O", *J. Chem. Phys.* **68**, 4047 (1978).
172. D. M. Hood, R. M. Pitzer, and H. F. Schaefer, "Equilibrium Geometry of the Trimethylenemethane and the Absence of an Adjacent Secondary Minimum on the Triplet Potential Energy Surface", *J. Am. Chem. Soc.* **100**, 2227 (1978).
173. D. M. Hood and H. F. Schaefer, "Singlet–Triplet Energy Separation for Silaethylene", *J. Chem. Phys.* **68**, 2985 (1978).
174. E. D. Jemmis, S. Alexandratos, P. R. Schleyer, A. Streitwieser, and H. F. Schaefer, "Ab Initio SCF-MO Study of Cyclopentadienylberyllium Hydride and Beryllocene", *J. Am. Chem. Soc.* **100**, 5695 (1978).
175. C. W. Bauschlicher, P. S. Bagus, and H. F. Schaefer, "A Model Study in Chemisorption: Molecular Orbital Cluster Theory for Atomic Hydrogen on Be(0001)", *IBM J. Res. Dev.* **22**, 213 (1978).
176. B. R. Brooks and H. F. Schaefer, "N(<sup>1</sup>A<sub>g</sub>), T(<sup>3</sup>B<sub>1u</sub>) States of Vertical Ethylene", *J. Chem. Phys.* **68**, 4839 (1978).
177. R. R. Lucchese, H. F. Schaefer, W. R. Rodwell, and L. Radom, "Fluorine Peroxide (FOOF): A Problem Molecule for Theoretical Structural Predictions", *J. Chem. Phys.* **68**, 2507 (1978).
178. R. R. Lucchese, M. P. Conrad, and H. F. Schaefer, "Correlated Wave Functions for the Water Molecule", *J. Chem. Phys.* **68**, 5292 (1978).
179. R. W. Wetmore and H. F. Schaefer, "Triplet Electronic States of Acetylene: cis and trans Structures and Energetics", *J. Chem. Phys.* **69**, 1648 (1978).
180. C. E. Dykstra and H. F. Schaefer, "Theoretical Methods and Their Application to Ketenes and Allenes", Chapter 1 of *The Chemistry of Ketenes and Allenes*, editor Saul Patai (Wiley/Interscience, London, 1980). Pages 1–44.

181. M. P. Conrad and H. F. Schaefer, "Role of Different Isomers of the  $\text{H}_2\text{CN}^+$  Ion in the Formation of Interstellar HCN and HNC", *Nature* **274**, 456 (1978).
182. M. P. Conrad and H. F. Schaefer, "Absence of an Energetically Viable Pathway for Triplet 1,2 Hydrogen Shifts. A Theoretical Study of the Vinylidene-Acetylene Isomerization", *J. Am. Chem. Soc.* **100**, 7820 (1978).
183. W. D. Laidig and H. F. Schaefer, "Structures of Energetics of Planar and Tetrahedral Dilithiomethane: A Near Degeneracy of Singlet and Triplet Electronic States", *J. Am. Chem. Soc.* **100**, 5972 (1978).
184. B. R. Brooks and H. F. Schaefer, "The BERKELEY System. III. General Configuration-Interaction Methods for Open-Shell Molecular Electronic States", *Int. J. Quantum Chem.* **14**, 603 (1978).
185. B. R. Brooks and H. F. Schaefer, "Sudden Polarization: The Pyramidalization of Twisted Ethylene", *J. Am. Chem. Soc.* **101**, 307 (1979).
186. D. M. Hood, H. F. Schaefer, and R. M. Pitzer, "Planar  $^3A'_2$  - Orthogonal  $^1B_1$  Energy Separation for Trimethylenemethane", *J. Am. Chem. Soc.* **100**, 8009 (1978).
187. W. C. Swope, Y. P. Lee, and H. F. Schaefer, "Diatomic Sulfur: Low-Lying Bound Molecular Electronic States of  $S_2$ ", *J. Chem. Phys.* **70**, 947 (1979).
188. M. E. Zandler, J. D. Goddard, and H. F. Schaefer, "Effects of Electron Correlation on the Geometrical Structure of HCCN", *J. Am. Chem. Soc.* **101**, 1072 (1979).
189. M. Trenary, M. E. Casida, B. R. Brooks, and H. F. Schaefer, "Three Isomers of the Al-C<sub>2</sub>H<sub>2</sub> System", *J. Am. Chem. Soc.* **101**, 1638 (1979).
190. B. R. Brooks and H. F. Schaefer, "The Graphical Unitary Group Approach to the Electron Correlation Problem. Methods and Preliminary Applications", *J. Chem. Phys.* **70**, 5092 (1979).
191. M. P. Conrad, R. M. Pitzer, and H. F. Schaefer, "Geometrical Structure and Energetics of Closs's Diradical: 1,3-Cyclopentadiyl", *J. Am. Chem. Soc.* **101**, 2245 (1979).
192. J. D. Goddard and H. F. Schaefer, "The Photodissociation of Formaldehyde: Potential Energy Surface Features", *J. Chem. Phys.* **70**, 5117 (1979).
193. D. M. Hood, R. M. Pitzer, and H. F. Schaefer, "Electronic Structure of Homoleptic Transition Metal Hydrides: TiH<sub>4</sub>, VH<sub>4</sub>, CrH<sub>4</sub>, FeH<sub>4</sub>, CoH<sub>4</sub>, NiH<sub>4</sub>", *J. Chem. Phys.* **71**, 705 (1979).
194. N. C. Handy, J. D. Goddard, and H. F. Schaefer, "Generalization of the Direct Configuration Interaction Method to the Hartree-Fock Interacting Space for Doublets, Quartets, and Open Shell Singlets. Applications to NO<sub>2</sub> and NO<sub>2</sub><sup>-</sup>", *J. Chem. Phys.* **71**, 426 (1979).
195. C. F. Bender, T. N. Rescigno, H. F. Schaefer, and A. E. Orel, "Potential Energy Curves for Diatomic Zinc and Cadmium", *J. Chem. Phys.* **71**, 1122 (1979).
196. J. D. Goddard, N. C. Handy, and H. F. Schaefer, "Gradient Techniques for Open-Shell Restricted Hartree-Fock and Multi-Configuration Self-Consistent Field Methods", *J. Chem. Phys.* **71**, 1525 (1979).
197. H. F. Schaefer, "The 1,2 Hydrogen Shift: A Common Vehicle for the Disappearance of Evanescent Molecular Species", *Acc. Chem. Res.* **12**, 288 (1979).
198. W. C. Swope, Y. P. Lee, and H. F. Schaefer, "Sulfur Oxide: Low-Lying Bound Molecular Electronic States of SO", *J. Chem. Phys.* **71**, 3761 (1979).
199. M. E. Casida, M. L. Chen, R. D. MacGregor, and H. F. Schaefer, "Walsh's Rules and Small Bond Angle States of Triatomic Dihydride Molecules", *Isr. J. Chem.* **19**, 127 (1980).
200. R. M. Pitzer and H. F. Schaefer, "Conformational Preferences and Electronic Structures of Ni(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub> and Ni(C<sub>2</sub>H<sub>4</sub>)<sub>3</sub>", *J. Am. Chem. Soc.* **101**, 7176 (1979).
201. W. D. Laidig and H. F. Schaefer, "1,1 Dilithioethylene: A Ground State Triplet Olefin with Nearly Free Rotation about the Double Bond", *J. Am. Chem. Soc.* **101**, 7184 (1979).
202. B. R. Brooks, W. D. Laidig, P. Saxe, N. C. Handy, and H. F. Schaefer, "The Loop-Driven Graphical Unitary Group Approach: A Powerful Method for the Variational Description of Electron Correlation", *Phys. Scr.* **21**, 312 (1980).
203. J. Demuynck and H. F. Schaefer, "The Gas-Phase Structure of Transition Metal Dihydrides", *J. Chem. Phys.* **72**, 311 (1980).
204. A. Komornicki, J. D. Goddard, and H. F. Schaefer, "The Reaction of Acetylene with Fulminic Acid. The Prototype 1,3-Dipolar Cycloaddition", *J. Am. Chem. Soc.* **102**, 1763 (1980).
205. R. W. Wetmore, H. F. Schaefer, P. C. Hiberty, and J. I. Brauman, "Dipole-Supported States: A Very Low-Lying Excited State of the Acetaldehyde Enolate Anion", *J. Am. Chem. Soc.* **102**, 5470 (1980).
206. M. L. Chen and H. F. Schaefer, "Potential Energy Surface for the Li + HF → LiF + H Reaction", *J. Chem. Phys.* **72**, 4376 (1980).
207. L. Radom, H. F. Schaefer, and M. A. Vincent, "The C<sub>7</sub>H<sub>6</sub> Isomers: Cycloheptatrienylidene and Phenylcarbene", *Nouv. J. Chem.* **4**, 411 (1980).
208. B. R. Brooks, W. D. Laidig, P. Saxe, and H. F. Schaefer, "A Multiconfiguration Self-Consistent-Field Formalism Utilizing the Two-Particle Density Matrix and Unitary Group Approach", *J. Chem. Phys.* **72**, 3837 (1980). Also W. D. Laidig and H. F. Schaefer, "The Loop-Driven Graphical Unitary Group Approach Applied to the MCSCF Problem", in *Recent Developments and Applications of Multiconfiguration Hartree-Fock Methods*, editor M. Dupuis, Proceedings No. 10 of the National Resource for Computation in Chemistry, February, 1981. Pages 23-26.
209. P. Saxe, Y. Yamaguchi, P. Pulay, and H. F. Schaefer, "Transition State Vibrational Analysis for the Methyl Isocyanide Rearrangement CH<sub>3</sub>NC → CH<sub>3</sub>CN", *J. Am. Chem. Soc.* **102**, 3718 (1980).
210. B. R. Brooks, W. D. Laidig, P. Saxe, J. D. Goddard, Y. Yamaguchi, and H. F. Schaefer, "Analytic Gradients from Correlated Wave Functions via the Two Particle Density Matrix and the Unitary Group Approach", *J. Chem. Phys.* **72**, 4652 (1980).
211. W. C. Swope, H. F. Schaefer, and D. R. Yarkony, "A Genealogical Electronic Coupling Procedure Incorporating the Hartree-Fock Interacting Space and Suitable for Degenerate Point Groups. Application to Excited States of BH<sub>3</sub>", *J. Chem. Phys.* **73**, 407 (1980).
212. P. Saxe and H. F. Schaefer, "Can Cyclopropyne Really Be Made?" *J. Am. Chem. Soc.* **102**, 3239 (1980).
213. W. D. Laidig and H. F. Schaefer, "Some Characteristics of the Intravalence Triplet-Triplet Electronic Transition in HCN", *J. Chem. Phys.* **73**, 1470 (1980).

214. W. D. Laidig, P. Saxe, and H. F. Schaefer, "Multiconfiguration Self-Consistent-Field Study of the Importance of Triply- and Quadruply-Excited Electronic Configurations in the Water Molecule", *J. Chem. Phys.* **73**, 1765 (1980).
215. Y. Yamaguchi and H. F. Schaefer, "A Systematic Theoretical Study of Harmonic Vibrational Frequencies: The Ammonium Ion  $\text{NH}_4^+$  and Other Simple Molecules", *J. Chem. Phys.* **73**, 2310 (1980).
216. K. S. Kim and H. F. Schaefer, "Geometric Isomerism in Triplet Carbenes: Carbohydroxycarbene", *J. Am. Chem. Soc.* **102**, 5389 (1980).
217. D. J. Fox, D. Ray, P. C. Rubesin, and H. F. Schaefer, "The Prototype Aluminum-Carbon Single, Double, and Triple Bonds:  $\text{Al-CH}_3$ ,  $\text{Al=CH}_2$ , and  $\text{Al=CH}$ ", *J. Chem. Phys.* **73**, 3246 (1980).
218. T. L. Allen, J. D. Goddard, and H. F. Schaefer, "A Possible Role for Triplet  $\text{H}_2\text{CN}^+$  Isomers in the Formation of HCN and HNC in Interstellar Clouds", *J. Chem. Phys.* **73**, 3255 (1980).
219. S. K. Gray, W. H. Miller, Y. Yamaguchi, and H. F. Schaefer, "Reaction Path Hamiltonian: Tunneling Effects in the Unimolecular Isomerization  $\text{HNC} \rightarrow \text{HCN}$ ", *J. Chem. Phys.* **73**, 2733 (1980).
220. J. Demuynck, D. J. Fox, Y. Yamaguchi, and H. F. Schaefer, "Triplet Methylnitrene: An Indefinitely Stable Species in the Absence of Collisions", *J. Am. Chem. Soc.* **102**, 6204 (1980).
221. S. P. So, R. W. Wetmore, and H. F. Schaefer, "Excited Singlet Electronic States of Acetylene: *cis* and *trans* Structures and Energetics", *J. Chem. Phys.* **73**, 5706 (1980).
222. J. D. Goddard, Y. Yoshioka, and H. F. Schaefer, "Methylsilylene, Silaethylene, and Silylmethylene: Energies, Structures, and Unimolecular Reactivities", *J. Am. Chem. Soc.* **102**, 7644 (1980).
223. S. C. DeCastro, H. F. Schaefer, and R. M. Pitzer, "Electronic Structure of the  $\text{N}_4^+$  Molecular Ion", *J. Chem. Phys.*, **74**, 550 (1981).
224. Y. Osamura, J. D. Goddard, H. F. Schaefer, and K. S. Kim, "Near Degenerate Rearrangement Between the Radical Cations of Formaldehyde and Hydroxymethylene", *J. Chem. Phys.* **74**, 617 (1981).
225. H. F. Schaefer, "Approaching the Hartree-Fock Limit for Organotransition Metal Complexes", *J. Mol. Struct.* **76**, 117 (1981).
226. Y. Yoshioka, J. D. Goddard, and H. F. Schaefer, "Analytic Configuration Interaction Gradient Studies of  $\text{SH}_4$ , Sulfurane", *J. Chem. Phys.* **74**, 1855 (1981).
227. Y. Osamura, H. F. Schaefer, S. K. Gray, and W. H. Miller, "Vinylidene: A Very Shallow Minimum on the  $\text{C}_2\text{H}_2$  Potential Energy Surface. Static and Dynamical Considerations", *J. Am. Chem. Soc.* **103**, 1904 (1981).
228. M. L. Chen, R. W. Wetmore, and H. F. Schaefer, "Mechanisms of the  $\text{H} + \text{O}_3$  Reaction", *J. Chem. Phys.*, **74**, 2938 (1981).
229. S. K. Gray, W. H. Miller, Y. Yamaguchi, and H. F. Schaefer, "Tunneling in the Unimolecular Decomposition of Formaldehyde: A More Quantitative Study", *J. Am. Chem. Soc.* **103**, 1900 (1981).
230. J. D. Goddard, Y. Yamaguchi, and H. F. Schaefer, "Features of the  $\text{H}_2\text{CO}$  Potential Energy Hypersurface Pertinent to Formaldehyde Photodissociation", *J. Chem. Phys.* **75**, 3459 (1981).
231. W. D. Laidig and H. F. Schaefer, "Large Multiconfiguration Self-Consistent-Field Wavefunctions for the Ozone Molecule", *J. Chem. Phys.* **74**, 3411 (1981).
232. Y. Osamura and H. F. Schaefer, "Internal Rotation Barrier and Transition State for Glyoxal", *J. Chem. Phys.* **74**, 4576 (1981).
233. B. R. Brooks, W. D. Laidig, P. Saxe, J. D. Goddard, and H. F. Schaefer, "New Directions for the Loop-Driven Graphical Unitary Approach: Analytic Gradients and an MCSCF Procedure", in "The Unitary Group for the Evaluation of Electronic Energy Matrix Elements", *Lecture Notes in Chemistry* Vol. 22, editor J. Hinze (Spring-Verlag, Berlin, 1981). Pages 158-176.
234. P. Saxe, H. F. Schaefer, and N. C. Handy, "Exact Solution (Within a Double-Zeta Basis Set) of Schrödinger's Electronic Equation for Water", *Chem. Phys. Lett.* **79**, 202 (1981).
235. Y. Osamura and H. F. Schaefer, "Toward the Spectroscopic Identification of Vinylidene,  $\text{H}_2\text{C=C:}$ ", *Chem. Phys. Lett.* **79**, 412 (1981).
236. P. Saxe, H. F. Schaefer, and N. C. Handy, "Methylene Singlet-Triplet Separation: An Explicit Variational Treatment of Many-Body Correlation Effects", *J. Phys. Chem.* **85**, 745 (1981).
237. D. Spangler, J. J. Wendoloski, M. Dupuis, M. L. Chen, and H. F. Schaefer, "Geometry and Electronic Structure of  $(\text{CO})_3\text{NiCH}_2$ . A Model Transition Metal Carbene", *J. Am. Chem. Soc.* **103**, 3958 (1981).
238. Y. Yoshioka, J. D. Goddard, and H. F. Schaefer, "Theoretical Challenge to the Experimentally Determined Geometrical Structure of Dimethylsilaethylene", *J. Am. Chem. Soc.* **103**, 2452 (1981).
239. Y. Yoshioka, H. F. Schaefer, and K. D. Jordan, "Theoretical Investigation of the Electron Affinity of  $\text{CO}_2$ ", *J. Chem. Phys.* **75**, 1040 (1981).
240. L. Farnell, J. Kao, L. Radom, and H. F. Schaefer, "Structures and Stabilities of Isomeric [10] Annulenes", *J. Am. Chem. Soc.* **103**, 2147 (1981).
241. M. R. Hoffman and H. F. Schaefer, "Hydroxycarbene (HCOH) and Protonated Formaldehyde: Two Potentially Observable Interstellar Molecules", *Astrophys. J.* **249**, 563 (1981).
242. M. A. Vincent and H. F. Schaefer, "Diborane(4),  $(\text{B}_2\text{H}_4)$ : The Boron Hydride Analogue of Ethylene", *J. Am. Chem. Soc.* **103**, 5677 (1981).
243. H. F. Schaefer, "Quantum Chemistry", *Encyclopedia of Science and Technology*, 5th ed. (McGraw-Hill, New York, 1982). Pages 164-168.
244. R. M. Pitzer, J. D. Goddard, and H. F. Schaefer, "Bis-(cyclobutadiene) Nickel: Geometrical and Electronic Structure", *J. Am. Chem. Soc.* **103**, 5681 (1981).
245. Y. Osamura, Y. Yamaguchi, and H. F. Schaefer, "Analytic Configuration Interaction (CI) Gradient Techniques for Potential Energy Hypersurfaces. A Method for Open-Shell Molecular Wave Functions", *J. Chem. Phys.* **75**, 2919 (1981).
246. Y. Osamura, H. F. Schaefer, M. Dupuis, and W. A. Lester, Jr., "A Unimolecular Reaction  $\text{ABC} \rightarrow \text{A} + \text{B} + \text{C}$  Involving Three Product Molecules and a Single Transition State. Photodissociation of Glyoxal:  $\text{HCOHCO} \rightarrow \text{H}_2 + \text{CO} + \text{CO}$ ", *J. Chem. Phys.* **75**, 5828 (1981).

247. Y. Yoshioka and H. F. Schaefer, "Theoretical Studies of the 1,2 Hydrogen Shift. 11. The Controversial Barrier Height Between Silaethylene and Methylsilylene", *J. Am. Chem. Soc.* **103**, 7366 (1981).
248. K. S. Kim, S. P. So, and H. F. Schaefer, "Structure and Energetics of Realistic Carbynes: (Carbohydroxy)carbyne, (HOCOC:)", *J. Am. Chem. Soc.* **104**, 1457 (1982).
249. J. D. Goddard, Y. Osamura, and H. F. Schaefer, "Complete Theoretical Structures for the Classical and Nonclassical Forms of the 2-Norbornyl Cation and for Edge-Protonated Norticyclene", *J. Am. Chem. Soc.* **104**, 3258 (1982).
250. Y. Osamura, Y. Yamaguchi, and H. F. Schaefer, "Generalization of Analytic Configuration Interaction (CI) Gradient Techniques for Potential Energy Hypersurfaces, Including a Solution to the coupled Perturbed Hartree–Fock Equations for Multiconfiguration SCF Molecular Wave Functions", *J. Chem. Phys.* **77**, 383 (1982).
251. Y. Osamura, Y. Yamaguchi, P. Saxe, M. A. Vincent, J. F. Gaw, and H. F. Schaefer, "Unified Theoretical Treatment of Analytic First and Second Energy Derivatives in Open-Shell Hartree–Fock Theory", *Chem. Phys.* **72**, 131 (1982).
252. H. F. Schaefer, "The Silicon–Carbon Double Bond: a Healthy Rivalry Between Theory and Experiment", *Acc. Chem. Res.* **15**, 283 (1982).
253. M. A. Vincent, Y. Yoshioka, and H. F. Schaefer, "High Spin Electronic States of the Experimentally Observed Molecular Ions  $\text{MnCH}_2^+$  and  $\text{CrCH}_2^+$ ", *J. Phys. Chem.* **86**, 3905 (1982).
254. P. Saxe, D. J. Fox, H. F. Schaefer, and N. C. Handy, "The Shape-Driven Graphical Unitary Group Approach to the Electron Correlation Problem. Application to the Ethylene Molecule", *J. Chem. Phys.* **77**, 5584 (1982).
255. P. Saxe, Y. Yamaguchi, and H. F. Schaefer, "Analytic Second Derivatives in Restricted Hartree–Fock Theory. A Method for High-Spin Open-Shell Molecular Wave Functions", *J. Chem. Phys.* **77**, 5647 (1982).
256. G. P. Raine, H. F. Schaefer, and R. C. Haddon, "The Dimers of Carbon Monoxide and Carbon Monosulfide. Chemically Bound Triplet Electronic Ground States", *J. Am. Chem. Soc.* **105**, 194 (1983).
257. M. A. Vincent and H. F. Schaefer, "Isomeric Structures of  $\text{CH}_2\text{LiF}$ , the Prototype Carbenoid", *J. Chem. Phys.* **77**, 6103 (1982).
258. D. J. Fox and H. F. Schaefer, "Terminal vs. Bridge Bonding of Methylene to Metal Systems:  $\text{Al}_2\text{CH}_2$  as a Model System", *J. Chem. Phys.* **78**, 328 (1983).
259. G. Fitzgerald, P. Saxe, and H. F. Schaefer, "Singlet Cyclobutene: A Relative Minimum on the  $\text{C}_4\text{H}_4$  Potential Energy Hypersurfaces?" *J. Am. Chem. Soc.* **105**, 690 (1983).
260. P. Saxe and H. F. Schaefer, "Cyclic  $D_{6h}$  Hexaazabenzene – A Relative Minimum on the  $\text{N}_6$  Potential Energy Hypersurface?" *J. Am. Chem. Soc.* **105**, 1760 (1983).
261. Y. Yamaguchi, J. F. Gaw, and H. F. Schaefer, "Molecular Clustering About a Positive Ion. Structures, Energetics and Vibrational Frequencies of the Protonated Hydrogen Clusters  $\text{H}_3^+$ ,  $\text{H}_5^+$ ,  $\text{H}_7^+$ ,  $\text{H}_9^+$ ", *J. Chem. Phys.* **78**, 4074 (1983).
262. S. Saebo, L. Radom, and H. F. Schaefer, "The Weakly Exothermic Rearrangement of Methoxy Radical ( $\text{CH}_3\text{O}$ ) to the Hydroxymethyl Radical ( $\text{CH}_2\text{OH}$ )", *J. Chem. Phys.* **78**, 845 (1983).
263. M. R. Hoffmann, Y. Yoshioka, and H. F. Schaefer, "Vibrational Frequencies for Silaacetylene and its Silylidene and Vinylidene Isomers", *J. Am. Chem. Soc.* **105**, 1084 (1983).
264. M. A. Vincent, P. Saxe, and H. F. Schaefer, "Rotational Invariance in Analytic First, Second, and Third Energy Derivative Studies in Molecular Electronic Structure Theory", *Chem. Phys. Lett.* **94**, 351 (1983).
265. Y. Yamaguchi, Y. Osamura, G. Fitzgerald, and H. F. Schaefer, "Analytic Force Constants for Post-Hartree–Fock Wave Functions: The Simplest Case", *J. Chem. Phys.* **78**, 1607 (1983).
266. J. Bicerano, H. F. Schaefer, and W. H. Miller, "Structure and Tunneling Dynamics of Malonaldehyde, A Theoretical Study", *J. Am. Chem. Soc.* **105**, 2550 (1983).
267. Y. Osamura, Y. Yamaguchi, P. Saxe, D. J. Fox, M. A. Vincent, and H. F. Schaefer, "Analytic Second Derivative Techniques for Self-Consistent-Field Wave Functions. A New Approach to the Solution of the Coupled Perturbed Hartree–Fock Equations", *J. Mol. Struct. (Kenichi Fukui Issue)* **103**, 183 (1983).
268. P. S. Bagus, H. F. Schaefer, and C. W. Bauschlicher, "The Convergence of the Cluster Model for the Study of Chemisorption:  $\text{Be}_{36}\text{H}$ ", *J. Chem. Phys.* **78**, 1390 (1983).
269. K. S. Kim, H. F. Schaefer, L. Radom, J. A. Pople, and J. S. Binkley, "Vibrational Frequencies of the HCCN Molecule. A Near Degeneracy Between Bent Cyano-carbene and Linear Allene-Related Geometries", *J. Am. Chem. Soc.* **105**, 4148 (1983).
270. M. A. Vincent, H. F. Schaefer, A. Schier, and H. Schmidbaur, "Molecular and Electronic Structure of Phosphonium Cyclopropylide ( $\text{H}_3\text{P}=\text{C}(\text{CH}_2)_2$ ): A Theoretical Study", *J. Am. Chem. Soc.* **105**, 3806 (1983).
271. G. Fitzgerald and H. F. Schaefer, "Structures, Energetics, and Vibrational Frequencies of Cyclopropyne", *Isr. J. Chem.* **23**, 93 (1983).
272. M. A. Vincent and H. F. Schaefer, "Some Unexpected Relationships Between First, Second and Third Derivative Electron Repulsion Integrals for Diatomic and Triatomic Molecules", *Theor. Chim. Acta* **64**, 21 (1983).
273. M. E. Colvin, G. P. Raine, H. F. Schaefer, and M. Dupuis, "Infrared Intensities of  $\text{H}_3\text{O}^+$ ,  $\text{H}_2\text{DO}^+$ ,  $\text{HD}_2\text{O}^+$ , and  $\text{D}_3\text{O}^+$ ", *J. Chem. Phys.* **79**, 1551 (1983).
274. R. S. Grev and H. F. Schaefer, "Transition State and Barrier Height for the Silanediyl Insertion Reaction  $\text{SiH}_2 + \text{H}_2 \rightarrow \text{SiH}_4$ ", *J. Chem. Soc., Chem. Commun.* 785 (1983).
275. M. E. Colvin, R. S. Grev and H. F. Schaefer, and J. Bicerano, " $\tilde{X}^1\text{A}_1$ ,  $\tilde{a}^3\text{B}_1$ , and  $\tilde{\text{A}}^1\text{B}_1$  Electronic States of Silylenes. Structures and Vibrational Frequencies of  $\text{SiH}_2$ ,  $\text{SiHF}$ , and  $\text{SiF}_2$ ", *Chem. Phys. Lett.* **99**, 399 (1983).
276. G. Fitzgerald and H. F. Schaefer, "In Pursuit of Cyclobutene: Stable and Potentially Observable Species", *Ind. Chem. News* **4**, No. 7, July 1983, page 32.
277. Y. Yamaguchi, Y. Osamura, and H. F. Schaefer "Analytic Energy Second Derivatives for Two-Configuration Self-Consistent-Field Wavefunctions. Application to Twisted Ethylene and to the Trimethylene Diradical", *J. Am. Chem. Soc.* **105**, 7506 (1983).



278. K. Raghavachari, R. C. Haddon, P. R. Schleyer, and H. F. Schaefer, "Effects of Electron Correlation on the Energies of 2-Norbornyl Cation Structures. Evaluation of the Nonclassical Stabilization Energy", *J. Am. Chem. Soc.* **105**, 5915 (1983).
279. M. R. Hoffmann, W. D. Laidig, K. S. Kim, D. J. Fox, and H. F. Schaefer, "Electronic Symmetry Breaking in Polyatomic Molecules. Multiconfiguration Self-Consistent-Field Study of the Cyclopropenyl Radical,  $C_3H_3$ ", *J. Chem. Phys.* **80**, 338 (1984).
280. G. P. Raine, H. F. Schaefer, and N. C. Handy, "The  $HO_2^+$  Molecular Ion. Geometrical Structure and Vibrational Frequencies", *J. Chem. Phys.* **80**, 319 (1984).
281. D. J. Fox, Y. Osamura, M. R. Hoffmann, J. F. Gaw, G. Fitzgerald, Y. Yamaguchi, and H. F. Schaefer, "Analytic Energy Second Derivatives for General Correlated Wavefunctions, Including a Solution of the First-Order Coupled-Perturbed Configuration-Interaction Equations", *Chem. Phys. Lett.* **102**, 17 (1983).
282. J. Breulet and H. F. Schaefer, "Conrotatory and Disrotatory Stationary Points for the Electrocyclic Isomerization of Cyclobutene to *cis*-Butadiene", *J. Am. Chem. Soc.* **106**, 1221 (1984).
283. M. R. Hoffmann, D. J. Fox, J. F. Gaw, Y. Osamura, Y. Yamaguchi, R. S. Grev, G. Fitzgerald, H. F. Schaefer, P. J. Knowles, and N. C. Handy, "Analytic Energy Second Derivatives for General MCSCF Wavefunctions", *J. Chem. Phys.* **80**, 2660 (1984).
284. H. F. Schaefer, "Applications of Molecular Quantum Mechanics to Problems in Chemistry", in *Chemistry for the Future*, editor H. Gr̄unewald (Pergamon, Oxford, 1984). Pages 247–253.
285. T. J. Lee and H. F. Schaefer, "Vibrational Frequencies and Infrared Intensities for  $H_2CN^+$ , Protonated HCN", *J. Chem. Phys.* **80**, 2977 (1984).
286. N. C. Handy, R. J. Harrison, P. J. Knowles, and H. F. Schaefer, "An Accurate Variational Wavefunction for Lithium Hydride", *J. Phys. Chem.* **88**, 4852 (1984).
287. W. D. Laidig, Y. Yamaguchi, and H. F. Schaefer, "Where to Look for the Electronic Spectrum of Hydrogen Isocyanide, HNC", *J. Chem. Phys.* **80**, 3069 (1984).
288. R. S. Grev and H. F. Schaefer, "An Energetically Low-Lying Silacyclopropyne Isomer of  $SiC_2$ ", *J. Chem. Phys.* **80**, 3552 (1984).
289. J. F. Gaw, Y. Yamaguchi, M. A. Vincent, and H. F. Schaefer, "Vibrational Frequency Shifts in Hydrogen-Bonded Systems: The Hydrogen Fluoride Dimer and Trimer", *J. Am. Chem. Soc.* **106**, 3133 (1984).
290. L. M. Ziurys, D. P. Clemens, R. J. Saykally, M. E. Colvin, and H. F. Schaefer, "A Search for Interstellar Silicon Nitride", *Astrophys. J.* **281**, 219 (1984).
291. M. E. Colvin, J. Breulet, and H. F. Schaefer, "When Might Silylenes Behave More Like Carbenes?  $SiHLi$ , a Triplet Silylene", *Tetrahedron Symposium-in-Print* **41**, 1429 (1985).
292. T. Carrington, L. M. Hubbard, H. F. Schaefer, and W. H. Miller "Vinylidene: Potential Energy Surface and Unimolecular Reaction Dynamics", *J. Chem. Phys.* **80**, 4347 (1984).
293. M. J. Frisch, J. S. Binkley, and H. F. Schaefer, "Ab Initio Calculation of Reaction Energies. Basis Set Dependence of Relative Energies on the  $FH_2$  and  $H_2CO$  Potential Energy Surfaces", *J. Chem. Phys.* **81**, 1882 (1984).
294. T. J. Lee, D. J. Fox, H. F. Schaefer, and R. M. Pitzer, "Analytic Second Derivatives for Renner-Teller Potential Energy Surfaces. Examples of the Five Distinct Cases", *J. Chem. Phys.* **81**, 356 (1984).
295. H. F. Schaefer, *Quantum Chemistry: The Development of Ab Initio Methods in Molecular Electronic Structure Theory* (Clarendon Press, Oxford England, 1984). 142 pages. Reprinted in paperback by Dover Publications (Mineola, NY, 2004).
296. G. Fitzgerald and H. F. Schaefer, "The Cyclic, Two-Hydrogen-Bond, Form of the  $HO_2$  Dimer", *J. Chem. Phys.* **81**, 362 (1984).
297. Y. Yamaguchi and H. F. Schaefer, "Equilibrium Geometries for Triplet Trimethylene,  $CH_2CH_2CH_2$ ", *J. Am. Chem. Soc.* **106**, 5115 (1984).
298. J. Breulet, T. J. Lee, and H. F. Schaefer, "Comparison Between the *s-Cis* and *Gauche* Conformers of 1,3-Butadiene", *J. Am. Chem. Soc.* **106**, 6250 (1984).
299. C. E. Dykstra and H. F. Schaefer, "Computer Technology in Quantum Chemistry", in *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules*, editor C. E. Dykstra (D. Reidel, Dordrecht, Holland, 1984). Pages 197–202.
300. G. P. Raine and H. F. Schaefer, "Vibrational Frequencies for the Classical and Nonclassical Forms of Protonated Acetylene –  $C_2H_3^+$ ", *J. Chem. Phys.* **81**, 4034 (1984).
301. N. C. Handy and H. F. Schaefer, "On the Evaluation of Analytic Energy Derivatives for Correlated Wavefunctions", *J. Chem. Phys.* **81**, 5031 (1984).
302. G. Frenking and H. F. Schaefer, "The Nature of the Boron–Carbon Double Bond in 2,4-Diboramethylenecyclopropane", *Chem. Phys. Lett.* **109**, 521 (1984).
303. T. J. Lee, A. Bunge, and H. F. Schaefer, "Toward the Laboratory Identification of Cyclopropenylidene", *J. Am. Chem. Soc.* **107**, 137 (1985).
304. J. F. Gaw, Y. Yamaguchi, and H. F. Schaefer, "Analytic Third Derivatives for Self-Consistent-Field Wave Functions", *J. Chem. Phys.* **81**, 6395 (1984).
305. M. E. Colvin and H. F. Schaefer, "Silacyclobutadiene: Singlet and Triplet Geometries, Vibrational Frequencies, and Electronic Structures", *Faraday Symp. Chem. Soc.* **19**, 39 (1984).
306. G. Frenking and H. F. Schaefer, "The Silaformyl Radical  $HSiO$  and its Energetically Lower-Lying Isomer  $SiOH$ ", *J. Chem. Phys.* **82**, 4585 (1985).
307. M. J. Frisch, B. Liu, J. S. Binkley, H. F. Schaefer, and W. H. Miller, "Further Theoretical Examination of the  $F + H_2$  Entrance Channel Barrier", *Chem. Phys. Lett.* **114**, 1 (1985).
308. M. J. Frisch, A. C. Scheiner, H. F. Schaefer, and J. S. Binkley, "The Malonaldehyde Equilibrium Geometry: A Major Structural Shift Due to the Effects of Electron Correlation", *J. Chem. Phys.* **82**, 4194 (1985).
309. M. J. Frisch, H. F. Schaefer, and J. S. Binkley, "Theoretical Study of the Structure and Spectroscopic Characteristics of Protonated Carbon Dioxide", *J. Phys. Chem.* **89**, 2192 (1985).
310. R. S. Grev and H. F. Schaefer, "Geometrical Structure and Vibrational Frequencies of Several Electronic States of  $Si_2C$ ", *J. Chem. Phys.* **82**, 4126 (1985).
311. H. F. Schaefer, "Fifth American Conference on Theoretical Chemistry", *J. Phys. Chem.* **89**, 2121 (1985).

312. M. R. Hoffmann and H. F. Schaefer, "The Treatment of Triple Excitations within the Coupled Cluster Description of Molecular Electronic Structure", *J. Chem. Phys.* **83**, 703 (1985).
313. T. J. Lee and H. F. Schaefer, "Systematic Study of Molecular Anions Within the Self-Consistent-Field Approximation:  $\text{OH}^-$ ,  $\text{CN}^-$ ,  $\text{C}_2\text{H}^-$ ,  $\text{NH}_2^-$ , and  $\text{CH}_3^-$ ", *J. Chem. Phys.* **83**, 1784 (1985).
314. A. C. Scheiner and H. F. Schaefer, "Why the Energetic Minimum Al - Vinylidene is Not Observed in Low-Temperature Aluminum + Acetylene Reactions", *J. Am. Chem. Soc.* **107**, 4451 (1985).
315. G. Fitzgerald and H. F. Schaefer, "Analytic Energy Derivative Methods for Excited States of the Same Symmetry as the Electronic Ground State", *J. Chem. Phys.* **83**, 1162 (1985).
316. M. R. Hoffmann and H. F. Schaefer, "A Full Coupled-Cluster Singles, Doubles, and Triples Model for the Descriptions of Electron Correlation", *Adv. Quantum Chem.* **18**, 207 (1986).
317. J. F. Gaw and H. F. Schaefer, "Molecular Structures and Energetics for the Lowest Triplet States of Glyoxal", *J. Chem. Phys.* **83**, 1741 (1985).
318. H. F. Schaefer and Y. Yamaguchi, "A New Dimension to Quantum Chemistry: Theoretical Methods for the Analytic Evaluation of First, Second, and Third Derivatives of the Molecular Electronic Energy with Respect to Nuclear Coordinates", *J. Mol. Struct.* **135** (Robert S. Mulliken Issue) 369 (1986).
319. R. S. Grev and H. F. Schaefer, "The Ground State of  $\text{Si}_3$ . Two Near Degenerate Isomers", *Chem. Phys. Lett.* **119**, 111 (1985).
320. T. J. Lee, H. F. Schaefer, and E. A. Magnusson, "Geometrical Structures of Four Conformers of the Phosphocanium Ion,  $\text{P}(\text{C}_2\text{H}_5)_2^+$ . A Phosphorous Sandwich?" *J. Am. Chem. Soc.* **107**, 7239 (1985).
321. M. E. Colvin, H. F. Schaefer, and J. Bicerano, "SiLiF: The Competition between Electronic Effects Favoring Singlet and Triplet Ground States. A Case Study", *J. Chem. Phys.* **83**, 4581 (1985).
322. R. Murphy, H. F. Schaefer, R. H. Nobes, L. Radom, and R. M. Pitzer, "The Equilibrium Geometry of  $\text{F}_2^+$  in its Ground Electronic State. A Simple Example of the Effects of Symmetry Breaking on an Observable Molecular Property", *Int. Rev. Phys. Chem.* **5** (David P. Craig Issue) 229 (1986).
323. T. L. Allen, A. C. Scheiner, Y. Yamaguchi, and H. F. Schaefer, "Low-Lying Triplet States of Diphosphene,  $\text{HP}=\text{PH}$ , and Diphosphinylidene,  $\text{H}_2\text{P}=\text{P}$ ", *Chem. Phys. Lett.* **121**, 154 (1985).
324. E. Magnusson and H. F. Schaefer, "Multiple d-Type Basis Functions for Molecules Containing Second Row Atoms", *J. Chem. Phys.* **83**, 5721 (1985).
325. G. Fitzgerald, T. J. Lee, H. F. Schaefer, and R. J. Bartlett, "The Open Chain or Chemically Bonded Structure of  $\text{H}_2\text{O}_4$ : the Hydroperoxyl Radical Dimer", *J. Chem. Phys.* **83**, 6275 (1985).
326. H. F. Schaefer, "The  $\text{F} + \text{H}_2$  Potential Energy Surface: The Ecstasy and the Agony" (Feature Article), *J. Phys. Chem.* **89**, 5336 (1985).
327. M. R. Hoffmann and H. F. Schaefer, "MCSCF Energy Derivatives Using Fock Operator Methods", in *Geometrical Derivatives of Energy Surfaces and Molecular Properties*, editors P. Jorgensen and J. Simons (D. Reidel, Dordrecht, Holland, 1986). Pages 63–77.
328. H. F. Schaefer, "Methylene: A Paradigm for Computational Quantum Chemistry", *Science* **231**, 1100 (1986).
329. R. Murphy and H. F. Schaefer, "Vibrational Frequencies of Small Metal Clusters. The Beryllium Tetramer", in *Applied Quantum Chemistry*, editors V. H. Smith, H. F. Schaefer, and K. Morokuma (D. Reidel, Dordrecht, Holland, 1986). Pages 431–438.
330. *Book*: V. H. Smith, H. F. Schaefer, and K. Morokuma, Co-editors, *Applied Quantum Chemistry* (D. Reidel, Dordrecht, Holland, 1986).
331. M. J. Frisch, J. E. Del Bene, J. S. Binkley, and H. F. Schaefer, "Extensive Theoretical Studies of the Hydrogen-Bonded Complexes  $(\text{H}_2\text{O})_2$ ,  $(\text{H}_2\text{O})_2\text{H}^+$ ,  $(\text{HF})_2$ ,  $(\text{HF})_2\text{H}^+$ ,  $\text{F}_2\text{H}^-$ , and  $(\text{NH}_3)_2$ ", *J. Chem. Phys.* **84**, 2279 (1986).
332. Y. Yamaguchi, M. J. Frisch, J. F. Gaw, H. F. Schaefer, and J. S. Binkley, "Analytic Evaluation and Basis Set Dependence of Intensities of Infrared Spectra", *J. Chem. Phys.* **84**, 2262 (1986).
333. D. A. Clabo and H. F. Schaefer, "The Silicon Analogue of Benzene-Hexasilabenzene ( $\text{Si}_6\text{H}_6$ )", *J. Chem. Phys.* **84**, 1664 (1986).
334. M. J. Frisch, Y. Yamaguchi, J. F. Gaw, and H. F. Schaefer, "Analytic Raman Intensities from Molecular Electronic Wave Functions", *J. Chem. Phys.* **84**, 531 (1986).
335. Y. Yamaguchi, M. J. Frisch, T. J. Lee, H. F. Schaefer, and J. S. Binkley, "Analytic Evaluation of Infrared Intensities and Polarizabilities by Two-Configuration Self-Consistent Field Wave Functions", *Theor. Chim. Acta* **69**, 337 (1986).
336. W. D. Allen and H. F. Schaefer, "Ab Initio Studies of the Low-Lying Electronic States of Ketene", *J. Chem. Phys.* **84**, 2212 (1986).
337. Y. Osamura, Y. Yamaguchi, and H. F. Schaefer, "Second-Order Coupled Perturbed Hartree-Fock Equations for Closed-Shell and Open-Shell Self-Consistent-Field Wavefunctions", *Chem. Phys.* **103**, 227 (1986).
338. W. D. Allen, J. E. Bertie, M. V. Falk, B. A. Hess, G. B. Mast, D. A. Othen, L. J. Schaad, and H. F. Schaefer, "The Experimental Vibrational Spectra, Vibrational Assignment and Normal Coordinate Analysis of Thiirane- $\text{h}_4$  and - $\text{d}_4$  and cis- and trans-1,2-Dideuteriothiirane; and Ab Initio Theoretical IR Spectra of Thiirane, Thiirene and Isotopically Substituted Derivatives", *J. Chem. Phys.* **84**, 4211 (1986).
339. G. Frenking, R. B. Remington, and H. F. Schaefer, "Structures and Energies of Singlet Silacyclopropenylidene and 14 Higher Lying  $\text{C}_2\text{SiH}_2$  Isomers", *J. Am. Chem. Soc.* **108**, 2169 (1986).
340. M. Dupuis, G. Fitzgerald, B. Hammond, W. A. Lester, and H. F. Schaefer, "Theoretical Study of the  $\text{H} + \text{O}_3 \leftrightarrow \text{OH} + \text{O}_2 \leftrightarrow \text{O} + \text{HO}_2$  System", *J. Chem. Phys.* **84**, 2691 (1986).
341. N. C. Handy, Y. Yamaguchi, and H. F. Schaefer, "The Diagonal Correction to the Born-Oppenheimer Approximation: Its Effect on the Singlet-Triplet Splitting of  $\text{CH}_2$  and Other Molecular Effects", *J. Chem. Phys.* **84**, 4481 (1986).

342. R. B. Remington, T. J. Lee, and H. F. Schaefer, "[5] Paracyclophane: Molecular Structure and Implications for Aromaticity", *Chem. Phys. Lett.* **124**, 199 (1986).
343. J. S. Binkley, M. J. Frisch, and H. F. Schaefer, "Vibrational Frequencies and Infrared Intensities for Malonaldehyde: A Post-Hartree-Fock Theoretical Study", *Chem. Phys. Lett.* **126**, 1 (1986).
344. G. E. Scuseria, M. Duran, R. G. A. R. Maclagan, and H. F. Schaefer, "Halocarbenes CHF, CHCl, and CHBr: Geometries, Singlet-Triplet Separations, and Vibrational Frequencies", *J. Am. Chem. Soc.* **108**, 3248 (1986).
345. G. E. Scuseria, T. J. Lee, R. J. Saykally, and H. F. Schaefer, "Nitrogen Quadrupole Coupling Constants for HCN and  $\text{H}_2\text{CN}^+$ : Explanation of the Absence of Fine Structure in the Microwave Spectrum of Interstellar  $\text{H}_2\text{CN}^+$ ", *J. Chem. Phys.* **84**, 5711 (1986).
346. J. E. Rice, R. D. Amos, N. C. Handy, T. J. Lee, and H. F. Schaefer, "The Analytic Configuration Interaction Gradient Method: Application to the Cyclic and Open Isomers of the  $\text{S}_3$  Molecule", *J. Chem. Phys.* **85**, 963 (1986).
347. D. A. Clabo and H. F. Schaefer, "Fluorine Peroxide (FOOF): A Continuing Problem for Normally Reliable Theoretical Methods", *Int. J. Quantum Chem.* (Andrew C. Hurley Issue) **31**, 429 (1987).
348. D. A. Clabo and H. F. Schaefer, "Tetrasilatetrahydrene", *J. Am. Chem. Soc.* **108**, 4344 (1986).
349. G. E. Scuseria and H. F. Schaefer, "Vibrational Frequencies and Geometries for the Open HF Trimer", *Chem. Phys.* **107**, 33 (1986).
350. W. D. Allen and H. F. Schaefer, "Geometrical Structures, Force Constants, and Vibrational Spectra of SiH, SiH<sub>2</sub>, SiH<sub>3</sub>, and SiH<sub>4</sub>", *Chem. Phys.* **108**, 243 (1986).
351. R. S. Grev and H. F. Schaefer, "The Ultraviolet Spectrum of Dimethylsilylene", *J. Am. Chem. Soc.* **108**, 5804 (1986).
352. T. J. Lee and H. F. Schaefer, "The Classical and Nonclassical Forms of Protonated Acetylene,  $\text{C}_2\text{H}_3^+$ . Structures, Vibrational Frequencies, and Infrared Intensities from Explicitly Correlated Wave Functions", *J. Chem. Phys.* **85**, 3437 (1986).
353. T. J. Lee, N. C. Handy, J. E. Rice, A. C. Scheiner, and H. F. Schaefer, "The Efficient Evaluation of Configuration Interaction Analytic Energy Second Derivatives: Application to Hydrogen Thioperoxide, HSOH", *J. Chem. Phys.* **85**, 3930 (1986).
354. M. E. Colvin, J. Kobayashi, J. Bicerano, and H. F. Schaefer, "The Infrared Spectrum of Silaethylene", *J. Chem. Phys.* **85**, 4563 (1986).
355. G. E. Scuseria, T. J. Lee, and H. F. Schaefer, "Accelerating the Convergence of the Coupled-Cluster Approach. The Use of the DIIS Method", *Chem. Phys. Lett.* **130**, 236 (1986).
356. J. F. Gaw, Y. Yamaguchi, H. F. Schaefer, and N. C. Handy, "Generalization of Analytic Energy Third Derivatives for the RHF Closed-Shell Wave Function: Derivative Energy and Integral Formalisms and the Prediction of Vibration-Rotation Interaction Constants", *J. Chem. Phys.* **85**, 5132 (1986).
357. J. E. Rice, T. J. Lee, and H. F. Schaefer, "Molecular Structure and Infrared Spectrum of Protonated Nitrous Oxide", *Chem. Phys. Lett.* **130**, 333 (1986).
358. J. F. Gaw, Y. Yamaguchi, R. B. Remington, Y. Osamura, and H. F. Schaefer, "Analytic Energy Third Derivatives for Open-Shell Self-Consistent Field Wavefunctions", *Chem. Phys.* **109**, 237 (1986).
359. T. L. Allen, A. C. Scheiner, Y. Yamaguchi, and H. F. Schaefer, "Theoretical Studies of Diphospene and Diphosphinylidene in Their Closed Shell States, Low-Lying Open-Shell Singlet and Triplet States, and Transition States. Search for a Stable Bridged Structure", *J. Am. Chem. Soc.* **108**, 7579 (1986).
360. C. L. Janssen, W. D. Allen, H. F. Schaefer, and J. M. Bowman, "The Infrared Spectrum of the Hydrogen Bifluoride Anion: Unprecedented Variation with Level of Theory", *Chem. Phys. Lett.* **131**, 352 (1986).
361. A. C. Scheiner, G. E. Scuseria, and H. F. Schaefer, "Mechanism of the Photodissociation of s-Tetrazine: A Unimolecular Triple Dissociation", *J. Am. Chem. Soc.* **108**, 8160 (1986).
362. T. J. Lee, J. E. Rice, and H. F. Schaefer, "The Infrared Spectrum of the Acetylene Radical Cation  $\text{C}_2\text{H}_2^+$ . A Theoretical Study Using SCF, MCSCF, and CI Methods", *J. Chem. Phys.* **86**, 3051 (1987).
363. G. E. Scuseria, A. C. Scheiner, T. J. Lee, J. E. Rice, and H. F. Schaefer, "The Closed-Shell Coupled Cluster Single and Double Excitation (CCSD) Model for the Description of Electron Correlation. A Comparison with Configuration Interaction (CID) Results", *J. Chem. Phys.* **86**, 2881 (1987).
364. R. A. Whiteside, J. S. Binkley, M. E. Colvin, and H. F. Schaefer, "Parallel Algorithms for Quantum Chemistry. 1. Integral Transformations on a Hypercube Processor", *J. Chem. Phys.* **86**, 2185 (1987).
365. M. Okamura, L. I. Yeh, D. Normand, J. J. H. van den Biesen, S. W. Bustamente, Y. T. Lee, T. J. Lee, N. C. Handy, and H. F. Schaefer, "Radiative Decay Lifetimes of  $\text{CH}_2^+$ ", *J. Chem. Phys.* **86**, 3807 (1987).
366. J. E. Rice, T. J. Lee, R. B. Remington, W. D. Allen, D. A. Clabo, and H. F. Schaefer, "[5] Paracyclophane: An Important Example of Ring Strain and Aromaticity in Hydrocarbon Compounds", *J. Am. Chem. Soc.* **109**, 2902 (1987).
367. Y. Yamaguchi, J. F. Gaw, R. B. Remington, and H. F. Schaefer, "The  $\text{H}_5^+$  Potential Energy Hypersurface: Characterization of Ten Distinct Energetically Low-Lying Stationary Points", *J. Chem. Phys.* **86**, 5072 (1987).
368. B. A. Hess, W. D. Allen, D. Michalska, L. J. Schaad, and H. F. Schaefer, "An Ab Initio Study of the Vibrational Spectrum of Bicyclo[1.1.0]but-1(3)-ene", *J. Am. Chem. Soc.* **109**, 1615 (1987).
369. Y. Osamura, Y. Yamaguchi, and H. F. Schaefer, "Generalization of Analytic Energy Derivatives for Configuration Interaction Wave Functions", *Theor. Chim. Acta* **72**, 71 (1987).
370. B. H. Lengsfeld, S. Havriliak, M. E. Colvin, and H. F. Schaefer, "Analytic MCSCF Infrared Intensities: Application to Formaldehyde", *Chem. Phys. Lett.* **135**, 340 (1987).
371. J. E. Rice and H. F. Schaefer, "A Multiconfiguration Self-Consistent-Field (MCSCF) Study of the Bent and Linear Conformations of HCCN", *J. Chem. Phys.* **86**, 7051 (1987).

372. A. Rajca, J. E. Rice, A. Streitwieser, and H. F. Schaefer, "Metaphosphate and Trimethylenemetaphosphate ( $(\text{P}(\text{CH}_2)_3^-)$  Anions: Do They Have Three Double Bonds to Phosphorus?", *J. Am. Chem. Soc.* **109**, 4189 (1987).
373. Y. Osamura, Y. Yamaguchi, and H. F. Schaefer, "Correspondence Between Higher Order Energy Derivative Formalisms for Restricted Hartree-Fock and Correlated Wavefunctions", *Theor. Chim. Acta* **72**, 93 (1987).
374. A. C. Scheiner and H. F. Schaefer, "The Electronic Spectrum of s-Tetrazine: Structures and Vibrational Frequencies of the Ground and Excited Electronic States", *J. Chem. Phys.* **87**, 3539 (1987).
375. H. F. Schaefer, "Yuan T. Lee - 1986 Nobel Prize in Chemistry", in *Nobel Prize Winners*, editor Tyler Wasson (H. W. Wilson, New York, 1987). Pages 617-619.
376. C. L. Janssen and H. F. Schaefer, "Cycloheptatrienyldiene Singlet-Triplet Energetics: Theory Responds", *J. Am. Chem. Soc.* **109**, 5030 (1987).
377. R. S. Grev and H. F. Schaefer, "Cyclopolysilanes: Structure, Strain, and the Form of the SOMO in their Radical-Anions", *J. Am. Chem. Soc.* **109**, 6569 (1987).
378. T. J. Lee, G. E. Scuseria, J. E. Rice, A. C. Scheiner, and H. F. Schaefer, "Comparison of Single and Double Excitation Coupled Cluster and Configuration Interaction Theories: Determination of Structure and Equilibrium Properties of Diatomic Molecules", *Chem. Phys. Lett.* **139**, 134 (1987).
379. G. E. Scuseria, A. C. Scheiner, J. E. Rice, T. J. Lee, and H. F. Schaefer, "Analytic Evaluation of Energy Gradients for the Single and Double Excitation Coupled Cluster (CCSD) Wave Function: A Comparison with Configuration Interaction (CISD, CISDT, and CISDTQ) Results for the Harmonic Vibrational Frequencies, Infrared Intensities, Dipole Moment, and Inversion Barrier of Ammonia", *Int. J. Quantum Chem. Symp.* **21**, 495 (1987).
380. R. S. Grev and H. F. Schaefer, "Hetero-Substituted Cyclopolysilanes: Unusual Structures and a New Model of Bonding in 1,3-Disubstituted Four-Membered Rings", *J. Am. Chem. Soc.* **109**, 6577 (1987).
381. A. C. Scheiner, G. E. Scuseria, J. E. Rice, T. J. Lee, and H. F. Schaefer, "Analytic Evaluation of Energy Gradients for the Single and Double Excitation Coupled Cluster (CCSD) Wave Function: Theory and Application", *J. Chem. Phys.* **87**, 5361 (1987).
382. G. E. Scuseria and H. F. Schaefer, "The Nuclear Quadrupole Moment of  $^{14}\text{N}$ . A Theoretical Prediction from Full Valence Shell and Full Configuration Interaction Atomic Wavefunctions", *J. Chem. Phys.* **87**, 4020 (1987).
383. M. Duran, Y. Yamaguchi, Y. Osamura, and H. F. Schaefer, "Analytical Energy Third Derivatives for Two-Configuration Self-Consistent-Field Wavefunctions", *J. Mol. Struct. (Michael J. S. Dewar Issue)* **163**, 389 (1988).
384. W. D. Allen and H. F. Schaefer, "An Examination of the  $2^1\text{A}_1$  States of Formaldehyde and Ketene Including Analytic Configuration Interaction Energy First Derivatives for Singlet Excited Electronic States of the Same Symmetry as the Ground State", *J. Chem. Phys.* **87**, 7076 (1987).
385. Y. T. Chang, Y. Yamaguchi, W. H. Miller, and H. F. Schaefer, "An Analysis of the Infrared and Raman Spectra of the Formic Acid Dimer ( $\text{HCOOH}$ ) $_2$ ", *J. Am. Chem. Soc.* **109**, 7245 (1987).
386. T. J. Lee, W. D. Allen, and H. F. Schaefer, "The Analytic Evaluation of Energy First Derivatives for Two-Configuration Self-Consistent-Field Configuration Interaction (TCSCF-CI) Wave Functions. Application to Ozone and Ethylene", *J. Chem. Phys.* **87**, 7062 (1987).
387. B. S. Thies, R. S. Grev, and H. F. Schaefer, "Dimethyldisilyne: A Fleetingly Observed Species Incorporating a Triple Bond?", *Chem. Phys. Lett.* **140**, 355 (1987).
388. C. P. Blahous and H. F. Schaefer, "Geometrical Structure and Vibrational Frequencies for the Oxygen Analogue of Hexasulfur", *J. Phys. Chem. (Massimo Simonetta Memorial Issue)* **92**, 959 (1988).
389. D. A. Clabo, W. D. Allen, R. B. Remington, Y. Yamaguchi, and H. F. Schaefer, "A Systematic Study of Molecular Vibrational Anharmonicity and Vibration-Rotation Interaction by Self-Consistent-Field Higher-Derivative Methods. Asymmetric Top Molecules", *Chem. Phys.* **123**, 187 (1988).
390. E. D. Simandiras, R. D. Amos, N. C. Handy, T. J. Lee, J. E. Rice, R. B. Remington, and H. F. Schaefer, "Second-Order Perturbation Theory and Configuration Interaction Theory Applied to Medium-Sized Molecules: Cyclopropane, Ethylenimine, Ethylene Oxide, Fluoroethane, and Acetaldehyde", *J. Am. Chem. Soc.* **110**, 1388 (1988).
391. G. E. Scuseria and H. F. Schaefer, "The Optimization of Molecular Orbitals for Coupled Cluster Wavefunctions", *Chem. Phys. Lett.* **142**, 354 (1987).
392. B. Kim, H. S. Johnston, D. A. Clabo, and H. F. Schaefer, "Vertical Electronic Spectrum of  $\text{NO}_3$ :  $^2\text{A}_2'$ ,  $^2\text{E}''$ ,  $^2\text{A}_2'$ ,  $^2\text{B}_1$ , and  $^2\text{E}'$  States", *J. Chem. Phys.* **88**, 3204 (1988).
393. B. F. Yates, D. A. Clabo, and H. F. Schaefer, "Cyclic Isomers of Singlet  $\text{Si}_4\text{H}_4$  Related to Tetrasilacyclobutadiene", *Chem. Phys. Lett.* **143**, 421 (1988).
394. M. Duran, Y. Yamaguchi, R. B. Remington, and H. F. Schaefer, "Analytic Energy Second Derivatives for Paired-Excited Multi-Configuration Self-Consistent-Field Wavefunctions. Application of the PEMCSCF Model to  $\text{H}_2\text{O}$ ,  $\text{CH}_2$ ,  $\text{HCN}$ ,  $\text{HCC}$ ,  $\text{HCO}$ ,  $\text{NH}_3$ ,  $\text{CH}_4$ , and  $\text{C}_2\text{H}_4$ ", *Chem. Phys.* **122**, 201 (1988).
395. M. Duran, Y. Yamaguchi, and H. F. Schaefer, "Analytic Energy Second Derivatives for Open-Shell Two-Configuration Self-Consistent-Field Wave Functions: Application to Carbyne and Silyne Least-Motion Insertion Reactions", Proceedings of the Sixth American Conference on Theoretical Chemistry (ACTC), *J. Phys. Chem.* **92**, 3070 (1988).
396. G. E. Scuseria and H. F. Schaefer, "Variational Studies of the Importance of Triple and Quadruple Excitations on the Barrier Height for  $\text{F} + \text{H}_2 \rightarrow \text{FH} + \text{H}$ ", *J. Chem. Phys.* **88**, 7024 (1988).
397. T. J. Lee, J. E. Rice, W. D. Allen, R. B. Remington, and H. F. Schaefer, "How Bent can a Benzene Be? The Molecular Structure, Infrared Spectrum and Energetics of [6] Paracyclophane", *Chem. Phys.* **123**, 1 (1988).
398. E. T. Seidl and H. F. Schaefer, "Theoretical Studies of Oxygen Rings: Cyclotetraoxygen,  $\text{O}_4$ ", *J. Chem. Phys.* **88**, 7043 (1988).
399. W. D. Allen and H. F. Schaefer, "Reaction Paths for the Dissociation of  $\tilde{a}^3\text{A}'' \text{CH}_2\text{CO} \rightarrow \tilde{\text{X}}^3\text{B}_1 \text{CH}_2 + \tilde{\text{X}}^1\Sigma^+ \text{CO}$ ", *J. Chem. Phys.* **89**, 329 (1988).

400. G. E. Scuseria and H. F. Schaefer, "Analytic Evaluation of Energy Gradients for the Single, Double, and Linearized Triple Excitation Coupled Cluster CCSDT-1 Wavefunction: Theory and Applications", *Chem. Phys. Lett.* **146**, 23 (1988).
401. T. J. Lee, R. B. Remington, Y. Yamaguchi, and H. F. Schaefer, "The Effects of Triple and Quadruple Excitations in Configuration Interaction Procedures for the Quantum Mechanical Prediction of Molecular Properties", *J. Chem. Phys.* **89**, 408 (1988).
402. B. H. Besler, G. E. Scuseria, A. C. Scheiner, and H. F. Schaefer, "A Systematic Theoretical Study of Harmonic Vibrational Frequencies: The Single and Double Excitation Coupled Cluster (CCSD) Method", *J. Chem. Phys.* **89**, 360 (1988).
403. G. E. Scuseria and H. F. Schaefer, "Equilibrium Structures and Vibrational Frequencies for Diatomic Molecules. An Assessment of the CCSDT-1 Method, Incorporating Coupled Cluster Single, Double, and Linearized Triple Excitations", *Chem. Phys. Lett.* **148**, 205 (1988).
404. H. Koch, G. E. Scuseria, A. C. Scheiner, and H. F. Schaefer, "The Infrared Spectrum of Water. Basis Set Dependence at the Single and Double Excitation Coupled Cluster (CCSD) Level of Theory", *Chem. Phys. Lett.* **149**, 118 (1988).
405. R. L. DeKock, R. S. Grev, and H. F. Schaefer, "The Valence Isoelectronic Molecules CCO, CNN, SiCO, SiNN in their Triplet Ground States: Theoretical Predictions of Structures and Infrared Spectra", *J. Chem. Phys.* **89**, 3016 (1988).
406. B. F. Yates, H. F. Schaefer, T. J. Lee, and J. E. Rice, "The Infrared Spectrum of F<sup>-</sup>-H<sub>2</sub>O", *J. Am. Chem. Soc.* **110**, 6327 (1988).
407. W. Thiel, G. E. Scuseria, H. F. Schaefer, and W. D. Allen, "The Anharmonic Force Fields of HOF and F<sub>2</sub>O", *J. Chem. Phys.* **89**, 4965 (1988).
408. T. J. Lee, J. E. Rice, R. B. Remington, and H. F. Schaefer, "The Molecular Structures and Energetics of [7]Paracyclophane and [8]Paracyclophane. An Investigation of the Boundaries of Aromaticity", *Chem. Phys. Lett.* **150**, 63 (1988).
409. R. S. Grev, G. E. Scuseria, A. C. Scheiner, H. F. Schaefer, and M. S. Gordon, "Relative Energies of Silaethylene and Methylsilylene", *J. Am. Chem. Soc.* **110**, 7337 (1988).
410. H. F. Schaefer, "A History of Ab Initio Computational Quantum Chemistry: 1950–1960", *Tetrahedron Comput. Methodol.* **1**, 97 (1988).
411. W. Thiel, Y. Yamaguchi, and H. F. Schaefer, "The Anharmonic Force Fields of Silyl Fluoride and Silyl Chloride", *J. Mol. Spectrosc.* **132**, 193 (1988).
412. T. P. Hamilton and H. F. Schaefer, "Silaketene: A Product of the Reaction Between Silylene and Carbon Monoxide?" *J. Chem. Phys.* **90**, 1031 (1989).
413. G. E. Scuseria, C. L. Janssen, and H. F. Schaefer, "An Efficient Reformulation of the Closed-Shell Coupled Cluster Single and Double Excitation (CCSD) Equations", *J. Chem. Phys.* **89**, 7382 (1988).
414. M. Duran, Y. Yamaguchi, R. B. Remington, Y. Osamura, and H. F. Schaefer, "Analytic Energy Third Derivatives for Paired-Excited Multi-Configuration Self-Consistent-Field Wavefunctions", *J. Chem. Phys.* **90**, 334 (1989).
415. T. J. Lee, J. E. Rice, G. E. Scuseria, and H. F. Schaefer, "Theoretical Investigations of Molecules Composed Only of Fluorine, Oxygen, and Nitrogen: Determination of the Equilibrium Structures of FOOF, (NO)<sub>2</sub>, and FNNF and the Transition State Structure for FNNF Cis–Trans Isomerization", *Theor. Chim. Acta* **75**, 81 (1989).
416. G. E. Scuseria and H. F. Schaefer, "A New Implementation of the Full CCSDT Model for Molecular Electronic Structure", *Chem. Phys. Lett.* **152**, 382 (1988).
417. H. F. Schaefer, "The Infrared Spectra of Polyatomic Molecular Ions: A Profitable Alliance Between Theory and Experiment", in *Ion and Cluster Ion Spectroscopy and Structure*, editor J. P. Maier (Elsevier, Amsterdam, 1989). Pages 109–
418. E. T. Seidl and H. F. Schaefer, "The Silanoic Acid Dimer (HSiOOH)<sub>2</sub>: A Simple Molecular System Incorporating Two Very Strong Hydrogen Bonds", *J. Am. Chem. Soc.* **111**, 1569 (1989).
419. A. C. Scheiner, H. F. Schaefer, and B. Liu, "The  $\tilde{X}^1A_1$  and  $\tilde{a}^3B_2$  States of *o*-Benzynes: A Theoretical Characterization of Equilibrium Geometries, Harmonic Vibrational Frequencies, and the Singlet–Triplet Energy Gap", *J. Am. Chem. Soc.* **111**, 3118 (1989).
420. G. E. Scuseria and H. F. Schaefer, "The Photodissociation of Formaldehyde: A Coupled Cluster Study Including Connected Triple Excitations of the Transition State Barrier Height for H<sub>2</sub>CO → H<sub>2</sub> + CO", *J. Chem. Phys.* **90**, 3629 (1989).
421. G. E. Scuseria and H. F. Schaefer, "Is Coupled Cluster Singles and Doubles (CCSD) More Computationally Intensive Than Quadratic Configuration Interaction (QCISD)?" *J. Chem. Phys.* **90**, 3700 (1989).
422. W. D. Allen, D. A. Horner, R. L. DeKock, R. B. Remington, and H. F. Schaefer, "The Lithium Superoxide Radical: Symmetry Breaking Phenomena and Potential Energy Surfaces", *Chem. Phys.* **133**, 11 (1989).
423. P. W. Harland, R. G. A. R. MacLagan, and H. F. Schaefer, "Structure and Energies of C<sub>2</sub>NH<sub>2</sub><sup>+</sup> Isomers", *J. Chem. Soc., Faraday Trans. 2* **85**, 187 (1989).
424. B. F. Yates and H. F. Schaefer, "Tetrasilacyclobutadienyliene: The Lowest Energy Cyclic Isomer of Singlet Si<sub>4</sub>H<sub>4</sub>?" *Chem. Phys. Lett.* **155**, 563 (1989).
425. T. P. Hamilton and H. F. Schaefer, "Sodium Pentaphosphacyclopentadiene (NaP<sub>5</sub>) and the Pentaphosphacyclopentadienide Ion (P<sub>5</sub><sup>-</sup>): Theoretical Predictions of Molecular Structures, Infrared and Raman Spectra", *Angew. Chem.* **101**, 500 (1989) (German); *Angew. Chem. Int. Ed. Engl.* **28**, 485 (1989).
426. T. P. Hamilton and H. F. Schaefer, "The Reaction of Methane with Molecular Oxygen: A Semi-Quantitative Estimate of The Activation Energy", *J. Chem. Phys.* **90**, 6391 (1989).
427. H. F. Schaefer, "The Third Age of Quantum Chemistry", *Chimia* **43**, 1 (1989).
428. G. E. Scuseria, T. J. Lee, A. C. Scheiner, and H. F. Schaefer, "Ordering of the O–O Stretching Vibrational Frequencies in Ozone", *J. Chem. Phys.* **90**, 5635 (1989).
429. H. F. Schaefer, "Computers and Molecular Quantum Mechanics: 1965–1988, A Personal Perspective", in *Nuclear and Atomic Physics at One Gigaflop*, editors C. Bottcher, M. R. Strayer, and J. B. McGrory (Harwood Academic Publishers, Chur, Switzerland, 1989). Pages 247–267.

430. R. L. DeKock, B. F. Yates, and H. F. Schaefer, "Electronic Structure of the  $^3\Sigma^-$  States of SiOSi and SiSiO," *Inorg. Chem.* **28**, 1680 (1989).
431. Y. Xie, G. E. Scuseria, B. F. Yates, Y. Yamaguchi, and H. F. Schaefer, "Methylnitrene: Theoretical Predictions of its Molecular Structure and Comparison with the Conventional C–N Single Bond in Methylamine ( $\text{CH}_3\text{–NH}_2$ )," *J. Am. Chem. Soc.* **111**, 5181 (1989).
432. Y. Xie, B. F. Yates, Y. Yamaguchi, and H. F. Schaefer, "The  $\pi$ -Bonded Complex Between Aluminum and Ethylene," *J. Am. Chem. Soc.* **111**, 6163 (1989).
433. Y. Xie, R. D. Davy, B. F. Yates, C. P. Blahous, Y. Yamaguchi, and H. F. Schaefer, "NO<sub>2</sub> Radical Spectroscopy: Vibrational Frequencies, Dipole Moment, and the Energy Difference Between the Bent and Linear Stationary Points on the Ground-State Potential Surface," *Chem. Phys.* **135**, 179 (1989).
434. R. S. Grev and H. F. Schaefer, "Reassignment of the Structure of Si(CO)<sub>2</sub> Based on Theoretically Predicted IR Spectra," *J. Am. Chem. Soc.* **111**, 5687 (1989).
435. R. S. Grev and H. F. Schaefer, "Why Metalloid-Substituted Unsaturated Compounds are Colored," *J. Am. Chem. Soc.* **111**, 6137 (1989).
436. M. E. Colvin, R. A. Whiteside, and H. F. Schaefer, "Quantum Chemical Methods for Massively Parallel Computers," in *Concurrent Computation in Chemical Calculations*, editor S. Wilson, Volume 3, *Methods in Computational Chemistry* (Plenum, New York, 1989). Pages 167–237.
437. C. Liang, R. D. Davy, and H. F. Schaefer, "Infrared Spectra of the Unknown Dialane (Al<sub>2</sub>H<sub>6</sub>) and Recently Observed Digallane (Ga<sub>2</sub>H<sub>6</sub>) Molecules," *Chem. Phys. Lett.* **159**, 393 (1989).
438. C. P. Blahous and H. F. Schaefer, "(NH)<sub>6</sub>: The Amino-Analog of Cyclohexane. A Laboratory for the Understanding of Lone-Pair Effects on Molecular Geometry," *J. Mol. Struct. Golden Volume* **200**, 591 (1989).
439. G. E. Scuseria and H. F. Schaefer, "The Unimolecular Triple Dissociation of Glyoxal: Transition State Structures Optimized by Configuration Interaction and Coupled Cluster Methods," *J. Am. Chem. Soc.* **111**, 7761 (1989).
440. K. S. Kim, H. S. Kim, S. Kim, J. H. Jang, and H. F. Schaefer, "Cyclododecaoxygen, O<sub>12</sub>: Comparison with the Experimentally Characterized S<sub>12</sub> Molecule," *J. Am. Chem. Soc.* **111**, 7746 (1989).
441. Y. Xie, B. F. Yates, and H. F. Schaefer, "The Wealth of Energetically Low-Lying Isomers for Very Simple Organometallic Systems. The Aluminum-Acetylene (Al–C<sub>2</sub>H<sub>2</sub>) System," *J. Am. Chem. Soc.* **112**, 517 (1990).
442. R. D. Davy and H. F. Schaefer, "Is There an Absence of Threefold Symmetry at the Equilibrium Geometry of the Ground Electronic State for NO<sub>3</sub>?" *J. Chem. Phys.* **91**, 4410 (1989).
443. G. E. Quelch, R. S. Grev, and H. F. Schaefer, "Concerning the Interaction of Atomic Silver with a Silicon Monoxide Ligand," *J. Chem. Soc., Chem. Commun.* 1498 (1989).
444. I. L. Alberts and H. F. Schaefer, "The Second Stable Conformer of 1,3-Butadiene. Geometry Optimizations with Configuration Interaction and Coupled Cluster Methods," *Chem. Phys. Lett.* **161**, 375 (1989).
445. Y. Xie and H. F. Schaefer, "The Bitetrahedral Molecule C<sub>8</sub>H<sub>6</sub>: The Shortest Possible C–C Bond Distance for a Saturated Hydrocarbon?" *Chem. Phys. Lett.* **161**, 516 (1989).
446. N. L. Allinger, R. S. Grev, B. F. Yates, and H. F. Schaefer, "The Syn Rotational Barrier in Butane," *J. Am. Chem. Soc.* **112**, 114 (1990).
447. R. S. Grev and H. F. Schaefer, "6-311G Is Not of Valence Triple-Zeta Quality," *J. Chem. Phys.* **91**, 7305 (1989).
448. G. E. Quelch, Y. Xie, B. F. Yates, Y. Yamaguchi, and H. F. Schaefer, "The HO<sub>2</sub><sup>+</sup> Molecular Ion. A Comparison of Theoretical Methods for the Prediction of Anharmonic Vibrational Frequencies," *Mol. Phys.* **68**, 1095 (1989).
449. T. P. Hamilton and H. F. Schaefer, "Vinylidene Radical Cation (H<sub>2</sub>CC<sup>+</sup>): A Sizable Barrier to Unimolecular Rearrangement to the Acetylene Radical Cation," *J. Phys. Chem.* **93**, 7560 (1989).
450. B. J. Smith, D. J. Swanton, J. A. Pople, H. F. Schaefer, and L. Radom, "Transition Structures for the Interchange of Hydrogen Atoms Within the Water Dimer," *J. Chem. Phys.* **92**, 1240 (1990).
451. E. T. Seidl and H. F. Schaefer, "Diketene and its Cyclic C<sub>4</sub>H<sub>4</sub>O<sub>2</sub> Isomers 1,3-Cyclobutanedione and 2,4-Dimethylene-1,3-Dioxetane," *J. Am. Chem. Soc.* **112**, 1493 (1990).
452. G. E. Scuseria, T. P. Hamilton, and H. F. Schaefer, "An Assessment of the Full Coupled Cluster Method Including All Single, Double, and Triple Excitations (CCSDT): The Diatomic Molecules LiH, Li<sub>2</sub>, BH, LiF, C<sub>2</sub>, BeO, CN<sup>+</sup>, BF, NO<sup>+</sup>, and F<sub>2</sub>," *J. Chem. Phys.* **92**, 568 (1990).
453. C. P. Blahous, Y. Xie, and H. F. Schaefer, "The Infrared Spectrum of Trimethylenemethane. Predictions of In-Plane Vibrational Frequencies from Correlated Wave Functions," *J. Chem. Phys.* **92**, 1174 (1990).
454. K. S. Kim, J. H. Jang, S. Kim, B.-J. Mhin, and H. F. Schaefer, "Potential New High Energy Density Materials: Cyclooctaoxygen O<sub>8</sub>, Including Comparisons with the Well-Known Cyclo-S<sub>8</sub> Molecule," *J. Chem. Phys.* **92**, 1887 (1990).
455. I. L. Alberts and H. F. Schaefer, "The Boron–Carbon Triple Bond (–B≡C–): Some Theoretical Predictions," *Chem. Phys. Lett.* **165**, 250 (1990).
456. R. S. Grev, B. J. DeLeeuw, and H. F. Schaefer, "Germanium–Germanium Multiple Bonds: The Singlet Electronic Ground State of Ge<sub>2</sub>H<sub>2</sub>," *Chem. Phys. Lett.* **165**, 257 (1990).
457. H. Koch, H. J. Aa. Jensen, P. Jørgensen, T. Helgaker, G. E. Scuseria, and H. F. Schaefer, "Coupled Cluster Energy Derivatives. Analytic Hessian for the Closed-Shell Coupled Cluster Singles and Doubles Wave Function: Theory and Applications," *J. Chem. Phys.* **92**, 4924 (1990).
458. C. Liang, T. P. Hamilton, and H. F. Schaefer, "Classical and non-Classical Forms of the Vinyl Cation: A Coupled Cluster Study," *J. Chem. Phys.* **92**, 3653 (1990).
459. Y. Yamaguchi, Y. Xie, R. S. Grev, and H. F. Schaefer, "What is the Lowest Energy Structure of the NS<sub>2</sub> Molecule?" *J. Chem. Phys.* **92**, 3683 (1990).
460. T. P. Hamilton and H. F. Schaefer, "The Triphosphorus Anion (P<sub>3</sub><sup>−</sup>): A Near Degeneracy Between Equilateral Triplet and Linear Singlet Electronic States," *Chem. Phys. Lett.* **166**, 303 (1990).

461. T. L. Allen, A. C. Scheiner, and H. F. Schaefer, "Theoretical Studies of Borylphosphine, Its Conjugate Base, and the Lithium Salt of its Conjugate Base. The Use of Orbital Kinetic Energies to Determine the Origin of the Driving Force for Changes in Molecular Geometry", *Inorganic Chem.* **29**, 1930 (1990).
462. J. Breidung, W. Schneider, W. Thiel, and H. F. Schaefer, "The Anharmonic Force Fields of PH<sub>3</sub>, PHF<sub>2</sub>, PF<sub>3</sub>, PH<sub>5</sub>, and H<sub>3</sub>PO", *J. Mol. Spectrosc.* **140**, 226 (1990).
463. B. T. Colegrove and H. F. Schaefer, "Disilyne (Si<sub>2</sub>H<sub>2</sub>) Revisited", *J. Phys. Chem.* (John A. Pople Issue) **94**, 5593 (1990).
464. G. E. Scuseria and H. F. Schaefer, "The Concerted Unimolecular Triple Dissociation of s-Tetrazine: Transition State Structural Optimizations Using Configuration Interaction and Coupled Cluster Methods", *J. Phys. Chem.* (John A. Pople Issue) **94**, 5552 (1990).
465. R. D. Davy and H. F. Schaefer, "The Structures and Vibrational Frequencies of the NNO Analogues NPO and PNO and their Protonated Forms", *J. Chem. Phys.* **92**, 5417 (1990).
466. K. M. Dunn, G. E. Scuseria, and H. F. Schaefer, "The Infrared Spectrum of Cyclotetraoxygen, O<sub>4</sub>: A Theoretical Investigation Employing the Single and Double Excitation Coupled Cluster (CCSD) Method", *J. Chem. Phys.* **92**, 6077 (1990).
467. Y. Xie and H. F. Schaefer, "Bond Distance Inversion in the Equilibrium Geometry of the Coupled Tricyclo [3.1.0.0<sup>2,6</sup>] Hexyl Molecule C<sub>12</sub>H<sub>14</sub>. A Puzzling Problem in Molecular Structure", *Chem. Phys. Lett.* **168**, 249 (1990).
468. W. D. Allen, Y. Yamaguchi, A. G. Csaszar, D. A. Clabo, R. B. Remington, and H. F. Schaefer, "A Systematic Study of Molecular Vibrational Anharmonicity and Vibration-Rotation Interaction by Self-Consistent Field Higher Derivative Methods. Linear Polyatomic Molecules", *Chem. Phys.* **145**, 427 (1990).
469. Y. Xie and H. F. Schaefer, "Aluminirene (HAlC<sub>2</sub>H<sub>2</sub>) and Aluminirane (HAlC<sub>2</sub>H<sub>4</sub>): The Aluminum Substituted Counterparts of Cyclopropene and Cyclopropane", *J. Am. Chem. Soc.* **112**, 5393 (1990).
470. C. Liang and H. F. Schaefer, "Electronic Structures of Linear C<sub>4</sub>, C<sub>6</sub>, C<sub>8</sub>, and C<sub>10</sub> Carbon Clusters and a Symmetry Breaking Phenomenon", *Chem. Phys. Lett.* **169**, 150 (1990).
471. T. L. Allen, A. C. Scheiner, and H. F. Schaefer, "Theoretical Studies of Diphosphene and Diphosphinylidene. 2. Some Unusual Features of the Radical Cations and Anions", *J. Phys. Chem.* (Kenneth S. Pitzer Issue) **94**, 7780 (1990).
472. M. M. Gallo and H. F. Schaefer, "The Infrared Spectrum of Difluorovinylidene, F<sub>2</sub>C=C:", *J. Chem. Phys.* **93**, 865 (1990).
473. R. S. Grev, I. L. Alberts, and H. F. Schaefer, "C<sub>3</sub><sup>+</sup> Is Bent", *J. Phys. Chem.* **94**, 3379 (1990).
474. N. C. Handy and H. F. Schaefer, "Forty Years of Quantum Chemistry", *J. Phys. Chem.* (John A. Pople Issue) **94**, 5417 (1990).
475. C. Meredith, R. D. Davy, and H. F. Schaefer, "Seven Isomers of Protonated Nitrosyl Fluoride", *J. Chem. Phys.* **93**, 1215 (1990).
476. Y. Xie and H. F. Schaefer, "The Silaformyl Radical HSiO and its SiOH Isomer", *J. Chem. Phys.* **93**, 1196 (1990).
477. S. Jin and H. F. Schaefer, "The NaSO → NaOS Potential Energy Hypersurface", *J. Chem. Phys.* **93**, 1799 (1990).
478. S. Jin, Y. Xie, and H. F. Schaefer, "The Characterization of Simple Organoaluminum Fragments: AlCH, AlCH<sub>2</sub>, and AlCH<sub>3</sub>", *Chem. Phys. Lett.* **170**, 301 (1990).
479. M. Shen, Y. Xie, H. F. Schaefer, and C. Deakynne, "Hydrogen Bonding Between the Nitrate Anion (Conventional and Peroxy Forms) and the Water Molecule", *J. Chem. Phys.* **93**, 3379 (1990).
480. T. P. Hamilton and H. F. Schaefer, "The Structure and Energetics of C<sub>2</sub>H<sub>4</sub>Br<sup>+</sup>: Ethylenebromonium Ion vs Bromoethyl Cations", *J. Am. Chem. Soc.* **112**, 8260 (1990).
481. I. L. Alberts, R. S. Grev, and H. F. Schaefer, "Geometrical Structures and Vibrational Frequencies of the Energetically Low-lying Isomers of SiC<sub>3</sub>", *J. Chem. Phys.* **93**, 5046 (1990).
482. J. D. Goddard and H. F. Schaefer, "Formyl Fluoride Photodissociation: Potential Energy Surface Features of Singlet HFCO", *J. Chem. Phys.* **93**, 4907 (1990).
483. C. L. Collins, R. D. Davy, and H. F. Schaefer, "Cyclopentadienylidene in Interstellar Space?", *Chem. Phys. Lett.* **171**, 259 (1990).
484. Y. Yamaguchi, Y. Xie, I. L. Alberts, R. S. Grev, and H. F. Schaefer, "The Electronic Spectra of SNS. Low-Lying Doublet States", *J. Chem. Phys.* **93**, 5053 (1990).
485. Y. Yamaguchi, I. L. Alberts, J. D. Goddard, and H. F. Schaefer, "Use of the Molecular Orbital Hessian for Self-Consistent-Field (SCF) Wavefunctions", *Chem. Phys.* **147**, 309 (1990).
486. G. E. Quelch, C. J. Marsden, and H. F. Schaefer, "Resolution of a Long-Standing Problem in Elemental Sulfur Chemistry: A Theoretical Study of Tetra-Sulfur", *J. Am. Chem. Soc.* **112**, 8719 (1990).
487. B. T. Colegrove and H. F. Schaefer, "Protonated Disilyne, Si<sub>2</sub>H<sub>3</sub><sup>+</sup>: Molecular Structures, Vibrational Frequencies and Infrared Intensities", *J. Chem. Phys.* **93**, 7230 (1990).
488. M. M. Gallo, T. P. Hamilton, and H. F. Schaefer, "Vinylidene—The Final Chapter?" *J. Am. Chem. Soc.* **112**, 8714 (1990).
489. J. R. Thomas, G. E. Quelch, and H. F. Schaefer, "The Unknown Unsubstituted Tetrazines: 1,2,3,4-Tetrazine and 1,2,3,5-Tetrazine", *J. Org. Chem.* **56**, 539 (1991).
490. R. S. Grev, H. F. Schaefer, and K. M. Baines, "Germasilene, H<sub>2</sub>Ge=SiH<sub>2</sub>, and its Isomers Silylgermylene and Germylsilylene: Bond Dissociation Energies,  $\pi$  Bond Energies, and Predictions of Isomeric Stability," *J. Am. Chem. Soc.* **112**, 9458 (1990).
491. C. P. Blahous, B. F. Yates, and H. F. Schaefer, "Symmetry-Breaking in the NO<sub>2</sub>  $\sigma$ -Radical: Construction of the <sup>2</sup>A<sub>1</sub> and <sup>2</sup>B<sub>2</sub> States with C<sub>s</sub> Symmetry CASSCF Wavefunctions", *J. Chem. Phys.* **93**, 8105 (1990).
492. M. Shen, Y. Xie, and H. F. Schaefer, "The Silyl Anion (SiH<sub>3</sub><sup>-</sup>): Harmonic Vibrational Frequencies and Infrared Intensities Predicted at the SCF, CISD, and CCSD Levels of Theory with Substantial Basis Sets", *J. Chem. Phys.* **93**, 8098 (1990).
493. C. Liang and H. F. Schaefer, "Carbon Clusters: The Structure of C<sub>10</sub> Studied with Configuration Interaction Methods", *J. Chem. Phys.* **93**, 8844 (1990).
494. B. F. Yates, Y. Yamaguchi, and H. F. Schaefer, "The Dissociation Mechanism of Triplet Formaldehyde", *J. Chem. Phys.* **93**, 8798 (1990).

495. C. Meredith, R. D. Davy, G. E. Quelch, and H. F. Schaefer, "Peroxy and Cyclic Isomers of  $\text{NO}_2$  and  $\text{NO}_2^-$ ", *J. Chem. Phys.* **94**, 1317 (1991).
496. G. E. Scuseria and H. F. Schaefer, "Diatomic Chromium ( $\text{Cr}_2$ ): Application of the Coupled Cluster Method Including All Single and Double Excitations (CCSD)", *Chem. Phys. Lett.* **174**, 501 (1990).
497. T. P. Hamilton and H. F. Schaefer, "New Variations in Two-Electron Integral Evaluation in the Context of Direct SCF Procedures", *Chem. Phys.* **150**, 163 (1991).
498. N. A. Burton, G. E. Quelch, M. M. Gallo, and H. F. Schaefer, "Cyclopentadienylidencarbene—A Stable Isomer of *o*-Benzyne?" *J. Am. Chem. Soc.* **113**, 764 (1991).
499. Y. Yamaguchi, I. L. Alberts, Y. Xie, and H. F. Schaefer, "The Electronic Spectrum of  $\text{NS}_2$ : Low-Lying Quartet States", *J. Chem. Phys.* **94**, 1277 (1991).
500. K. S. Kim, H. S. Kim, J. H. Jang, H. S. Kim, B.-J. Mhin, Y. Xie, and H. F. Schaefer, "Hydrogen Bonding Between the Water Molecule and the Hydroxyl Radical ( $\text{H}_2\text{O}\cdot\text{OH}$ ): The  $^2A''$   $^2A'$  Minima", *J. Chem. Phys.* **94**, 2057 (1991).
501. S.-J. Kim, T. P. Hamilton and H. F. Schaefer, "Structure and Energetics of the Lowest  $^1A_1$  and  $^1B_1$  States of Dichlorocarbene", *J. Chem. Phys.* **94**, 2063 (1991).
502. C. Meredith, G. E. Quelch, and H. F. Schaefer, "Open-Chain and Cyclic Protonated Ozone: The Ground-State Potential Energy Hypersurface", *J. Am. Chem. Soc.* **113**, 1186 (1991).
503. C. L. Janssen and H. F. Schaefer, "The Automated Solution of Second Quantization Equations with Applications to the Coupled Cluster Approach", *Theor. Chim. Acta* **79**, 1 (1991).
504. B. J. Duke, C. Liang, and H. F. Schaefer, "Properties of Small Group IIIA Hydrides Including the Cyclic and Pentacoordinate Structures of Trialane ( $\text{Al}_3\text{H}_6$ ) and Trigallane ( $\text{Ga}_3\text{H}_6$ ): Can Dialane Be Isolated?", *J. Am. Chem. Soc.* **113**, 2884 (1991).
505. B. T. Colegrove and H. F. Schaefer, "Trans -Dimethyldisilyne ( $\text{Si}_2(\text{CH}_3)_2$ ): An Achievable Synthetic Target", *J. Am. Chem. Soc.* **113**, 1557 (1991).
506. E. T. Seidl and H. F. Schaefer, "A New Configuration of 12-Crown-4", *J. Phys. Chem.* **95**, 3589 (1991).
507. E. T. Seidl and H. F. Schaefer, "Faced Fused Dicycubane ( $\text{C}_{12}\text{H}_8$ ) and its Dicycubane Isomer: Achievable Synthetic Targets?", *J. Am. Chem. Soc.* **113**, 1915 (1991).
508. R. D. Davy and H. F. Schaefer, "Dinitrogen Sulfide ( $\text{N}_2\text{S}$ ) and Its Protonated Isomers", *J. Am. Chem. Soc.* **113**, 1917 (1991).
509. B. J. Duke and H. F. Schaefer, "Arachno-2-Gallatetraborane(10),  $\text{H}_2\text{GaB}_3\text{H}_8$ : An *Ab Initio* Molecular Quantum Mechanical Study", *J. Chem. Soc., Chem. Commun.* 123 (1991).
510. M. Shen, Y. Xie, H. F. Schaefer, and C. A. Deakyne, "The  $\text{H}_2\text{O}_2\text{-NO}_2^-$  and  $\text{H}_2\text{NO}_4^-$  Isomers of the Nitrate Anion—Water Complex", *Chem. Phys.* **151**, 187 (1991).
511. C. Liang, Y. Xie, H. F. Schaefer, K. S. Kim, and H. S. Kim, "The Vibrational Spectra of Butatriene ( $\text{C}_4\text{H}_4$ ) and Pentatetraene ( $\text{C}_5\text{H}_4$ ): Is Pentatetraene Bent?" *J. Am. Chem. Soc.* **113**, 2452 (1991).
512. Y. Xie, H. F. Schaefer, and J. S. Thrasher, "The Conjunction of Aromaticity and Hypervalency: The  $\text{C}_5\text{H}_5\text{SF}_3$  Molecule 1,1,1-Trifluorothiabenzene", *J. Mol. Struct. (G. G. Hall—C. C. J. Roothaan Issue)* **234**, 247 (1991).
513. G. Vacek, B. T. Colegrove, and H. F. Schaefer, "Does Oxirene Exist? A Theoretical Inquiry Involving the Coupled-Cluster Method", *Chem. Phys. Lett.* **177**, 468 (1991).
514. A. C. Scheiner and H. F. Schaefer, "Benzyne: Higher Level Theoretical Evidence for the Weak Triple Bond", *Chem. Phys. Lett.* **177**, 471 (1991).
515. R. D. Davy, Y. Xie, and H. F. Schaefer, "Phosphoryl Nitride Isomeric Dimers, Trimers, and Tetramers:  $(\text{NPO})_x$  ( $x = 2-4$ )", *J. Am. Chem. Soc.* **113**, 4136 (1991).
516. R. D. Davy, Y. Xie, and H. F. Schaefer, "Stabilization of Three-Membered Rings by Protonation. The Cyclic Global Minimum of  $\text{HP}_2\text{O}^+$ , the Protonated Phosphorus Analogue of Nitrous Oxide", *J. Am. Chem. Soc.* **113**, 3697 (1991).
517. G. Vacek, B. T. Colegrove, and H. F. Schaefer, "The Infrared Spectrum of Silacyclopropenylidene", *J. Am. Chem. Soc.* **113**, 3192 (1991).
518. J. E. Fowler, I. L. Alberts, and H. F. Schaefer, "Mechanistic Study of the Electrocyclic Ring-Opening Reaction of Thirane", *J. Am. Chem. Soc.* **113**, 4768 (1991).
519. Y. Xie and H. F. Schaefer, "Hexalithiobenzene: A  $D_{6h}$  Equilibrium Geometry with Six Lithium Atoms in Bridging Positions", *Chem. Phys. Lett.* **179**, 563 (1991).
520. M. Shen, Y. Xie, Y. Yamaguchi, and H. F. Schaefer, "The Silyl Anion ( $\text{SiH}_3^-$ ): Cubic/Quartic Force Field and Anharmonic Contributions to the Fundamental Vibrational Frequencies", *J. Chem. Phys.* **94**, 8112 (1991).
521. T. P. Hamilton and H. F. Schaefer, "The Prototypical Zinc Carbene and Zinc Carbyne Molecules  $\text{ZnCH}_2$  and  $\text{HZnCH}$ : Triplet Electronic Ground States", *J. Chem. Soc., Chem. Commun.* 621 (1991).
522. T. P. Hamilton and H. F. Schaefer, "Do the Vinyl Isomers of  $\text{C}_2\text{H}_2\text{Cl}^+$  and  $\text{C}_2\text{H}_2\text{Br}^+$  Exist?", *J. Am. Chem. Soc.* **113**, 7147 (1991).
523. E. T. Seidl and H. F. Schaefer, "Theoretical Investigation of the Dimerization of Ketene: Does the  $2S + 2A$  Cycloaddition Reaction Exist?", *J. Am. Chem. Soc.* **113**, 5195 (1991).
524. S. Jin, B. T. Colegrove, and H. F. Schaefer, "Multiple Bonding in Perfluorodiphosphene (FPPF) and Perfluorodiphosphinylidene ( $\text{PPF}_2$ )", *Inorg. Chem.* **30**, 2969 (1991).
525. R. S. Grev, H. F. Schaefer and P. P. Gaspar, "In Search of Triplet Silylenes", *J. Am. Chem. Soc.* **113**, 5638 (1991).
526. M. J. van der Woerd, K. Lammertsma, B. J. Duke, and H. F. Schaefer, "Simple Mixed Hydrides of Boron, Aluminum, and Gallium:  $\text{AlBH}_6$ ,  $\text{AlGaH}_6$ , and  $\text{BGaH}_6$ ", *J. Chem. Phys.* **95**, 1160 (1991).
527. S. Q. Jin, Y. Xie, and H. F. Schaefer, "The Description of Elementary Organoaluminum Fragments:  $\text{AlCH}_x$  ( $x = 1, 2, 3$ )", *J. Chem. Phys.* **95**, 1834 (1991).
528. C. J. Marsden, B. J. Smith, J. A. Pople, H. F. Schaefer, and L. Radom, "Characterization of the Bifurcated Structure of the Water Dimer", *J. Chem. Phys.* **95**, 1825 (1991).
529. Y. Xie, H. F. Schaefer, P. Aped, K. Chen, and N. L. Allinger, "The Structure of the Bitetrahedryl Molecule — A Major Shift Due to Electron Correlation. Effects of Carbonyl Substituents, Implications for the Structure of Coupled Tricyclo [3.1.0.0<sup>2,6</sup>] Hexyl, and Extension to Cubylcubane", *Int. J. Quantum. Chem. (Enrico Clementi Issue)* **42**, 953 (1992).



530. R. S. Grev, C. L. Janssen, and H. F. Schaefer, "Concerning Zero-Point Vibrational Energy Corrections to Electronic Energies", *J. Chem. Phys.* **95**, 5128 (1991).
531. B. J. Duke, T. P. Hamilton, and H. F. Schaefer, "Chlorogallanes ( $\text{GaClH}_2$ ,  $\text{GaCl}_2\text{H}$ , and  $\text{GaCl}_3$ ) and their Dimer Isomers", *Inorg. Chem.* **30**, 4225 (1991).
532. N. A. Burton, Y. Yamaguchi, I. L. Alberts, and H. F. Schaefer, "Interpretation of Excited-State Hartree-Fock Analytic Derivative Anomalies for  $\text{NO}_2$  and  $\text{HCO}_2$  Using the Molecular Orbital Hessian", *J. Chem. Phys.* **95**, 7466 (1991).
533. Y. Yamaguchi, H. F. Schaefer, and J. E. Baldwin, "Reappraisal of the Disrotatory Transition State for the Ring Opening of Cyclopropane", *Chem. Phys. Lett.* **185**, 143 (1991).
534. D. A. Horner, W. D. Allen, A. G. Csaszar, and H. F. Schaefer, "Sodium Superoxide Radical:  $\tilde{X}^2A_2$  and  $\tilde{A}^2B_2$  Potential Energy Surfaces", *Chem. Phys. Lett.* **186**, 346 (1991).
535. E. T. Seidl and H. F. Schaefer, "Molecular Structure of Diketene: A Discrepancy Between Theory and Experiments?" *J. Phys. Chem.* **96**, 657 (1992).
536. M. Shen, H. F. Schaefer, C. Liang, J.-H. Lii, N. L. Allinger, and P. R. Schleyer, "Finite  $T_d$  Symmetry Models for Diamond: From Adamantane to Superadamantane ( $\text{C}_{35}\text{H}_{36}$ )", *J. Am. Chem. Soc.* **114**, 497 (1992).
537. H. A. Carlson, G. E. Quelch, and H. F. Schaefer, "How 'Stable' is Cyclobutyne? The Activation Energy for the Unimolecular Rearrangement to Butatriene", *J. Am. Chem. Soc.* **114**, 5344 (1992).
538. J. D. Goddard, Y. Yamaguchi, and H. F. Schaefer, "The Decarboxylation and Dehydration Reactions of Monomeric Formic Acid", *J. Chem. Phys.* **96**, 1158 (1992).
539. B. J. DeLeeuw, R. S. Grev, and H. F. Schaefer, "A Comparison and Contrast of Selected Saturated and Unsaturated Hydrides of Group 14 Elements:  $\text{C}_2\text{H}_6$ ,  $\text{Si}_2\text{H}_6$ ,  $\text{Ge}_2\text{H}_6$ , and  $\text{C}_2\text{H}_2$ ,  $\text{Si}_2\text{H}_2$ ,  $\text{Ge}_2\text{H}_2$ ", *J. Chem. Educ.* **69**, 441 (1992).
540. C. Meredith, G. E. Quelch, and H. F. Schaefer, "Investigation of XNO and XON (where X = Cl or Br) and Their Protonated Isomers", *J. Chem. Phys.* **96**, 480 (1992).
541. E. T. Seidl and H. F. Schaefer, "Is There a Transition State for the Unimolecular Dissociation of Cyclotetraoxygen( $\text{O}_4$ )?", *J. Chem. Phys.* **96**, 1176 (1992).
542. T. P. Hamilton and H. F. Schaefer, "The Use of Special Coordinate Axes in Direct and Semi-Direct Implementations of Second-Order Perturbation Theory, Including the Derivation of a Horizontal Recurrence Relation", *Can. J. Chem.* (Sigeru Huzinaga Issue) **70**, 416 (1992).
543. T. D. Crawford, N. A. Burton, and H. F. Schaefer, "Monofluorinated Hydrogen Sulfide (HFS): A Definitive Theoretical Prediction of the Infrared Spectrum", *J. Chem. Phys.* **96**, 2044 (1992).
544. D. A. Horner, R. S. Grev, and H. F. Schaefer, "Three-Membered Rings of Carbon, Silicon, and Germanium: An Analysis of Thermodynamic Stability to Fragmentation", *J. Am. Chem. Soc.* **114**, 2093 (1992).
545. M. Shen and H. F. Schaefer, "The Known and Unknown Group 13 Hydride Molecules  $\text{M}_2\text{H}_6$ : Diborane (6), Dialane (6), and Digallane (6)", *J. Chem. Phys.* **96**, 2868 (1992).
546. Y. Xie and H. F. Schaefer, "Naked Organosulfur Clusters: The Infrared Spectrum of the  $\text{C}_2\text{S}$  Molecule", *J. Chem. Phys.* **96**, 3714 (1992).
547. I. M. B. Nielsen, C. L. Janssen, N. A. Burton, and H. F. Schaefer, "(1,2)-Hydrogen Shift in Monovalent Carbon Compounds: The Methylcarbyne-Vinyl Radical Isomerization", *J. Phys. Chem.* **96**, 2490 (1992).
548. Y. Xie, H. F. Schaefer, J. H. Jang, B. J. Mhin, H. S. Kim, C. W. Yoon, and K. S. Kim, "Sulfur Clusters: Structure, Infrared, and Raman Spectra of Cyclo- $\text{S}_6$  and Comparison with the Hypothetical Cyclo- $\text{O}_6$  Molecule", *Mol. Phys.* **76**, 537 (1992).
549. S.-J. Kim, T. P. Hamilton, and H. F. Schaefer, "Phenylnitrene: Energetics, Vibrational Frequencies, and Molecular Structures", *J. Am. Chem. Soc.* **114**, 5349 (1992).
550. M. Shen and H. F. Schaefer, "The Fundamental Vibrational Frequencies of the Silyl Anion ( $\text{SiH}_3^-$ )", *Mol. Phys.* **76**, 467 (1992).
551. E. T. Seidl and H. F. Schaefer, "Equilibrium Geometry of the HCCN Triplet Ground State: Carbene or Allene? An Open-Shell Coupled Cluster Study Including Connected Triple Excitations", *J. Chem. Phys.* **96**, 4449 (1992).
552. M. M. Gallo and H. F. Schaefer, "Methylcarbene: The Singlet-Triplet Energy Separation", *J. Phys. Chem.* **96**, 1515 (1992).
553. C.-H. Hu, M. Shen, and H. F. Schaefer, "Toward the Infrared Spectroscopic Observation of  $\text{SiH}_5^+$ : The Silanium Ion", *Chem. Phys. Lett.* **190**, 543 (1992).
554. C. M. B. Marsh, T. P. Hamilton, Y. Xie, and H. F. Schaefer, "Ammonia Alane", *J. Chem. Phys.* **96**, 5310 (1992).
555. E. T. Seidl, R. S. Grev, and H. F. Schaefer, "Mechanistic, Structural, and Vibrational Aspects of the Dimerization of Silaethylene", *J. Am. Chem. Soc.* **114**, 3643 (1992).
556. C. D. Sherrill, E. T. Seidl, and H. F. Schaefer, "Closs's Diradical: Some Surprises on the Potential Energy Hypersurface", *J. Phys. Chem.* **96**, 3712 (1992).
557. J. R. Thomas, G. E. Quelch, E. T. Seidl, and H. F. Schaefer, "The Titane Molecule ( $\text{TiH}_4$ ): Equilibrium Geometry, Infrared and Raman Spectra of the First Spectroscopically Characterized Transition Metal Tetrahydride", *J. Chem. Phys.* **96**, 6857 (1992).
558. R. S. Grev and H. F. Schaefer, "Natural Orbitals From Single and Double Excitation Configuration Interaction Wave Functions: Their Use in Second-Order Configuration Interaction and Wave Functions Incorporating Limited Triple and Quadruple Excitations", *J. Chem. Phys.* **96**, 6850 (1992).
559. A. C. Scheiner and H. F. Schaefer, "Cyclopentadienylideneketene: Theoretical Consideration of An Infrared Spectrum Frequently Mistaken for Benzyne", *J. Am. Chem. Soc.* **114**, 4758 (1992).
560. B. Ma, Y. Xie, and H. F. Schaefer, "Tetraethynylethylene, A Molecule with Four Very Short C-C Single Bonds. Interpretation of the Infrared Spectrum", *Chem. Phys. Lett.* **191**, 521 (1992).
561. M. Shen, H. F. Schaefer, and H. Partridge, "The Remarkable Enneahydridorhenate Dianion:  $\text{ReH}_9^{2-}$ ", *Mol. Phys.* **76**, 995 (1992).
562. H. F. Schaefer, "Quantum Chemistry", *Encyclopedia of Science and Technology*, 7th ed. (McGraw-Hill, New York, 1992). Pages 587-591.
563. I. S. Ignatyev and H. F. Schaefer, "Difluorosulfurane ( $\text{SF}_2$ ): A Molecule Identified in the Laboratory?" *J. Phys. Chem.* **96**, 6247 (1992).

564. C. J. Marsden, G. E. Quelch, and H. F. Schaefer, "The  $S_3^{2+}$  Dication: The First 16-Valence-Electron Triatomic with an Equilateral Triangle Triplet Ground State?" *J. Am. Chem. Soc.* **114**, 6802 (1992).
565. I. S. Ignatyev and H. F. Schaefer, "Diazasilene (SiNN). A Comparison of Coupled Cluster Methods With Experiment and Local Density Functional Methods", *J. Phys. Chem.* **96**, 7632 (1992).
566. M. P. McGrath, L. Radom, and H. F. Schaefer, "Bow-lane: Toward Planar Tetracoordinate Carbon", *J. Org. Chem.* **57**, 4847 (1992).
567. G. E. Quelch, M. M. Gallo, and H. F. Schaefer, "Aspects of the Reaction Mechanism of Ethane Combustion. Conformations of the Ethylperoxy Radical", *J. Am. Chem. Soc.* **114**, 8239 (1992).
568. E. E. Bolton, B. J. DeLeeuw, J. E. Fowler, R. S. Grev, and H. F. Schaefer, "The Silicon-Carbon Symmetric Stretching Fundamental  $\nu_1$  of  $Si_2C$ : Nonintuitive Theoretical Behavior", *J. Chem. Phys.* **97**, 5586 (1992).
569. C. L. Collins, C. Meredith, Y. Yamaguchi, and H. F. Schaefer, "Advancing the Search for Cyclopropenylidene Carbene, The Exocyclic Ring Isomer of Diacetylene", *J. Am. Chem. Soc.* **114**, 8694 (1992).
570. R. S. Grev and H. F. Schaefer, "The Remarkable Mono-bridged Structure of  $Si_2H_2$ ", *J. Chem. Phys.* **97**, 7990 (1992).
571. O. G. Parchment, I. H. Hillier, D. V. S. Green, N. A. Burton, J. Morley, and H. F. Schaefer, "A Theoretical Study, Using *Ab Initio* Methods, of Tautomerism in 3-Amino-1,2,4-Triazole in Gas Phase and in Aqueous Solution", *J. Chem. Soc., Perkin Trans. 2* 1681 (1992).
572. A. A. Bliznyuk, M. Shen, and H. F. Schaefer, "The Dodecahedral  $N_{20}$  Molecule: Some Theoretical Predictions", *Chem. Phys. Lett.* **198**, 249 (1992).
573. C. Meredith, T. P. Hamilton, and H. F. Schaefer, "Oxy-water (Water Oxide): New Evidence for the Existence of a Structural Isomer of Hydrogen Peroxide", *J. Phys. Chem.* **96**, 9250 (1992).
574. R. S. Grev and H. F. Schaefer, "Thermochemistry of  $CH_n$ ,  $SiH_n$  ( $n = 0-4$ ) and the Cations  $SiH^+$ ,  $SiH_2^+$ , and  $SiH_3^+$ : A Converged Quantum Mechanical Approach", *J. Chem. Phys.* **97**, 8389 (1992).
575. J. R. Thomas, B. J. DeLeeuw, G. Vacek, and H. F. Schaefer, "A Systematic Theoretical Study of the Harmonic Vibrational Frequencies of Polyatomic Molecules: The Single, Double, and Perturbative Triple Excitation Coupled Cluster [CCSD(T)] Method", *J. Chem. Phys.* **98**, 1336 (1993).
576. Y. Yamaguchi, G. Vacek, and H. F. Schaefer, "Low-Lying Triplet Electronic States of Acetylene: *Cis*  $^3B_2$  and  $^3A_2$ , *Trans*  $^3B_u$  and  $^3A_u$ ", *Theor. Chim. Acta* (Per-Olov Löwdin Issue) **86**, 97 (1993).
577. R. C. Raffanetti, K. Ruedenberg, C. L. Janssen and H. F. Schaefer, "Efficient Use of Jacobi Rotations For Orbital Optimization and Localization", *Theor. Chim. Acta* (Per-Olov Löwdin Issue) **86**, 149 (1993).
578. R. S. Grev and H. F. Schaefer, "Rearrangement Barriers in Doubly Bonded Germanium Compounds", *Organometallics* **11**, 3489 (1992).
579. M. Shen, H. F. Schaefer, and H. Partridge, "Tungsten Hexahydride ( $WH_6$ ). An Equilibrium Geometry Far From Octahedral", *J. Chem. Phys.* **98**, 508 (1993).
580. J. G. G. Simon, A. Schweig, Y. Xie, and H. F. Schaefer, "The UV/VIS and IR Absorption Spectra of Benzocyclopropenone in Solid Argon at 12 K", *Chem. Phys. Lett.* **200**, 631 (1992).
581. C. L. Collins, Y. Yamaguchi, and H. F. Schaefer, "The Bending Frequency  $\delta_{NS}$  of Dinitrogen Sulfide ( $N_2S$ ): A Theoretical Analysis Demonstrating the Importance of Coriolis Coupling Terms", *J. Chem. Phys.* **98**, 4777 (1993).
582. B. Ma, Y. Xie, M. Shen, and H. F. Schaefer, " $PO_3^-(H_2O)_n$  Clusters. Molecular Anion Structures, Energetics and Vibrational Frequencies", *J. Am. Chem. Soc.* **115**, 1943 (1993).
583. M. S. Gordon, Y. Xie, Y. Yamaguchi, R. S. Grev, and H. F. Schaefer, "The Insertion Reactions of Monovalent Silicon: A Nonvanishing Barrier for the Silylyne Plus Hydrogen Reaction  $SiH + H_2$ ", *J. Am. Chem. Soc.* **115**, 1503 (1993).
584. B. J. DeLeeuw, J. T. Fermann, Y. Xie, and H. F. Schaefer, "Substitution Effects on the Properties of Unsaturated Carbenes: Fluorovinylidene ( $HFC=C:$ )", *J. Am. Chem. Soc.* **115**, 1039 (1993).
585. D. J. Tozer, N. C. Handy, R. D. Amos, J. A. Pople, R. H. Nobes, Y. Xie, and H. F. Schaefer, "Theory and Applications of Spin-Restricted Open-Shell Møller-Plesset Theory", *Mol. Phys.* **79**, 777 (1993).
586. M. Bühl and H. F. Schaefer, "Theoretical Characterization of the Transition Structure for a  $S_N2$  Reaction at Neutral Nitrogen", *J. Am. Chem. Soc.* **115**, 364 (1993).
587. G. Vacek, J. R. Thomas, B. J. DeLeeuw, Y. Yamaguchi, and H. F. Schaefer, "Isomerization Reactions on the Lowest Potential Energy Hypersurface of Triplet Vinylidene and Triplet Acetylene", *J. Chem. Phys.* **98**, 4766 (1993).
588. M. Shen, C. Liang, and H. F. Schaefer, "The Tetramer of Borane and Its Heavier Valence-Isoelectronic Analogues:  $M_4H_{12}$  with  $M = B, Al, \text{ and } Ga$ ", *Chem. Phys.* **171**, 325 (1993).
589. Z. Palagyi, R. S. Grev, and H. F. Schaefer, "Striking Similarities Between Elementary Silicon and Aluminum Compounds: Monobridged, Dibridged, Trans-Bent, and Vinylidene Isomers of  $Al_2H_2$ ", *J. Am. Chem. Soc.* **115**, 1936 (1993).
590. S.-J. Kim, T. P. Hamilton, and H. F. Schaefer, "Methylphosphinidene ( $CH_3P$ ) and its Rearrangement to Phosphaethylene ( $CH_2PH$ ): Toward the Observation of Ground-State Triplet  $CH_3P$ ", *J. Phys. Chem.* **97**, 1872 (1993).
591. C.-H. Hu, M. Shen, and H. F. Schaefer, "Glycine Conformational Analysis", *J. Am. Chem. Soc.* **115**, 2923 (1993).
592. M. Shen, I. S. Ignatyev, Y. Xie, and H. F. Schaefer, "[7]Circulene: A Remarkably Floppy Polycyclic Aromatic  $C_{28}H_{14}$  Isomer", *J. Phys. Chem.* **97**, 3212 (1993).
593. Z. Palagyi, H. F. Schaefer, and E. Kapuy, " $Ga_2H_2$ : Planar Dibridged, Vinylidene-Like, Monobridged, and Trans Equilibrium Geometries", *Chem. Phys. Lett.* **203**, 195 (1993).
594. J. M. Galbraith, G. Vacek, and H. F. Schaefer, " $ClF_2$ : Structure and Infrared Spectra of a Weakly Bound Triatomic Molecule", *J. Chem. Phys.* **98**, 8051 (1993).

595. T. P. Hamilton, Y. Xie, and H. F. Schaefer, "HP<sub>4</sub><sup>-</sup>: The Monoconjugate Base from Tetraphosphabicyclobutane. Evidence for an *Exo* Ground State Conformation in the Gas Phase", *Chem. Phys. Lett.* **208**, 106 (1993).
596. J. E. Fowler, T. P. Hamilton, and H. F. Schaefer, "The Nearly Octahedral Hexamethylsulfur and Hexamethylselenium Molecules: Lighter Counterparts to the Recently Synthesized Hexamethyltellurium", *J. Am. Chem. Soc.* **115**, 4155 (1993).
597. J. K. Lundberg, R. W. Field, C. D. Sherrill, E. T. Seidl, Y. Xie, and H. F. Schaefer, "Acetylene: Synergy Between Theory and Experiment", *J. Chem. Phys.* **98**, 8384 (1993).
598. G. Vacek, B. J. DeLeeuw, and H. F. Schaefer, "The  $\tilde{X}$  AlOH- $\tilde{X}$  HALO Isomerization Potential Energy Hypersurface", *J. Chem. Phys.* **98**, 8704 (1993).
599. Y. Yamaguchi, R. B. Remington, J. F. Gaw, H. F. Schaefer, and G. Frenking, "Use of Canonical Orbital Energy Derivatives for Closed-Shell Self-Consistent-Field (SCF) Wavefunctions", *J. Chem. Phys.* **98**, 8749 (1993).
600. Y. Xie and H. F. Schaefer, "Hydrogen Bonding Between the Water Molecule and the Hydroxyl Radical (H<sub>2</sub>O-OH): The Global Minimum", *J. Chem. Phys.* **98**, 8829 (1993).
601. Y. Yamaguchi, H. F. Schaefer, and I. L. Alberts, "A Mechanistic Study of the Ring Opening Reaction of Singlet Oxirane", *J. Am. Chem. Soc.* **115**, 5790 (1993).
602. M. Bühl, H. F. Schaefer, P. R. Schleyer, and R. Boese, "On the B-O Bond Length in Oxadiboriranes", *Angew. Chem. Int. Ed. Engl.* **32**, 1154 (1993).
603. J. R. Thomas, B. J. DeLeeuw, G. Vacek, T. D. Crawford, Y. Yamaguchi, and H. F. Schaefer, "The Balance Between Theoretical Method and Basis Set Quality: A Systematic Study of Equilibrium Geometries, Dipole Moments, Harmonic Vibrational Frequencies, and Infrared Intensities", *J. Chem. Phys.* **99**, 403 (1993).
604. A. A. Bliznyuk, H. F. Schaefer, and I. J. Amster, "Proton Affinities of Lysine and Histidine: A Theoretical Consideration of the Conflict Between Experimental Results from the Kinetic and Bracketing Methods", *J. Am. Chem. Soc.* **115**, 5149 (1993).
605. E. E. Bolton and H. F. Schaefer, "Nitromethylene (H-C-NO<sub>2</sub>): A Comparison of the Lowest Lying Triplet and Singlet States of a Highly Unconventional Carbene", *J. Am. Chem. Soc.* **115**, 6207 (1993).
606. R. S. Grev, B. J. DeLeeuw, Y. Yamaguchi, S. -J. Kim, and H. F. Schaefer, "The Cis Monobridged Equilibrium Geometries of Si<sub>2</sub>H<sub>2</sub>, Ge<sub>2</sub>H<sub>2</sub>, Al<sub>2</sub>H<sub>2</sub>, and Ga<sub>2</sub>H<sub>2</sub>: A Fundamentally New Type of Molecular Structure", in *Structures and Conformations of Non-Rigid Molecules*, NATO ASI Series C, Vol. 410, editors J. Laane, M. Dakkouri, B. van der Veken, and H. Oberhammer (Kluwer Academic Publishers, Dordrecht, Holland, 1993). Pages 325-342.
607. Z. Palagyi, H. F. Schaefer, and E. Kapuy, "Ge<sub>2</sub>H<sub>2</sub>: A Molecule with a Low-Lying Monobridged Equilibrium Geometry", *J. Am. Chem. Soc.* **115**, 6901 (1993).
608. P. R. Schreiner, S.-J. Kim, H. F. Schaefer, and P. R. Schleyer, "CH<sub>5</sub><sup>+</sup> - The Never-Ending Story or the Final Word?" *J. Chem. Phys.* **99**, 3716 (1993).
609. C.-H. Hu, H. F. Schaefer, Z. Hou, and K. D. Bayes, "The Attractive Quartet Potential Energy Surface for the CH( $\tilde{a}$   $^4\Sigma^-$ ) + CO Reaction: A Role for the  $\tilde{a}$   $^4A'$  State of the Ketenyl Radical in Combustion?" *J. Am. Chem. Soc.* **115**, 6904 (1993).
610. J. M. Galbraith, G. Vacek, and H. F. Schaefer, "The Vibrational Frequencies of Borane (BH<sub>3</sub>): A Comparison of High Level Theoretical Results", Golden Volume, *J. Mol. Struct.* **300**, 281 (1993).
611. H. F. Schaefer, "Banish Quantum Mechanics from General Chemistry?" *J. Chem. Educ.* **70**, 782 (1993).
612. C.-H. Hu, M. Shen, and H. F. Schaefer, "Is Dodecahedral P<sub>20</sub> Special?" *Theor. Chim. Acta* (Werner Kutzelnigg Issue) **88**, 29 (1994).
613. C.-H. Hu and H. F. Schaefer, "Cyanovinylidene: An Observable Unsaturated Carbene and a Possible Interstellar Molecule", *J. Phys. Chem.* **97**, 10681 (1993).
614. M. Bühl and H. F. Schaefer, "The S<sub>N</sub>2 Reaction of Neutral Nitrogen: Transition State Geometries and Intrinsic Barriers. An *Ab Initio* Study", *J. Am. Chem. Soc.* **115**, 9143 (1993).
615. Y. Yamaguchi, Y. Osamura, J. D. Goddard, and H. F. Schaefer, *A New Dimension to Quantum Chemistry: Analytic Derivative Methods in Ab Initio Molecular Electronic Structure Theory*, (Oxford University Press, England, 1994), 471 pages.
616. P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "The Mechanisms of Electrophilic Substitutions of Aliphatic Hydrocarbons: CH<sub>4</sub> + NO<sup>+</sup>", *J. Am. Chem. Soc.* **115**, 9659 (1993).
617. T. D. Crawford and H. F. Schaefer, "The Equilibrium Geometry of the  $\tilde{C}$   $^2A_2$  State of NO<sub>2</sub>", *J. Chem. Phys.* **99**, 7926 (1993).
618. C. Richards, C. Meredith, S. -J. Kim, G. E. Quelch, and H. F. Schaefer, "Is There a Potential Minimum Corresponding to Singlet Methylnitrene? A Study of the CH<sub>3</sub>N to CH<sub>2</sub>NH Rearrangement on the Lowest Singlet State Potential Energy Hypersurface", *J. Chem. Phys.* **100**, 481 (1994).
619. S.-J. Kim, P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "The Structure and Dissociation Energy of the Weakly Bound Complex CH<sub>5</sub><sup>+</sup>(H<sub>2</sub>)", *J. Phys. Chem.* **97**, 12232 (1993).
620. B. Ma, Y. Xie, M. Shen, P. R. Schleyer, and H. F. Schaefer, "Isomerization of PO<sub>3</sub><sup>-</sup>(H<sub>2</sub>O)<sub>n</sub> Clusters to H<sub>2</sub>PO<sub>4</sub><sup>-</sup>(H<sub>2</sub>O)<sub>n-1</sub>", *J. Am. Chem. Soc.* **115**, 11169 (1993).
621. H. F. Schaefer, "John A. Pople-Computational Chemistry Pioneer", Introductory Article, *Israel J. Chem.* **33**, 241, 355 (1993).
622. C. L. Collins, C.-H. Hu, Y. Yamaguchi, and H. F. Schaefer, "Ethynylvinylidene", *Israel J. Chem.* (John A. Pople Issue) **33**, 317 (1993).
623. Y. Yamaguchi, R. B. Remington, J. F. Gaw, H. F. Schaefer, and G. Frenking, "Canonical Orbital Energy Derivative Studies of the C<sub>2</sub>H<sub>2</sub> and H<sub>2</sub>CO Ground-State Potential Energy Hypersurfaces", *Chem. Phys.* **180**, 55 (1994).
624. J. W. de M. Carneiro, P. R. Schleyer, M. Saunders, R. B. Remington, H. F. Schaefer, A. Rauk, and T. S. Sorensen, "Protonated Ethane. A Theoretical Investigation of C<sub>2</sub>H<sub>7</sub><sup>+</sup> Structures and Energetics", *J. Am. Chem. Soc.* **116**, 3483 (1994).

625. T. A. Ramelot, C.-H. Hu, J. E. Fowler, B. J. DeLeeuw, and H. F. Schaefer, "Carbonyl-Water Hydrogen Bonding: The  $\text{H}_2\text{CO}-\text{H}_2\text{O}$  Prototype", *J. Chem. Phys.* **100**, 4347 (1994).
626. B. F. Yates and H. F. Schaefer, "The Inversion Barrier in  $\text{NF}_3^+$ ", *J. Chem. Phys.* **100**, 4459 (1994).
627. Y. Xie, H. F. Schaefer, G. Liang, and J. P. Bowen, "[10] Annulene: The Wealth of Energetically Low-Lying Structural Isomers of the Same  $(\text{CH})_{10}$  Connectivity", *J. Am. Chem. Soc.* **116**, 1442 (1994).
628. Y. Yamaguchi, G. Vacek, J. R. Thomas, B. J. DeLeeuw, and H. F. Schaefer, "First and Second Energy Derivative Analyses of the Vinylidene and Acetylene Triplet State Potential Energy Surfaces", *J. Chem. Phys.* **100**, 4969 (1994).
629. Y. Yamaguchi, H. F. Schaefer, and G. Frenking, "First and Second Energy Derivative Analyses for Open-Shell Self-Consistent-Field (SCF) Wavefunctions", *Mol. Phys.* **82**, 713 (1994).
630. B. Ma, H. M. Sulzbach, Y. Xie, and H. F. Schaefer, " $\pi$  Electron Delocalization and Compression in Acyclic Acetylenic Precursors to Multidimensional Carbon Networks: Comparison with Experiment for the Recently Synthesized Tris(trimethylsilyl) Substituted Tetraethynylmethane. Structures, Thermochemistry, Infrared Spectra, Polarizabilities, and Hyperpolarizabilities", *J. Am. Chem. Soc.* **116**, 3529 (1994).
631. J. T. Fermann, C. D. Sherrill, T. D. Crawford, and H. F. Schaefer, "Benchmark Studies of Electron Correlation in Six-Electron Systems", *J. Chem. Phys.* **100**, 8132 (1994).
632. B. Ma and H. F. Schaefer, "Toward the Observation of Silanone ( $\text{H}_2\text{SiO}$ ) and Hydroxysilylene ( $\text{HSiOH}$ ) via Microwave Spectroscopy", *J. Chem. Phys.* **101**, 2734 (1994).
633. H. M. Sulzbach, P. R. Schleyer, and H. F. Schaefer, "The Interrelationship Between Conformation and Theoretical Chemical Shifts. Case Study on Glycine and Glycine Amide", *J. Am. Chem. Soc.* **116**, 3967 (1994).
634. B. Ma and H. F. Schaefer, "Singlet Methylcarbene: Equilibrium Geometry or Transition State?" *J. Am. Chem. Soc.* **116**, 3539 (1994).
635. C. D. Sherrill and H. F. Schaefer, "The  $\tilde{A}^1A'$  State of Isocyanogen ( $\text{CNCN}$ )", *J. Chem. Phys.* **100**, 8920 (1994).
636. C. B. Kellogg, J. M. Galbraith, J. E. Fowler, and H. F. Schaefer, "Equilibrium Geometry of Isocyanomethylene ( $\text{HCNC}$ ) and Comparison to the Troublesome Isomer Cyanomethylene ( $\text{HCCN}$ )", *J. Chem. Phys.* **101**, 430 (1994).
637. C.-H. Hu, P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "Structure, Infrared Spectrum and Dissociation Energy of  $\text{SiH}_7^+$ ", *J. Phys. Chem.* **98**, 5040 (1994).
638. C.-H. Hu and H. F. Schaefer, "Reaction Barrier for the Methyl diazenyl Radical Decomposition ( $\text{CH}_3\text{N}_2 \rightarrow \text{CH}_3 + \text{N}_2$ )", *J. Chem. Phys.* **101**, 1289 (1994).
639. G. E. Quelch, M. M. Gallo, M. Shen, Y. Xie, H. F. Schaefer and D. Moncrief, "Aspects of the Reaction Mechanism of Ethane Combustion. Nature of the Intramolecular Hydrogen Transfer", *J. Am. Chem. Soc.* **116**, 4953 (1994).
640. P. R. Schreiner, H. F. Schaefer, and P. R. Schleyer, "The Structures, Energies, Vibrational and Rotational Frequencies, and Dissociation Energy of  $\text{GeH}_5^+$ ", *J. Chem. Phys.* **101**, 2141 (1994).
641. M. Shen and H. F. Schaefer, "Dodecahedral and Smaller Arsenic Clusters:  $\text{As}_n$ ,  $n = 2, 4, 12, 20$ ", *J. Chem. Phys.* **101**, 2261 (1994).
642. Y. Yamaguchi, B. J. DeLeeuw, G. Vacek, C. A. Richards, and H. F. Schaefer, "Comparative Energy Derivative Analyses of the  $\text{HBO}-\text{BOH}$  and  $\text{AlOH}-\text{HALO}$  Potential Energy Surfaces", *J. Chem. Phys.* **101**, 3006 (1994).
643. V. S. Mastryukov, H. F. Schaefer, and J. E. Boggs, "Self-Consistent Changes of Geometrical Parameters: Experiment and Theory", *Acc. Chem. Res.* **27**, 242 (1994).
644. Y. Xie, R. B. Remington, and H. F. Schaefer, "The Protonated Water Dimer: Extensive Theoretical Studies of  $\text{H}_5\text{O}_2^+$ ", *J. Chem. Phys.* **101**, 4878 (1994).
645. B. Ma, C. Meredith, and H. F. Schaefer, "Pyrophosphate Structures and Reactions: The Evaluation of Electrostatic Effects on the Pyrophosphates with and without Alkali Cations", *J. Phys. Chem.* **98**, 8216 (1994).
646. J. E. Baldwin, Y. Yamaguchi, and H. F. Schaefer, "Thermal Stereomutations of Cyclopropane and of Isotopically Labeled Cyclopropanes Assessed Through *Ab Initio* Computational Methods and Kinetic Isotope Effect Calculations", *J. Phys. Chem.* **98**, 7513 (1994).
647. P. R. Schreiner, H. F. Schaefer, and P. R. Schleyer, "The Structure and Stability of  $\text{BH}_5$ —Does Correlation Make it a Stable Molecule? Qualitative Changes at High Levels of Theory", *J. Chem. Phys.* **101**, 7625 (1994).
648. J. E. Fowler, J. M. Galbraith, G. Vacek, and H. F. Schaefer, "Substituted Oxirenes ( $\text{X}_2\text{C}_2\text{O}$ ,  $\text{X}=\text{BH}_2, \text{CH}_3, \text{NH}_2, \text{OH}, \text{F}$ ): Can They Be Made?" *J. Am. Chem. Soc.* **116**, 9311 (1994).
649. G. Vacek, J. M. Galbraith, Y. Yamaguchi, H. F. Schaefer, R. H. Nobes, A. P. Scott, and L. Radom, "Oxirene: To Be or Not To Be?" *J. Phys. Chem.* **98**, 8660 (1994).
650. J. E. Fowler and H. F. Schaefer, "The Tetramethyl Chalcogens ( $\text{Me}_4\text{S}$ ,  $\text{Me}_4\text{Se}$ ,  $\text{Me}_4\text{Te}$ ): Bonding and Structure", *J. Am. Chem. Soc.* **116**, 9596 (1994).
651. E. E. Bolton, H. F. Schaefer, W. D. Laidig, and P. R. Schleyer, "Singlet  $\text{C}_2\text{H}_2\text{Li}_2$ : Acetylenic and 1,2-Dilithioethene Isomers. A Remarkably Congested Potential Energy Hypersurface for a Simple Organometallic System", *J. Am. Chem. Soc.* **116**, 9602 (1994).
652. A. P. Scott, R. H. Nobes, H. F. Schaefer, and L. Radom, "The Wolff Rearrangement: The Relevant Portion of the Oxirene-Ketene Potential Energy Hypersurface," *J. Am. Chem. Soc.* **116**, 10165 (1994).
653. Y. Yamaguchi, C. A. Richards, and H. F. Schaefer, "High Level *Ab Initio* Study on the Ground-State Potential Energy Hypersurface of the  $\text{HCO}^+-\text{COH}^+$  System", *J. Chem. Phys.* **101**, 8945 (1994).
654. M. Ponder, J. E. Fowler, and H. F. Schaefer, "Proposed Intermediates in the Tautomerization of Benzofurazan 1-Oxide", *J. Organic Chem.* **59**, 6431 (1994).
655. Y. Xie and H. F. Schaefer, "The Electron Affinity of  $\text{CF}^+$ ", *J. Chem. Phys.* **101**, 10191 (1994).
656. H. F. Schaefer, J. R. Thomas, Y. Yamaguchi, B. J. DeLeeuw, and G. Vacek, "The Chemical Applicability of Standard Methods in *Ab Initio* Molecular Quantum Mechanics", in *Modern Electronic Structure Theory*, editor D. R. Yarkony (World Scientific Publishing, Singapore, 1995). Pages 3–54.

657. G. Vacek, V. S. Mastryukov, and H. F. Schaefer, "Deviations from Idealized Geometry: An *Ab Initio* Investigation of  $(\text{CH}_3)_2 \text{AX}_2$  Molecules [A = Si, Ge; X = F, Cl]", *J. Phys. Chem.* **98**, 11337 (1994).
658. H. M. Sulzbach, P. R. Schleyer, and H. F. Schaefer, "Influence of the Non-Planarity of the Amide Moiety on Computed Chemical Shifts in Peptide Analogues. Is the Amide Nitrogen Pyramidal?" *J. Am. Chem. Soc.* **117**, 2632 (1995).
659. Y. Yamaguchi, B. J. DeLeeuw, C. A. Richards, and H. F. Schaefer, "Application of the Energy Derivative Analysis Method to the *Cis* Monobridged Equilibrium Structures  $\text{Al}_2\text{H}_2$ ,  $\text{Si}_2\text{H}_2$ ,  $\text{Ga}_2\text{H}_2$ , and  $\text{Ge}_2\text{H}_2$  and the Comparable Stationary Points of  $\text{B}_2\text{H}_2$  and  $\text{C}_2\text{H}_2$ ", *J. Am. Chem. Soc.* **116**, 11922 (1994).
660. P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "The Electrophilic Reactions of Aliphatic Hydrocarbons: Substitution and Cleavage of Ethane by  $\text{NO}^+$ ", *J. Am. Chem. Soc.* **117**, 453 (1995).
661. J. E. Fowler, H. F. Schaefer, and K. N. Raymond, "The  $S_6$  Point Group Conformers of the Hexamethyl-Chalcogens:  $\text{Me}_6\text{S}$ ,  $\text{Me}_6\text{Se}$ , and  $\text{Me}_6\text{Te}$ ", *Inorg. Chem.* **35**, 279 (1996).
662. B. J. Duke, J. W. Gauld, and H. F. Schaefer, "The Structure of Hydridogallium and Hydridoaluminum Bis (Tetrahydroborates)", *Chem. Phys. Lett.* **230**, 306 (1994).
663. H. F. Schaefer, "Computers and Molecular Quantum Mechanics: 1965–1994, A Personal Perspective", pages 22–32, *Proceedings of the High Performance Computing Conference '94*, September 29–30, 1994, Singapore (National Supercomputing Research Centre, National University of Singapore, 81 Science Park Drive, #04–03 The Chadwick, Singapore Science Park, Singapore 0511). ISBN: 981-00-6013-0.
664. J. E. Fowler and H. F. Schaefer, "A Detailed Study of the Water Trimer Potential Energy Surface", *J. Am. Chem. Soc.* **117**, 446 (1995).
665. C. A. Richards, G. Vacek, B. J. DeLeeuw, Y. Yamaguchi, and H. F. Schaefer, "An *Ab Initio* Study on the Ground-State HBO–BOH System", *J. Chem. Phys.* **102**, 1280 (1995).
666. P. F. Souter, L. Andrews, A. J. Downs, T. M. Greene, B. Ma, and H. F. Schaefer, "Observed and Calculated Raman Spectra of the  $\text{Ga}_2\text{H}_6$  and  $\text{Ga}_2\text{D}_6$  Molecules", *J. Phys. Chem.* **98**, 12824 (1994).
667. C. M. B. Marsh and H. F. Schaefer, "Trimethylamine Alane and its Dissociation Products", *J. Phys. Chem.* **99**, 195 (1995).
668. C. L. Collins, K. G. Dyall, and H. F. Schaefer, "Relativistic and Correlation Effects in CuH, AgH, and AuH: Comparison of Various Relativistic Methods", *J. Chem. Phys.* **102**, 2024 (1995).
669. T. D. Crawford, K. W. Springer, and H. F. Schaefer, "A Contribution to the Understanding of the Structure of Xenon Hexafluoride", *J. Chem. Phys.* **102**, 3307 (1995).
670. P. R. Schreiner, D. L. Severance, W. L. Jorgensen, P. R. Schleyer, and H. F. Schaefer, "The Energy Difference Between the Classical and the Nonclassical 2-Norbornyl Cation in Solution, A Combined *Ab Initio*–Monte Carlo Aqueous Solution Study", *J. Am. Chem. Soc.* **117**, 2663 (1995).
671. M. L. Leininger, C. D. Sherrill, and H. F. Schaefer, " $\text{N}_8$ : A Structure Analogous to Pentalene and Other High Energy Density Minima", *J. Phys. Chem.* **99**, 2324 (1995).
672. C.-H. Hu and H. F. Schaefer, "The Mechanism of the Thermal Decomposition and the  $(n - \pi^*)$  Excited States of Azomethane", *J. Phys. Chem.* (Mostafa A. El-Sayed Issue) **99**, 7507 (1995).
673. H. M. Sulzbach, P. R. Schleyer, H. Jiao, Y. Xie, P. O'Leary, and H. F. Schaefer, "A [10] Annulene Isomer May Be Aromatic, After All!" *J. Am. Chem. Soc.* **117**, 1369 (1995).
674. C. D. Sherrill and H. F. Schaefer, "1-Silavinylidene: The First Unsaturated Silylene", *J. Phys. Chem.* **99**, 1949 (1995).
675. E. F. Archibong, P. R. Schreiner, J. Leszczynski, P. R. Schleyer, H. F. Schaefer, and R. Sullivan, "*Ab Initio* Prediction of the Structure, Harmonic Vibrational Frequencies and Dissociation Energy of the  $\text{H}_2\text{--GeH}_3^+\text{--H}_2$  Cluster Ion", *J. Chem. Phys.* **102**, 3667 (1995).
676. C. B. Kellogg and H. F. Schaefer, "The Ring and Superoxide Isomers of  $\text{SO}_2$ ", *J. Chem. Phys.* **102**, 4177 (1995).
677. B. J. DeLeeuw, Y. Yamaguchi, and H. F. Schaefer, "Chromium Dihydride ( $\text{CrH}_2$ ): Theoretical Evidence for a Bent  $^5\text{B}_2$  Ground State", *Mol. Phys.* **84**, 1109 (1995).
678. J. R. Thomas, B. J. DeLeeuw, P. O'Leary, H. F. Schaefer, B. J. Duke, and B. O'Leary, "The Ethylenedione Anion: Elucidation of the Intricate Potential Energy Hypersurface", *J. Chem. Phys.* **102**, 6525 (1995).
679. B. Ma, C. Meredith, and H. F. Schaefer, "Quest for a Metaphosphate Intermediate—the Mechanisms for Hydrolysis of Pyrophosphates with and without Catalysis", *J. Phys. Chem.* **99**, 3815 (1995).
680. B. Ma, Y. Yamaguchi, and H. F. Schaefer, "Spectroscopic Constants and Potential Energy Surfaces for the Possible Interstellar Molecules  $\text{AlNC}$  and  $\text{AlCN}$ ", *Mol. Phys.* **86**, 1331 (1995).
681. D. M. Miller, P. R. Schreiner, and H. F. Schaefer, "Singlet Methylcarbene: An Elusive Intermediate of the Thermal Decomposition of Diazoethane and Methyl diazirene", *J. Am. Chem. Soc.* **117**, 4137 (1995).
682. Y. Yamaguchi and H. F. Schaefer, "The  $\text{SiOH}^+\text{--HSiO}^+$  System. A High Level *Ab Initio* Quantum Mechanical Study", *J. Chem. Phys.* **102**, 5327 (1995).
683. P. O'Leary, J. R. Thomas, H. F. Schaefer, B. J. Duke, and B. O'Leary, "A Study of the Silagermylyne ( $\text{SiGeH}_2$ ) Molecule: A New Monobridged Structure", *Int. J. Quantum Chem. Symp.* **29**, 593 (1995).
684. H. M. Sulzbach, Y. Xie, and H. F. Schaefer, "[10] Annulene: Was Hückel Right?" *Proceedings of the Robert A. Welch Foundation 38th Conference on Chemical Research*, October 24–25, 1994, Houston, Texas, pages 28–43.
685. C.-H. Hu, B. Ma, and H. F. Schaefer, "The Synchronous Thermal Decomposition Mechanism of Azoisopropane", *Mol. Phys.* **85**, 769 (1995).
686. B. J. Duke, J. W. Gauld, and H. F. Schaefer, "A New Isomer of Triborane (9)", *J. Am. Chem. Soc.* **117**, 7753 (1995).
687. R. A. King, G. Vacek, and H. F. Schaefer, "1,3,5-Trisilabenzene: Has It Been Synthesized?" *J. Mol. Struct.* **358**, 1 (1995).

688. P. R. Schreiner, H. F. Schaefer, and P. R. Schleyer "Can  $\text{AlH}_5$  Exist?" *J. Chem. Phys.* **103**, 5565 (1995).
689. B. Ma, H. M. Sulzbach, R. B. Remington, and H. F. Schaefer, "The Structure, Strain Energy and Magnetic Susceptibility of [4] Paracyclophane and the Activation Energy for its Interconversion with 1,4 Tetramethylene Dewar Benzene", *J. Am. Chem. Soc.* **117**, 8392 (1995).
690. C. L. Collins, K. Morihashi, Y. Yamaguchi, and H. F. Schaefer, "Vibrational Frequencies of the HF Dimer from the Coupled Cluster Method Including All Single and Double Excitations Plus Perturbative Connected Triple Excitations [CCSD(T)]", *J. Chem. Phys.* **103**, 6051 (1995).
691. I. S. Ignatyev and H. F. Schaefer, "The Search for the Low-Lying States of the  $\text{Si}_2\text{C}_2^+$  Radical Cation", *J. Chem. Phys.* **103**, 7025 (1995).
692. C. M. B. Marsh and H. F. Schaefer, "Bisammonia Alane Does Not Incorporate Dative Bonds", *J. Phys. Chem.* **99**, 14309 (1995).
693. J. Leszczynski, J. Q. Huang, P. R. Schreiner, G. Vacek, J. Kapp, P. R. Schleyer, and H. F. Schaefer, "Molecular Geometries of Disilane, Silylgermane, and Digermane. Is there a Discrepancy between Experiment and Theory?" *Chem. Phys. Lett.* **244**, 252 (1995).
694. C. A. Richards, S.-J. Kim, Y. Yamaguchi, and H. F. Schaefer, "Dimethylcarbene: A Singlet Ground State?" *J. Am. Chem. Soc.* **117**, 10104 (1995).
695. Y. Yamaguchi, C. A. Richards, and H. F. Schaefer, "The  $\text{GeOH}^+-\text{HGeO}^+$  System: A Detailed Quantum Mechanical Study", *J. Chem. Phys.* **103**, 7975 (1995).
696. A. Gobbi, Y. Yamaguchi, G. Frenking, and H. F. Schaefer, "The Role of  $\sigma$  and  $\pi$  Stabilization in Benzene, Allyl Cation and Allyl Anion. A Canonical Orbital Energy Derivative Study", *Chem. Phys. Lett.* **244**, 27 (1995).
697. C.-H. Hu and H. F. Schaefer, "Structure and Decomposition Barrier of the Ethyldiazanyl Radical", *J. Mol. Struct.* (James E. Boggs Issue) **376**, 413 (1996).
698. Y. Xie and H. F. Schaefer, "Singlet-Triplet Splitting of Carbohydroxycarbene", *Mol. Phys.* **87**, 389 (1996).
699. E. E. Bolton, W. D. Laidig, P. R. Schleyer, and H. F. Schaefer, "Does Singlet 1,1 Dithioethene Really Prefer a Perpendicular Structure?" *J. Phys. Chem.* **99**, 17551 (1995).
700. G. Vacek, C. D. Sherrill, Y. Yamaguchi, and H. F. Schaefer, "The Anomalous Behavior of the Zeeman Anticrossing Spectra of  $\tilde{A}^1\text{A}_u$  Acetylene: Theoretical Considerations", *J. Chem. Phys.* **104**, 1774 (1996).
701. G. S. Tschumper, J. T. Fermann, and H. F. Schaefer, "Structures, Thermochemistry, and Electron Affinities of the  $\text{PF}_n$  and  $\text{PF}_n^-$  Series,  $n = 1-6$ ", *J. Chem. Phys.* **104**, 3676 (1996).
702. S. S. Wesolowski, T. D. Crawford, J. T. Fermann, and H. F. Schaefer, "Aluminum Monocarbonyl and Aluminum Isocarbonyl", *J. Chem. Phys.* **104**, 3672 (1996).
703. B. Ma, C. L. Collins, and H. F. Schaefer, "Periodic Trends for Transition Metal Dihydrides  $\text{MH}_2$ , Dihydride Dihydrogen Complexes  $\text{MH}_2\cdot\text{H}_2$  and Tetrahydrides  $\text{MH}_4$  ( $\text{M} = \text{Ti}, \text{V}, \text{and Cr}$ )", *J. Am. Chem. Soc.* **118**, 870 (1996).
704. S.-J. Kim, H. F. Schaefer, E. Kraka, and D. Cremer, "Dioxirane Vibrational Frequencies: An Unsettling Relationship Between Theory and Experiment", *Mol. Phys.* (A. David Buckingham Issue) **88**, 93 (1996).
705. R. A. King, J. M. Galbraith and H. F. Schaefer, "Negative Ion Thermochemistry: The Sulfur Fluorides  $\text{SF}_n/\text{SF}_n^-$  ( $n = 1-7$ )", *J. Phys. Chem.* (Boys/Shavitt Issue) **100**, 6061 (1996).
706. Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, "The  $\tilde{X}^3\text{B}_1$ ,  $\tilde{a}^1\text{A}_1$ ,  $\tilde{b}^1\text{B}_1$  and  $\tilde{c}^1\text{A}_1$  States of  $\text{CH}_2^+$ ", *J. Phys. Chem.* (James L. Kinsey Issue) **100**, 7911 (1996).
707. C. D. Sherrill and H. F. Schaefer, "Compact Variational Wavefunctions Incorporating Limited Triple and Quadruple Substitutions", *J. Phys. Chem.* (Boys/Shavitt Issue) **100**, 6069 (1996).
708. P. R. Schleyer, H. Jiao, H. M. Sulzbach, and H. F. Schaefer, "Highly Aromatic Planar All-*cis* -[10] Annulene Derivatives", *J. Am. Chem. Soc.* **118**, 2093 (1996).
709. T. D. Crawford and H. F. Schaefer, "A Comparison of Two Approaches to Perturbational Triple Excitation Corrections to the Coupled-Cluster Singles and Doubles Method for High-Spin Open-Shell Systems", *J. Chem. Phys.* **104**, 6259 (1996).
710. D. M. Miller, W. D. Allen, and H. F. Schaefer, "The Electron Affinity of  $\text{CF}_3$ ", *Mol. Phys.* **88**, 727 (1996).
711. H. H. Huang, Y. Xie, and H. F. Schaefer, "Can Oxywater Be Made?" *J. Phys. Chem.* (Boys/Shavitt Issue) **100**, 6076 (1996).
712. Y. Xie, W. D. Allen, Y. Yamaguchi, and H. F. Schaefer, "Is the Oxywater Radical Cation More Stable than Neutral Oxywater?" *J. Chem. Phys.* **104**, 7615 (1996).
713. H. M. Sulzbach, G. Vacek, P. R. Schreiner, J. M. Galbraith, P. R. Schleyer, and H. F. Schaefer, "NMR Chemical Shielding Surface of *N*-Acetyl-*N'* Methylalaninamide: A Density Functional Study", *J. Comput. Chem.* **18**, No. 1, 126 (1997).
714. N. C. Handy and H. F. Schaefer, "Molecular Quantum Mechanics: Methods and Applications", *J. Phys. Chem.* (Boys/Shavitt Issue) **100**, 6003 (1996).
715. C. D. Sherrill, G. Vacek, Y. Yamaguchi, and H. F. Schaefer, "The  $\tilde{A}^1\text{A}_u$  State and the  $\text{T}_2$  Potential Energy Surface of Acetylene: Implications for Triplet Perturbations in the Fluorescence Spectra of the  $\tilde{A}$  State", *J. Chem. Phys.* **104**, 8507 (1996).
716. H. M. Sulzbach, H. F. Schaefer, W. Klopper and H.-P. Lüthi, "Exploring the Boundary Between Aromatic and Olefinic Character: Bad News for Second-Order Perturbation Theory and Density Functional Schemes", *J. Am. Chem. Soc.* **118**, 3519 (1996).
717. B. Ma and H. F. Schaefer, "Singlet-Triplet Energy Separation and Barrier for Ring Closure for Trimethylenemethane and its Complexes", *Chem. Phys.* **207**, 31 (1996).
718. C. A. Richards, Y. Yamaguchi, S.-J. Kim, and H. F. Schaefer, "The  $\text{GaOH}-\text{HGaO}$  Potential Energy Hypersurface and the Necessity of Correlating the 3d Electrons", *J. Chem. Phys.* **104**, 8516 (1996).
719. H. F. Schaefer, "Odorless Chemistry: A Gentle Reductionist Companion to Experiment", *J. Chinese Chem. Soc.* **43**, 109 (1996).
720. J. R. Thomas, P. O'Leary, B. J. DeLeeuw, B. J. Duke, B. O'Leary, and H. F. Schaefer, "The Structurally-Rich Potential Energy Surface of the Algallylyne ( $\text{AlGaH}_2$ ) Molecule", *J. Phys. Chem.* **100**, 7372 (1996).
721. Y. Yamaguchi and H. F. Schaefer, "The  $\text{GeOH}-\text{HGeO}$  System. Are the 3d Electrons Core or Valence?" *J. Chem. Phys.* **104**, 9841 (1996).

722. J. M. Galbraith and H. F. Schaefer, "The Nitrosyl Azide ( $N_4O$ ) Potential Energy Hypersurface: A High Energy-Density Boom or Bust?" *J. Am. Chem. Soc.* **118**, 4860 (1996).
723. T. J. Van Huis, J. M. Galbraith, and H. F. Schaefer, "The Monochlorine Fluorides ( $ClF_n$ ) and their Anions ( $ClF_n^-$ ),  $n = 1-7$ : Structures and Energetics", *Mol. Phys. (A. David Buckingham Issue)* **89**, 607 (1996).
724. T. D. Crawford, H. F. Schaefer, and T. J. Lee, "On the Energy Invariance of Open-Shell Perturbation Theory with Respect to Unitary Transformations of Molecular Orbitals", *J. Chem. Phys.* **105**, 1060 (1996).
725. Y. Yamaguchi, Y. Xie, S.-J. Kim, and H. F. Schaefer, "The  $SiOH-HSiO$  System: A High Level Quantum Mechanical Study", *J. Chem Phys.* **105**, 1951 (1996).
726. B. C. Hoffman, C. D. Sherrill, and H. F. Schaefer, "Monomethyl Gallium: Prelude to Experiment", *J. Mol. Struct.* **370**, 93 (1996).
727. P. R. Schreiner, H. F. Schaefer, and P. R. Schleyer, "Alkyl Cation-Dihydrogen Complexes, Silonium and Germanium Cations. Theoretical Considerations", Volume 2, pages 125-160, *Advances in Gas-Phase Ion Chemistry*, editors N. Adams and L. M. Babcock (JAI Press, Greenwich, CT, 1996).
728. J. M. Galbraith and H. F. Schaefer, "Concerning the Applicability of Density Functional Methods to Atomic and Molecular Negative Ions", *J. Chem. Phys.* **105**, 862 (1996).
729. R. D. Davy and H. F. Schaefer, "Open Chain Versus Cyclic Fourteen Electron Triatomics. Molecular Structures and Vibrational Frequencies of  $P_2Si$ ,  $P_2C$ ,  $SiN_2$ , and  $Si_2S$ ", *Chem. Phys. Lett.* **255**, 171 (1996).
730. B. Ma, J.-H. Lii, H. F. Schaefer, and N. L. Allinger, "Systematic Comparison of Experimental, Quantum Mechanical, and Molecular Mechanical Bond Lengths for Organic Molecules", *J. Phys. Chem.* **100**, 8763 (1996).
731. C. D. Sherrill, C. G. Brandow, W. D. Allen, and H. F. Schaefer, "Cyclopropyne and Silacyclopropyne: A World of Difference", *J. Am. Chem. Soc.* **118**, 7158 (1996).
732. H. M. Sulzbach, E. E. Bolton, D. Lenoir, P. R. Schleyer, and H. F. Schaefer, "Tetra-*tert*-butylethylene: An Elusive Molecule With a Highly Twisted Double Bond. Can it be Made by Carbene Dimerization?", *J. Am. Chem. Soc.* **118**, 9908 (1996).
733. B. Ma, N. L. Allinger, and H. F. Schaefer, "Spectroscopic Constants and Potential Energy Surfaces for Silanone ( $H_2SiO$ ), Hydroxysilylene ( $HSiOH$ ), the Hydroxysilylene Dimer and the Disilylanyl Radical ( $Si_2H$ )", *J. Chem. Phys.* **105**, 5731 (1996).
734. P. R. Bunker, P. Jensen, Y. Yamaguchi, and H. F. Schaefer, "The Rovibrational Energy Levels of Quasi-linear  $\tilde{c}^1A_1$  Methylene", *J. Mol. Spectrosc.* **179**, 263 (1996).
735. X.-W. Li, Y. Xie, P. R. Schreiner, K. D. Gripper, R. C. Crittendon, C. F. Campana, H. F. Schaefer, and G. H. Robinson, "Cyclogallanes and Metalloaromaticity. Synthesis and Molecular Structure of Dipotassium Tris(2,6-dimesitylphenyl) cyclogallene,  $K_2[(Mes)_2C_6H_3]Ga_3$  ( $Mes = 2,4,6-Me_3C_6H_2$ ): A Structural and Theoretical Examination", *Organometallics* **15**, 3798 (1996).
736. H. F. Bettinger, P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "Ring Opening of Cyclopropylidene and Internal Rotation of Allene", *J. Phys. Chem.* **100**, 16147 (1996).
737. R. A. King, V. S. Mastryukov, and H. F. Schaefer, "The Electron Affinities of the Silicon Fluorides  $SiF_n$  ( $n = 1-5$ )", *J. Chem. Phys.* **105**, 6880 (1996).
738. C. B. Kellogg, E. Valeev, J. M. Galbraith, J. E. Fowler, and H. F. Schaefer, "The Elementary Reaction of Quartet Methylidyne ( $CH$ ) with Methane", *Mol. Phys.* **89**, 1659 (1996).
739. H. M. Sulzbach, D. Graham, J. C. Stephens, and H. F. Schaefer, "The Strange Case of the Ethane Radical Cation", *Acta Chem. Scand.* **51**, 547 (1997).
740. E. Kraka, Z. Konkoli, D. Cremer, J. E. Fowler, and H. F. Schaefer, "Difluorodioxirane—An Unusual Cyclic Peroxide", *J. Am. Chem. Soc.* **118**, 10595 (1996).
741. Y. Xie, P. R. Schreiner, H. F. Schaefer, X.-W. Li, and G. H. Robinson, "Are Cyclogallenes [ $M_2(GaH)_3$ ] ( $M = Li, Na, K$ ) Aromatic?" *J. Am. Chem. Soc.* **118**, 10635 (1996).
742. J. E. Baldwin, T. B. Freedman, Y. Yamaguchi, and H. F. Schaefer, "Secondary Deuterium Kinetic Isotope Effects on the Isomerization of the Trimethylene Diradical to Cyclopropane", *J. Am. Chem. Soc.* **118**, 10934 (1996).
743. P. R. Bunker, P. Jensen, Y. Yamaguchi, and H. F. Schaefer, "High Level *Ab Initio* Calculation of the Rotation-Vibration Energies in the  $\tilde{c}^1A_1$  State of Methylene  $CH_2$ ", *J. Phys. Chem.* **100**, 18088 (1996).
744. P. R. Schreiner, W. L. Karney, P. R. Schleyer, W. T. Borden, T. P. Hamilton, and H. F. Schaefer, "Carbene Rearrangements Unsurpassed: The  $C_7H_6$  Potential Energy Surface Revealed", *J. Org. Chem.* **61**, 7030 (1996).
745. Y. Yamaguchi and H. F. Schaefer, "The  $^3A_2$ ,  $^1A_2$ ,  $^3B_2$ , and  $^1B_2$  Electronic States of  $CH_2$ : Small Bond Angle States", *J. Chem. Phys.* **106**, 1819 (1997).
746. C. D. Sherrill, T. J. Van Huis, Y. Yamaguchi, and H. F. Schaefer, "Full Configuration Interaction Benchmarks for the  $\tilde{X}^3B_1$ ,  $\tilde{a}^1A_1$ ,  $\tilde{b}^1B_1$ , and  $\tilde{c}^1A_1$  States of Methylene", *J. Mol. Struct. (THEOCHEM)* (Issue on *Ab Initio* Benchmark Studies) **400**, 139 (1997).
747. R. A. Morris, W. B. Knighton, A. A. Viggiano, B. C. Hoffman, and H. F. Schaefer, "The Gas-Phase Acidity of  $H_3PO_4$ ", *J. Chem. Phys.* **106**, 3545 (1997).
748. Y. Xie, P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "The Naphthylcarbene Potential Energy Hypersurface," *J. Am. Chem. Soc.* **119**, 1370 (1997).
749. J. C. Stephens, E. E. Bolton, and H. F. Schaefer, and L. Andrews "Quantum Mechanical Frequencies and Matrix Assignments for  $Al_2H_2$ ", *J. Chem. Phys.* **107**, 119 (1997).
750. H. F. Schaefer, "The Reachable Dream: Some Steps Toward the Realization of Molecular Quantum Mechanics by Computer", *J. Mol. Struct. (WATOC Jerusalem Symposium Issue)* **398**, 199 (1997).
751. T. J. Van Huis and H. F. Schaefer, "The  $ClO_4$  Radical: Experiment versus Theory", *J. Chem. Phys.* **106**, 4028 (1997).
752. R. D. Davy and H. F. Schaefer, "Aluminum-Phosphorus Compounds with Low Coordination Numbers: Structures, Energies, and Vibrational Frequencies of the  $AlPH_2$ ,  $AlPH_3$ , and  $AlPH_4$  Isomers, and the  $H_3Al-PH_3$  Adduct", *J. Phys. Chem. A* **101**, 3135 (1997).

753. H. F. Schaefer, "The World Association of Theoretically Oriented Chemists (WATOC) 1996–1999", *J. Mol. Struct. (WATOC Jerusalem Symposium Issue)* **398**, xiii (1997).
754. J. T. Fermann, B. C. Hoffmann, G. S. Tschumper, and H. F. Schaefer, "The Hydroperoxyl Radical Dimer: Triplet Ring or Singlet String?" *J. Chem. Phys.* **106**, 5102 (1997).
755. N. L. Allinger, J. T. Fermann, W. D. Allen, and H. F. Schaefer, "The Torsional Conformations of Butane: Definitive Energetics from *Ab Initio* Methods", *J. Chem. Phys.* **106**, 5143 (1997).
756. P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer, "Why the Classical and Nonclassical Norbornyl Cations Do Not Resemble the 2-endo and 2-exo-Norbornyl Solvolysis Transition States", *J. Org. Chem.* **62**, 4216 (1997).
757. S. S. Wesolowski, J. T. Fermann, T. D. Crawford, and H. F. Schaefer, "The Weakly Bound Dinitrogen Tetroxide Molecule: High Level Single Reference Wavefunctions are Good Enough", *J. Chem. Phys.* **106**, 7178 (1997).
758. C. B. Kellogg and H. F. Schaefer, "Coupled-Cluster Vibrational Frequencies for Open, Ring, and Superoxide Sulfur Dioxide", *Theor. Chem. Acc.* **96**, 7 (1997).
759. A. Tian, F. Ding, L. Zhang, Y. Xie, and H. F. Schaefer, "New Isomers of N<sub>8</sub> without Double Bonds", *J. Phys. Chem. A* **101**, 1946 (1997).
760. J. M. Galbraith and H. F. Schaefer, "Hydrogen Bridging in Molecules Containing Atoms Beyond the First Row", *J. Mol. Struct. (Lionel Salem Issue)* **424**, 7 (1998).
761. R. A. King and H. F. Schaefer, "Molecular Geometry and Vibrational Frequency Predictions from the CISD [TQ] Wavefunction: The Water Molecule", *Spectrochim. Acta A (Issue on Ab Initio and Ab Initio Derived Force Fields: State of the Science)* **53**, 1163 (1997).
762. Y. Yamaguchi and H. F. Schaefer, "The 3d Rydberg (<sup>3</sup>A<sub>2</sub>) Electronic State Observed by Herzberg and Shoosmith for Methylene", *J. Chem. Phys.* **106**, 8753 (1997).
763. I. S. Ignatyev, Y. Xie, W. D. Allen, and H. F. Schaefer, "Mechanism of the C<sub>2</sub>H<sub>5</sub> + O<sub>2</sub> Reaction", *J. Chem. Phys.* **107**, 141 (1997).
764. G. S. Tschumper, Y. Yamaguchi, and H. F. Schaefer, "A High Level Theoretical Investigation of the Cyclic Hydrogen Fluoride Trimer", *J. Chem. Phys.* **106**, 9627 (1997).
765. J. C. Rienstra-Kiracofe and H. F. Schaefer, "Revision of the Experimental Electron Affinity of BO", *J. Chem. Phys.* **106**, 8278 (1997).
766. A. Y. Timoshkin, H. F. Bettinger, and H. F. Schaefer, "The Chemical Vapor Deposition of Aluminum Nitride: Unusual Cluster Formation in the Gas Phase", *J. Am. Chem. Soc.* **119**, 5668 (1997).
767. Y. Yamaguchi, T. J. Van Huis, C. D. Sherrill, and H. F. Schaefer, "The  $\tilde{X}^1A_1$ ,  $\tilde{a}^3B_1$ ,  $\tilde{A}^1B_1$ , and  $\tilde{B}^1A_1$  Electronic State of SiH<sub>2</sub>", *Theor. Chem. Acc. (Jan Almlöf Memorial Issue)* **97**, 341 (1997).
768. M. L. Leininger, T. J. Van Huis, and H. F. Schaefer, "Protonated High Energy Density Materials: N<sub>4</sub> Tetrahedron and N<sub>8</sub> Octahedron", *J. Phys. Chem. A* **101**, 4460 (1997).
769. I. M. B. Nielsen, W. D. Allen, A. G. Császár, and H. F. Schaefer, "Toward Resolution of the Silicon Dicarbide (SiC<sub>2</sub>) Saga: *Ab Initio* Excursions in the Web of Polytopism", *J. Chem. Phys.* **107**, 1195 (1997).
770. G. S. Tschumper and H. F. Schaefer, "Predicting Electron Affinities with Density Functional Theory: Some Positive Results for Negative Ions", *J. Chem. Phys.* **107**, 2529 (1997).
771. T. D. Crawford, J. F. Stanton, P. G. Szalay, and H. F. Schaefer, "The  $\tilde{C}^2A_2$  Excited State of NO<sub>2</sub>: Evidence for a C<sub>S</sub> Equilibrium Structure and a Failure of Some Spin-Restricted Reference Wavefunctions", *J. Chem. Phys.* **107**, 2525 (1997).
772. R. D. Davy and H. F. Schaefer, "Structure, Spectra, and Reaction Energies of the Aluminum–Phosphorus Rings (HAl–PH)<sub>2</sub> and (H<sub>2</sub>Al–PH<sub>2</sub>)<sub>2</sub> and the (HAl–PH)<sub>4</sub> Cluster", *J. Phys. Chem. A* **101**, 5707 (1997).
773. R. D. Davy and H. F. Schaefer, "Structure, Spectra, and Reaction Energies of the Aluminum–Nitrogen (HAl–NH)<sub>2</sub> and (H<sub>2</sub>Al–NH<sub>2</sub>)<sub>2</sub> Rings, and the (HAl–NH)<sub>4</sub> Cluster", *Inorg. Chem.* **37**, 2291 (1998).
774. H. M. Sulzbach, M. S. Platz, H. F. Schaefer, and C. M. Hadad, "Hydrogen Migration vs. Carbon Migration in Dialkylcarbenes. A Study of the Preferred Product in the Carbene Rearrangements of Ethylmethylcarbene, Cyclobutylidene, 2-Norbornylidene and 2-Bicyclo[2.1.1]-hexylidene", *J. Am. Chem. Soc.* **119**, 5682 (1997).
775. T. J. Van Huis, Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, "The  $\tilde{X}^1A_1$ ,  $\tilde{a}^3B_1$ ,  $\tilde{A}^1B_1$ , and  $\tilde{B}^1A_1$  Electronic States of PH<sub>2</sub><sup>+</sup>", *J. Phys. Chem. A* **101**, 6955 (1997).
776. I. S. Ignatyev and H. F. Schaefer, "Silacyanogen", *J. Chem. Phys.* **107**, 5776 (1997).
777. B. Ma, H. F. Schaefer, and N. L. Allinger, "Computational Studies of Phosphate Derivatives", in *Recent Research Developments in Chemical Sciences*, editor S. G. Pandalai (Transworld Research Network, Trivandrum, 1997). Pages 37–57. ISBN: 81-86846-02-6.
778. H. F. Schaefer, "Quantum Mechanical Computations", in *Macmillan Encyclopedia of Chemistry*, editor J. J. Lagowski (Macmillan, New York, 1997). Pages 1276–1281.
779. R. A. King, N. D. Pettigrew, and H. F. Schaefer, "The Electron Affinities of the Perfluorocarbons C<sub>2</sub>F<sub>n</sub>, n = 1–6", *J. Chem. Phys.* **107**, 8536 (1997).
780. M. L. Leininger and H. F. Schaefer "Molecular Geometry and Vibrational Frequencies of Ozone from Compact Variational Wave Functions Explicitly Including Triple and Quadruple Substitutions", *J. Chem. Phys.* **107**, 9059 (1997).
781. Y. Yamaguchi and H. F. Schaefer, "An *An Initio* Study on the Four Electronically Lowest-Lying States of CH<sub>2</sub> Using the State-Averaged Complete Active Space Second-Order Configuration Interaction Method", *Chem. Phys. (Sigrid D. Peyerimhoff Issue)* **225**, 23 (1997).
782. T. D. Crawford, T. J. Lee, and H. F. Schaefer, "A New Spin-Restricted Triple Excitation Correction for Coupled Cluster Theory", *J. Chem. Phys.* **107**, 7943 (1997).
783. B. C. Hoffman, C. D. Sherrill, and H. F. Schaefer, "Comparison Between Molecular Geometry and Harmonic Vibrational Frequency Predictions from CIS-D[TQ] and CISDTQ Wave Functions for Hydrogen Sulfide", *J. Chem. Phys.* **107**, 10616 (1997).
784. I. S. Ignatyev and H. F. Schaefer, "Effects of Fluorination on Methylene Insertion Reactions", *J. Am. Chem. Soc.* **119**, 12306 (1997).



785. T. D. Crawford, T. J. Lee, N. C. Handy, and H. F. Schaefer, "Spin-Restricted Brueckner Orbitals for Coupled-Cluster Wavefunctions", *J. Chem. Phys.* **107**, 9980 (1997).
786. T. D. Crawford, J. F. Stanton, W. D. Allen, and H. F. Schaefer, "Hartree-Fock Orbital Instability Envelopes in Highly Correlated Single-Reference Wave Functions", *J. Chem. Phys.* **107**, 10626 (1997).
787. J. Gu, K. Chen, Y. Xie, H. F. Schaefer, R. A. Morris, and A. A. Viggiano, "The Electron Affinities of PF and PF<sub>2</sub>", *J. Chem. Phys.* **108**, 1050 (1998).
788. C. D. Sherrill and H. F. Schaefer, "The Configuration Interaction Method: Advances in Highly Correlated Approaches", *Adv. Quantum Chem.* **34**, 143 (1999).
789. C. D. Sherrill, M. L. Leininger, T. J. Van Huis, and H. F. Schaefer, "Structures and Vibrational Frequencies in the Full Configuration Interaction Limit: Predictions for Four Electronic States of Methylene Using a Triple-Zeta Plus Double Polarization (TZ2P) Basis", *J. Chem. Phys.* **108**, 1040 (1998).
790. H. F. Bettinger, P. R. Schleyer, P. R. Schreiner, and H. F. Schaefer, "Ring Opening of Substituted Cyclopropylidenes to Cyclic Allenes", *J. Org. Chem.* **62**, 9267 (1997).
791. Y. Xie, P. R. Schreiner, H. F. Schaefer, X.-W. Li, and G. H. Robinson, "Are Heterocyclic 2 $\pi$ -Electron Aromatic Systems HC—Ga(H)—CH, M[HGa—C(H)—GaH], [HGa—C(H)—GaH]<sup>-</sup>, HSi—Ga(H)—SiH, M[HGa—Si(H)—GaH] (M = Li, Na, and K), and [HGa—Si(H)—GaH]<sup>-</sup> Stable?" *Organometallics* **17**, 114 (1998).
792. H. F. Bettinger, P. R. Schleyer, P. R. Schreiner, and H. F. Schaefer, "Computational Analyses of Prototype Carbene Structures and Reactions", in *Modern Electronic Structure Theory and Applications in Organic Chemistry*, editor E. R. Davidson (World Scientific, Singapore, 1998). Pages 89–170.
793. H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "[3<sub>6</sub>](1,2,3,4,5,6)Cyclophane—A Molecular Pinwheel And Its Correlated Inversion: NMR And Energetic Considerations", *J. Am. Chem. Soc.* **120**, 1074 (1998).
794. H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Tetraphenyldihydrocyclobutarenes—What Causes the Extremely Long 1.72 Å C—C Single Bond?" *Chem. Commun.* 769 (1998).
795. H. F. Bettinger, P. R. Schreiner, H. F. Schaefer, and P. R. Schleyer, "Rearrangements on the C<sub>6</sub>H<sub>6</sub> Potential Energy Surface and the Topomerization of Benzene", *J. Am. Chem. Soc.* **120**, 5741 (1998).
796. Y. Yamaguchi, S. S. Wesolowski, T. J. Van Huis, and H. F. Schaefer, "The Unimolecular Dissociation of H<sub>2</sub>CO on the Lowest Triplet Potential-Energy Surface", *J. Chem. Phys.* **108**, 5281 (1998).
797. B. Ma, H. F. Schaefer, and N. L. Allinger, "Theoretical Studies of the Potential Energy Surfaces and Compositions of the D—Aldo— and D—KetoHexoses", *J. Am. Chem. Soc.* **120**, 3411 (1998).
798. E. F. Valeev and H. F. Schaefer, "The Protonated Water Dimer: Brueckner Methods Remove the Spurious C<sub>1</sub> Symmetry Minimum", *J. Chem. Phys.* **108**, 7197 (1998).
799. M. L. Leininger, C. D. Sherrill, W. D. Allen, and H. F. Schaefer, "Benchmark Configuration Interaction Spectroscopic Constants for X <sup>1</sup>Σ<sub>g</sub><sup>+</sup> C<sub>2</sub> and X <sup>1</sup>Σ<sup>+</sup> CN<sup>+</sup>", *J. Chem. Phys.* **108**, 6717 (1998).
800. G. S. Tschumper and H. F. Schaefer, "A Comparison Between the CISD[TQ] Wave Function and Other Highly Correlated Methods: Molecular Geometry and Harmonic Vibrational Frequencies of MgH<sub>2</sub>", *J. Chem. Phys.* **108**, 7511 (1998).
801. J. Gu, Y. Xie and H. F. Schaefer, "The Barrier Height for Decomposition of HN<sub>2</sub>", *J. Chem. Phys.* **108**, 8029 (1998).
802. J. C. Rienstra-Kiracofe, D. E. Graham, and H. F. Schaefer, "Medium Ring Compounds and their Anions: A Systematic Density Functional Theory Study", *Mol. Phys.* **94**, 767 (1998).
803. Y. Xie, R. S. Grev, J. Gu, H. F. Schaefer, P. R. Schleyer, J. Su, X.-W. Li, and G. H. Robinson, "The Nature of the Gallium—Gallium Triple Bond", *J. Am. Chem. Soc.* **120**, 3773 (1998).
804. S. S. Wesolowski, J. M. Galbraith, and H. F. Schaefer, "Isomerization Pathway of the Aluminum Monocarbonyl/Isocarbonyl Pair, AlCO/AlOC: Evidence of a Cyclic Minimum", *J. Chem. Phys.* **108**, 9398 (1998).
805. A. G. Császár, W. D. Allen, and H. F. Schaefer, "In Pursuit of the *Ab Initio* Limit for Conformational Energy Prototypes", *J. Chem. Phys.* **108**, 9751 (1998).
806. C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer, "Experimental and *Ab Initio* Study of the Infrared Spectra of Ionic Species Derived from SF<sub>6</sub> and SF<sub>4</sub> and Trapped in Solid Neon", *J. Chem. Phys.* **108**, 9639 (1998).
807. J. C. Stephens, Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, "The  $\tilde{X}^3B_1$ ,  $\tilde{a}^1A_1$ ,  $\tilde{b}^1B_1$ , and  $\tilde{c}^1\Sigma_g^+$  Electronic States of NH<sub>2</sub><sup>+</sup>", *J. Phys. Chem. A* **102**, 3999 (1998).
808. S. Re, Y. Osamura, Y. Suzuki, and H. F. Schaefer, "Structures and Stability of Hydrated Clusters of Hydrogen Chloride, HCl(H<sub>2</sub>O)<sub>n</sub>, n = 1–5", *J. Chem. Phys.* **109**, 973 (1998).
809. K. Fukuzawa, Y. Osamura, and H. F. Schaefer, "Are Neutral–Neutral Reactions Effective for the Carbon-Chain Growth of Cyanopolyynes and Polyacetylenes in Interstellar Space?" *Astrophys. J.* **505**, 278 (1998).
810. T. J. Van Huis, M. L. Leininger, C. D. Sherrill, and H. F. Schaefer, "Full Configuration Interaction Energies, Geometries, and Quartic Force Fields of the Nitrenium Ion", *Collect. Czech. Chem. Commun.* (Rudolf Zahradnik Issue) **63**, 1107 (1998).
811. E. F. Valeev, H. M. Botee, and H. F. Schaefer, "Is F<sub>3</sub><sup>+</sup> Viable? A High Level *Ab Initio* Comparison of F<sub>3</sub><sup>+</sup> and Cl<sub>3</sub><sup>+</sup>", *J. Chem. Phys.* **109**, 1772 (1998).
812. S. S. Wesolowski, E. M. Johnson, M. L. Leininger, T. D. Crawford, and H. F. Schaefer, "Definitive *Ab Initio* Structure for the  $\tilde{X}^2A'$  H<sub>2</sub>PO Radical and Resolution of the P–O Stretching Mode Assignment", *J. Chem. Phys.* **109**, 2694 (1998).
813. J. H. Jang, J. G. Lee, H. Lee, Y. Xie, and H. F. Schaefer, "Molecular Structures and Vibrational Frequencies of Iron Carbonyls: Fe(CO)<sub>5</sub>, Fe<sub>2</sub>(CO)<sub>9</sub>, and Fe<sub>3</sub>(CO)<sub>12</sub>", *J. Phys. Chem. A* **102**, 5298 (1998).
814. Y. Yamaguchi, J. C. Rienstra-Kiracofe, J. C. Stephens, and H. F. Schaefer, "The Hydroxyethynyl Radical (CCOH): An Accessible Isomer of the Ketenyl Radical (HCCO)?" *Chem. Phys. Lett.* **291**, 509 (1998).
815. T. M. Miller, J. V. Seeley, W. B. Knighton, R. F. Meads, A. A. Viggiano, R. A. Morris, J. M. Van Doren, J. Gu, and H. F. Schaefer, "Electron Attachment to PCl<sub>3</sub> and POCl<sub>3</sub>, 296–552 K", *J. Chem. Phys.* **109**, 578 (1998).

816. X.-W. Li, Y. Xie, J. Su, H. F. Schaefer, and G. H. Robinson "Synthesis and Molecular Structure of (Mes<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>)B(Br)N(H)[(i-Pr<sub>2</sub>C<sub>6</sub>H<sub>3</sub>)] and an *Ab Initio* Examination of CH<sub>3</sub>BBr<sub>2</sub> and CH<sub>3</sub>B(Br)NH<sub>2</sub>", *Main Group Chem.* **2**, 323 (1998).
817. H. F. Bettinger, P. R. Schreiner, P. R. Schleyer, and H. F. Schaefer "Carbenes—A Testing Ground for Electronic Structure Methods", in *Encyclopedia of Computational Chemistry*, editor P. R. Schleyer (Wiley, Chichester, England, 1998). Pages 183–196.
818. R. A. King, W. D. Allen, B. Ma, and H. F. Schaefer, "The Fragmentation Surface of Triplet Ketene", *Faraday Discuss. Chem. Soc.* **110**, 23 (1998).
819. Y. Xie and H. F. Schaefer, "The Molecular Structure and Infrared and Raman Spectra of SCCCS", *J. Mol. Struct.* **460**, 117 (1999).
820. G. S. Tschumper, M. D. Kelty, and H. F. Schaefer, "Subtle Basis Set Effects on Hydrogen Bonded Systems", *Mol. Phys.* (Bowen Liu Memorial Issue) **96**, 493 (1999).
821. S. T. Brown, T. J. Van Huis, B. C. Hoffman, and H. F. Schaefer, "Excited Electronic States of Carbon Disulfide", *Mol. Phys.* (Bowen Liu Memorial Issue) **96**, 693 (1999).
822. C. Pak, Y. Xie, T. J. Van Huis, and H. F. Schaefer, "The Electron Affinities of the Bromine Fluorides, BrF<sub>n</sub> (n = 1–7)", *J. Am. Chem. Soc.* **120**, 11115 (1998).
823. H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "NF<sub>3</sub>—Viable or Not?" *J. Am. Chem. Soc.* **120**, 11439 (1998).
824. B. C. Hoffman and H. F. Schaefer, "Mg<sup>+</sup>NO and Mg<sup>+</sup>ON: Potentially Important Ionospheric Species", *Int. J. Mass Spectrom. Ion Processes* (Michael T. Bowers Issue) **185/186/187**, 961 (1999).
825. T. D. Crawford, J. F. Stanton, J. C. Saeh, and H. F. Schaefer, "Structure and Energetics of Isomers of the Interstellar Molecule C<sub>5</sub>H", *J. Am. Chem. Soc.* **121**, 1902 (1999).
826. J. C. Stephens, Y. Yamaguchi, and H. F. Schaefer, "The Adiabatic and Vertical Ionization Potentials of NH<sub>2</sub> to the Three Lowest-Lying States of NH<sub>2</sub><sup>+</sup>", *J. Mol. Struct.* (Keiji Morokuma Issue) **461/462**, 41 (1999).
827. H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Tetradecahydrobenzenes—Singlet–Triplet Energy Separations and Vibrational Frequencies", *J. Am. Chem. Soc.* **121**, 2829 (1999).
828. M. B. Walsh, R. A. King, and H. F. Schaefer, "The Structures, Electron Affinities, and Energetic Stabilities of TiO<sub>n</sub> and TiO<sub>n</sub><sup>−</sup> (n = 1–3)", *J. Chem. Phys.* **110**, 5224 (1999).
829. N. R. Brinkmann, G. S. Tschumper, and H. F. Schaefer, "Electron Affinities of the Oxides of Aluminum, Silicon, Phosphorus, Sulfur, and Chlorine", *J. Chem. Phys.* **110**, 6240 (1999).
830. T. D. Crawford and H. F. Schaefer, "An Introduction to Coupled Cluster Theory for Computational Chemists", *Rev. Comput. Chem.* **14**, 33–136 (1999).
831. S. Portmann, J. M. Galbraith, H. F. Schaefer, and H. P. Lüthi, "Some New Structures of C<sub>28</sub>", *Chem. Phys. Lett.* **301**, 98 (1999).
832. S. S. Wesolowski, J. M. Gonzales, P. R. Schleyer, and H. F. Schaefer, "3-Ethynylcyclopropene: A Highly Suspicious Crystal Structure", *J. Chem. Soc., Chem. Commun.* 439 (1999).
833. B. C. Hoffman, Y. Yamaguchi, and H. F. Schaefer, "The  $\tilde{X}^1A_1$ ,  $\tilde{a}^3B_1$ , and  $\tilde{A}^1B_1$  Electronic States of the Aluminum Dihydride Anion", *J. Phys. Chem. A* **103**, 1886 (1999).
834. R. A. Morris, T. M. Miller, J. F. Paulson, A. A. Viggiano, M. T. Feldmann, R. A. King, and H. F. Schaefer, "Formation of CF<sub>3</sub>O<sup>−</sup> in the Gas Phase", *J. Chem. Phys.* **110**, 8436 (1999).
835. G. Tarczay, A. G. Csaszar, W. Klopper, V. Szalay, W. D. Allen, and H. F. Schaefer, "The Barrier to Linearity of Water", *J. Chem. Phys.* **110**, 11971 (1999).
836. H. F. Bettinger, H. M. Sulzbach, P. R. Schleyer, and H. F. Schaefer, "Aza[10]annulene: The Next Higher Aromatic Analogue of Pyridine", *J. Org. Chem.* **64**, 3278 (1999).
837. S. T. Brown, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "A Systematic Application of Density Functional Theory to Some Carbon Containing Molecules and their Anions", *J. Phys. Chem. A* **103**, 4056 (1999).
838. R. A. Provencal, J. B. Paul, K. Roth, C. Chapo, R. N. Casaes, R. J. Saykally, G. S. Tschumper, and H. F. Schaefer, "Infrared Cavity Ringdown Absorption Spectroscopy of Methanol Clusters: Single Donor Hydrogen Bonding", *J. Chem. Phys.* **110**, 4258 (1999).
839. R. I. Kaiser, I. Hahndorf, L. C. L. Huang, Y. T. Lee, H. F. Bettinger, P. R. Schleyer, H. F. Schaefer, and P. R. Schreiner, "Crossed Beams Reaction of Atomic Carbon, C(<sup>3</sup>P<sub>1</sub>), with d<sub>6</sub>-Benzene, C<sub>6</sub>D<sub>6</sub> (X <sup>1</sup>A<sub>1g</sub>): Observation of the Per-Deutero-1,2-Didehydrocycloheptatrienyl Radical, C<sub>7</sub>D<sub>5</sub>(X <sup>2</sup>B<sub>2</sub>)", *J. Chem. Phys.* **110**, 6091 (1999).
840. T. J. Van Huis, S. S. Wesolowski, Y. Yamaguchi, and H. F. Schaefer, "Scratching the Surface of the Water Dication", *J. Chem. Phys.* **110**, 11856 (1999).
841. S. T. Brown, Y. Yamaguchi, and H. F. Schaefer, "An *Ab Initio* Study on the Ground and First Excited Electronic States of Disilaketonyl Radical (HSiSiO)", *J. Chem. Phys.* **111**, 227 (1999).
842. A. Y. Timoshkin, A. V. Suvorov, H. F. Bettinger, and H. F. Schaefer, "The Role of the Terminal Atoms in the Donor–Acceptor Complexes MX<sub>3</sub>–D (M = Al, Ga, In; X = F, Cl, Br, I; D = YH<sub>3</sub>, YX<sub>3</sub>, X<sup>−</sup>; Y = N, P, As)," *J. Am. Chem. Soc.* **121**, 5687 (1999).
843. G. S. Tschumper, J. M. Gonzalez, and H. F. Schaefer, "Assignment of the Infrared Spectra of the Methanol Trimer", *J. Chem. Phys.* **111**, 3027 (1999).
844. Y. Xie, H. F. Schaefer, X.-Y. Fu, and R.-Z. Liu, "The Infrared Spectrum of the NO Dimer Cation: Problems for Density Functional Theory and a Muddled Relationship to Experiment", *J. Chem. Phys.* **111**, 2532 (1999).
845. I. S. Ignatyev and H. F. Schaefer, "Bromine Halides: The Neutral Molecules BrClF<sub>n</sub> (n = 1–5) and their Anions; Structures, Energetics, and Electron Affinities", *J. Am. Chem. Soc.* **121**, 6904 (1999).
846. V. S. Mastryukov, M. Hofmann, and H. F. Schaefer, "Structure and Conformations of Cyclopentasilane, Si<sub>5</sub>H<sub>10</sub>", *J. Phys. Chem. A* **103**, 5581 (1999).
847. H. F. Bettinger, J. C. Rienstra-Kiracofe, B. C. Hoffman, H. F. Schaefer, J. E. Baldwin, and P. R. Schleyer, "Structural Isomerization of Cyclopropane: A New Mechanism Through 1-Propylidene", *J. Chem. Soc., Chem. Commun.* 1515 (1999).

848. M. Hofmann and H. F. Schaefer, "The  $[\text{C}_6\text{H}_{10}]^+$  Hyper-surface: The Parent Radical Cation Diels–Alder Reaction and Alternative Pathways", *J. Am. Chem. Soc.* **121**, 6719 (1999).
849. N. Takagi, K. Fukuzawa, Y. Osamura, and H. F. Schaefer, "Ion–Molecule Reactions Producing  $\text{HC}_3\text{NH}^+$  in Interstellar Space: Forbiddenness of the Reaction between Cyclic  $\text{C}_3\text{H}_3^+$  and the N Atom", *Astrophys. J.* **525**, 791 (1999).
850. Q. Li, W. Xu, Y. Xie, and H. F. Schaefer, "The Electron Affinities of the Selenium Fluorides  $\text{SeF}_n$  ( $n = 1-7$ )", *J. Phys. Chem. A* **103**, 7496 (1999).
851. Q. Li, G. Li, W. Xu, Y. Xie, and H. F. Schaefer, "Structures, Thermochemistry, and Electron Affinities of the Germanium Fluorides,  $\text{GeF}_n/\text{GeF}_n^-$  ( $n = 1-5$ )", *J. Chem. Phys.* **111**, 7945 (1999).
852. N. Balucani, O. Asvany, A. H. H. Chang, S. H. Lin, Y. T. Lee, R. I. Kaiser, H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Crossed Beam Reaction of Cyano Radicals with Hydrocarbon Molecules I: Dynamics of Cyanobenzene ( $\text{C}_6\text{H}_5\text{CN}$ ;  $X^1\text{A}_1$ ) and Perdeutero Cyanobenzene ( $\text{C}_6\text{D}_5\text{CN}$ ;  $X^1\text{A}_1$ ) Formation from Reaction of  $\text{CN}(X^2\Sigma^+)$  with Benzene,  $\text{C}_6\text{H}_6(X^1\text{A}_1\text{g})$  and  $d_6$ -Benzene,  $\text{C}_6\text{D}_6(X^1\text{A}_1\text{g})$ ", *J. Chem. Phys.* **111**, 7457 (1999).
853. N. Balucani, O. Asvany, A. H. H. Chang, S. H. Lin, Y. T. Lee, R. I. Kaiser, H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Crossed Beam Reaction of Cyano Radicals with Hydrocarbon Molecules II: Chemical Dynamics of 1,1-Cyanomethylallene ( $\text{CNCH}_2\text{CCCH}_2$ ;  $X^1\text{A}'$ ) Formation from Reaction of  $\text{CN}(X^2\Sigma^+)$  with Dimethylacetylene,  $\text{CH}_3\text{CCCH}_3(X^1\text{A}_1')$ ", *J. Chem. Phys.* **111**, 7472 (1999).
854. H. F. Bettinger, C. Pak, Y. Xie, P. v. R. Schleyer, and H. F. Schaefer, "The Thermodynamic Stabilities of Tricyclic Tetraene  $\text{C}_{12}\text{H}_{12}$  Hydrocarbons", *J. Chem. Soc. Perkin Trans. (Robert Squires Memorial Issue) 2*, 2377 (1999).
855. I. S. Ignatyev, H. F. Schaefer, R. B. King and S. T. Brown, "Binuclear Homoleptic Nickel Carbonyls: Incorporation of Ni–Ni Single, Double, and Triple Bonds,  $\text{Ni}_2(\text{CO})_x$  ( $x = 5, 6, 7$ )", *J. Am. Chem. Soc.* **122**, 1989 (2000).
856. M. Hofmann and H. F. Schaefer, "Pathways for the Reaction of the Butadiene Radical Cation  $[\text{C}_4\text{H}_6]^+$  with Ethylene", *J. Phys. Chem. A* **103**, 8895 (1999).
857. R. A. King, T. D. Crawford, J. F. Stanton, and H. F. Schaefer, "Conformations of [10]Annulene: More Bad News for Density Functional Theory", *J. Am. Chem. Soc.* **121**, 10788 (1999).
858. N. A. Richardson, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "Examining Trends in the Tetravalent Character of Group 14 Elements (C, Si, Ge, Sn, Pb) with Acids and Hydroperoxides", *J. Am. Chem. Soc.* **121**, 10813 (1999).
859. Y. Yamaguchi, B. C. Hoffman, J. C. Stephens, and H. F. Schaefer, "The Three Lowest-Lying Electronic States of  $\text{NH}_2$ ", *J. Phys. Chem. A* **103**, 7701 (1999).
860. P. R. Bunker, O. Bludsky, P. Jensen, S. S. Wesolowski, T. J. Van Huis, Y. Yamaguchi, and H. F. Schaefer, "The  $\text{H}_2\text{O}^{2+}$  Ground-State Potential Energy Surface", *J. Mol. Spectrosc.* **198**, 371 (1999).
861. K. Aarset, A. G. Császár, E. L. Sibert, W. D. Allen, H. F. Schaefer, W. Klopper, and J. Noga, "Anharmonic Force Field, Vibrational Energies, and Barrier to Inversion of  $\text{SiH}_3^-$ ", *J. Chem. Phys.* **112**, 4053 (2000).
862. J. C. Rienstra-Kiracofe, G. B. Ellison, B. C. Hoffman, and H. F. Schaefer, "The Electron Affinities of  $\text{C}_3\text{O}$  and  $\text{C}_4\text{O}$ ", *J. Phys. Chem. A (William A. Goddard Issue)* **104**, 2273 (2000).
863. Y. Yamaguchi, N. D. K. Petraco, S. T. Brown, and H. F. Schaefer, "The 1-Silaketenyl Radical ( $\text{HSiCO}$ ): Ground and First Excited Electronic States", *J. Chem. Phys.* **112**, 2168 (2000).
864. N. D. K. Petraco, S. T. Brown, Y. Yamaguchi, and H. F. Schaefer, "The Silaketenyldene ( $\text{SiCO}$ ) Molecule: Characterization of the  $\tilde{X}^3\Sigma^-$  and  $\tilde{A}^3\Pi$  States", *J. Chem. Phys.* **112**, 3201 (2000).
865. R. A. King, W. D. Allen, and H. F. Schaefer, "On Apparent Quantized Transition-State Thresholds in the Photofragmentation of Acetaldehyde", *J. Chem. Phys.* **112**, 5585 (2000).
866. Y. Xie, H. F. Schaefer, and G. H. Robinson, "The Gallium–Gallium Triple Bond in a Realistic Model. A Density Functional Theory Study of  $\text{Na}_2[(\text{C}_6\text{H}_5)_2\text{C}_6\text{H}_3\text{Ga-GaC}_6\text{H}_3(\text{C}_6\text{H}_5)_2]$ ", *Chem. Phys. Lett.* **317**, 174 (2000).
867. N. D. K. Petraco, S. S. Wesolowski, M. L. Leininger, and H. F. Schaefer, "Coupled Cluster Studies of the Hyperfine Splitting Constants of the Thioformyl Radical", *J. Chem. Phys.* **112**, 6245 (2000).
868. N. A. Richardson, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "An Examination of the Stabilities of Group 14 (C, Si, Ge, Sn, Pb) Congeners of Dihydroxycarbene and Dioxirane; Comparison to Formic Acid and Hydroperoxycarbene Congeners", *Inorg. Chem.* **38**, 6271 (1999).
869. R. A. Provencal, R. N. Casaes, K. Roth, J. B. Paul, C. N. Chapo, R. J. Saykally, G. Tschumper, and H. F. Schaefer, "Hydrogen Bonding in Alcohol Clusters: A Comparative Study by Infrared Cavity Ringdown Laser Absorption Spectroscopy", *J. Phys. Chem. A* **104**, 1423 (2000).
870. R. I. Kaiser, O. Asvany, Y. T. Lee, H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Crossed Beam Reaction of Phenyl Radicals with Unsaturated Hydrocarbon Molecules. I. Chemical Dynamics of Phenylmethylacetylene ( $\text{C}_6\text{H}_5\text{CCCH}_3$ ;  $X^1\text{A}'$ ) Formation from Reaction of  $\text{C}_6\text{H}_5$  ( $X^2\text{A}_1$ ) with Methylacetylene,  $\text{CH}_3\text{CCH}(X^1\text{A}_1)$ ", *J. Chem. Phys.* **112**, 4994 (2000).
871. S. T. Brown, Y. Yamaguchi, and H. F. Schaefer, "The  $\tilde{X}^3\Sigma^-$  and  $\tilde{A}^3\Pi$  Electronic States of Ketenylidene ( $\text{CCO}$ ): Analysis of the Renner-Teller Effect in the Upper State", *J. Phys. Chem. A (Marilyn Jacox Issue)* **104**, 3603 (2000).
872. M. Hofmann, D. Scheschkewitz, A. Ghaffari, G. Geiseler, W. Massa, H. F. Schaefer, and A. Berndt, "Two Electron Aromatics with Classical and Non-Classical Homobridges", *J. Molecular Modeling (Paul Schleyer Issue)* **6**, 257 (2000).
873. X.-W. Li, P. Wei, B. C. Beck, Y. Xie, H. F. Schaefer, J. Su and G. H. Robinson, "Synthesis and Molecular Structure of an Unusual –Ga–Ga–Ga– Linked Organometallic", *J. Chem. Soc., Chem. Commun.* 453 (2000).

874. Y. Xie, H. F. Schaefer, Y. Wang, X.-Y. Fu, and R.-Z. Liu, "Electron Affinities of the Bromine Oxides  $\text{BrO}_n$ ,  $n = 1-4$ ", *Mol. Phys.* **98**, 879 (2000).
875. D. Scheschkewitz, A. Ghaffari, P. Amseis, M. Unverzagt, G. Subramanian, M. Hofmann, P. R. Schleyer, H. F. Schaefer, G. Geiseler, W. Massa, and A. Berndt, "Bishomoaromatic 1,2,4-Triboracyclopentane Dianions: Strong Three-Center/Two-Electron Bonds Among Three Boron Atoms", *Angew. Chem. Int. Ed. Engl.* **39**, 1272 (2000).
876. C. J. Barden, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "Homonuclear 3d Transition-Metal Diatomics: A Systematic Density Functional Theory Study", *J. Chem. Phys.* **113**, 690 (2000).
877. A. Wittkopp, M. Prall, P. R. Schreiner, and H. F. Schaefer, "Is  $\text{SH}_4$ , the Simplest 10 S-4 Sulfurane, Isolable?" *Phys. Chem. Chem. Phys.* (Reinhart Ahlrichs Issue) **2**, 2239 (2000).
878. C. J. Barden and H. F. Schaefer, "The Singlet-Triplet Separation in Dichlorocarbene: A Surprising Difference between Theory and Experiment", *J. Chem. Phys.* **112**, 6515 (2000).
879. Y. Yamaguchi, S. T. Brown, N. D. K. Petraco, and H. F. Schaefer, "The 2-Silaketenyl Radical ( $\text{HCSiO}$ ): Ground and First Excited Electronic States", *J. Mol. Struct.* (Norman L. Allinger Issue) **556**, 293 (2000).
880. M. L. Leininger, W. D. Allen, H. F. Schaefer, and C. D. Sherrill, "Is Møller-Plesset Perturbation Theory a Convergent *Ab Initio* Method?" *J. Chem. Phys.* **112**, 9213 (2000).
881. B. K. Decker, N. G. Adams, L. M. Babcock, T. D. Crawford, and H. F. Schaefer, "Thermokinetic Proton Transfer and *Ab Initio* Studies of the  $[\text{2H,S,O}]^+$  System. The Proton Affinity of  $\text{HSO}^-$ ", *J. Phys. Chem. A* **104**, 4636 (2000).
882. Y. Xie and H. F. Schaefer, "The Puzzling Infrared Spectra of the Nitric Oxide Dimer Radical Cation: A Systematic Application of Brueckner Methods", *Mol. Phys.* **98**, 955 (2000).
883. S. S. Wesolowski, E. F. Valeev, R. A. King, V. Baranovski, and H. F. Schaefer, "The Not-So-Peculiar Case of Calcium Oxide: A Weakness in Atomic Natural Orbital Basis Sets for Calcium", *Mol. Phys.* (Charlotte Froese Fischer Issue) **98**, 1227 (2000).
884. J. M. Gonzales, R. A. King, and H. F. Schaefer, "Analyses of the  $\text{ScO}^-$  and  $\text{ScO}_2^-$  Photoelectron Spectra," *J. Chem. Phys.* **113**, 567 (2000).
885. S. S. Wesolowski, R. A. King, H. F. Schaefer, and M. A. Duncan, "Coupled Cluster Electronic Spectra for the  $\text{Ca}^+$ -Acetylene  $\pi$  Complex and Comparisons to its Alkaline Earth Analogues", *J. Chem. Phys.* **113**, 701 (2000).
886. H. F. Schaefer, "Quantum Mechanical Computations of Potential Energy Hypersurfaces", a vignette published in *Physical Chemistry*, 2nd ed., by R. S. Berry, S. A. Rice, and J. Ross (Oxford University Press, New York, 2000). Pages 882-888
887. H. F. Bettinger, P. R. Schleyer, P. R. Schreiner, H. F. Schaefer, R. I. Kaiser, and Y. T. Lee, "The Reaction of Benzene with Ground-State Carbon Atom,  $\text{C}(^3\text{P})$ ", *J. Chem. Phys.* **113**, 4250 (2000).
888. N. D. K. Petraco, S. T. Brown, Y. Yamaguchi, and H. F. Schaefer, "The 2-Silaketenylidene ( $\text{CSiO}$ ) Radical: Electronic Structure of the  $\tilde{\text{X}}^3\Sigma^-$  and  $\tilde{\text{A}}^3\Pi$  States", *J. Phys. Chem. A* (C. Bradley Moore Issue) **104**, 10165 (2000).
889. A. G. Császár, W. D. Allen, Y. Yamaguchi, and H. F. Schaefer, "*Ab Initio* Determination of Accurate Ground Electronic State Potential Energy Hypersurfaces for Small Molecules", in *Computational Molecular Spectroscopy*, editors P. R. Bunker and P. Jensen (Wiley, New York, 2000). Pages 15-68.
890. Y. Xie, H. F. Schaefer, and R. B. King, "Binuclear Homoleptic Iron Carbonyls: Incorporation of Formal Iron-Iron Single, Double, Triple, and Quadruple Bonds,  $\text{Fe}_2(\text{CO})_x$ , ( $x = 9, 8, 7, 6$ )", *J. Am. Chem. Soc.* **122**, 8746 (2000).
891. E. F. Valeev and H. F. Schaefer, "Evaluation of Two-Electron Integrals for Explicit  $r_{12}$  Theories", *J. Chem. Phys.* **113**, 3990 (2000).
892. S.-J. Kim and H. F. Schaefer, "Dimethyldioxirane, Carbonyl Oxide, and the Transition State Connecting Them: Electronic Structures, Relative Energies, and Vibrational Frequencies", *J. Phys. Chem. A* **104**, 7892 (2000).
893. J. C. Rienstra-Kiracofe, W. D. Allen, and H. F. Schaefer, "The  $\text{C}_2\text{H}_5 + \text{O}_2$  Reaction Mechanism: High-Level *Ab Initio* Characterizations", Feature Article, *J. Phys. Chem. A* **104**, 9823 (2000).
894. T. D. Crawford, S. S. Wesolowski, E. F. Valeev, R. A. King, M. L. Leininger, and H. F. Schaefer, "The Past, Present, and Future of Quantum Chemistry", in *Chemistry for the 21st Century*, editors E. Keinan and I. Schechter (Wiley-VCH, Weinheim, Germany, 2001). Pages 219-246.
895. C. Pak, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "Electron Affinities of Silicon Hydrides:  $\text{SiH}_n$  ( $n = 0-4$ ) and  $\text{Si}_2\text{H}_n$  ( $n = 0-6$ )", *J. Phys. Chem. A* **104**, 11232 (2000).
896. M. Hofmann and H. F. Schaefer, "Structure and Reactivity of the Vinylcyclopropane Radical Cation", *J. Mol. Struct.* (Alfred Bauder Issue) **599**, 95 (2001).
897. A. Y. Timoshkin, H. F. Bettinger, and H. F. Schaefer, "A Theoretical Approach to the Single-Source Precursor Concept: Quantum Chemical Modeling of Gas-Phase Reactions", *J. Cryst. Growth* **222**, 170 (2001).
898. R. I. Kaiser, C. C. Chiong, O. Asvany, Y. T. Lee, F. Stahl, P. R. Schleyer, and H. F. Schaefer, "Chemical Dynamics of  $\text{d}_1$ -Methyldiacetylene ( $\text{CH}_3\text{CCCD}$ ;  $\tilde{\text{X}}^1\text{A}'_1$ ) and  $\text{d}_1$ -Ethylnylallene ( $\text{H}_2\text{CCCH}(\text{C}_2\text{D})$ ;  $\tilde{\text{X}}^1\text{A}'_1$ ) Formation from Reaction of  $\text{C}_2\text{D}$  ( $\tilde{\text{X}}^2\Sigma^+$ ) with Methylacetylene,  $\text{CH}_3\text{CCH}$  ( $\tilde{\text{X}}^1\text{A}'_1$ )", *J. Chem. Phys.* **114**, 3488 (2001).
899. R. A. King, H. P. Lüthi, H. F. Schaefer, F. Glarner, and U. Burger "The Photohydration of N-Alkylpyridinium Salts, Interplay between Theory and Experiment", *Chem. Eur. J.* **7**, 1734 (2001).
900. F. Stahl, P. R. Schleyer, H. F. Bettinger, R. I. Kaiser, Y. T. Lee, and H. F. Schaefer, "Reaction of the Ethynyl Radical,  $\text{C}_2\text{H}$ , with Methylacetylene,  $\text{CH}_3\text{CCH}$ , Under Single Collision Conditions: Implications for Astrochemistry", *J. Chem. Phys.* **114**, 3476 (2001).
901. C. J. Barden and H. F. Schaefer, "Quantum Chemistry in the Twenty-First Century", Cover Article, *Pure Appl. Chem.* **72**, 1405 (2000).

902. N. R. Brinkman, S. S. Wesolowski, and H. F. Schaefer, "Coupled-Cluster Characterization of the Ground and Excited States of the CH<sub>2</sub>N and CH<sub>2</sub>P Radicals", *J. Chem. Phys.* **114**, 3055 (2001).
903. J. P. Kenny, R. B. King, and H. F. Schaefer, "Cobalt-Cobalt Multiple Bonds in Homoleptic Carbonyls? Co<sub>2</sub>(CO)<sub>x</sub> (x = 8, 7, 6, 5) Structures, Energetics, and Vibrational Spectra", *Inorg. Chem.* **40**, 900 (2001).
904. J. C. Rienstra-Kiracofe, C. J. Barden, S. T. Brown, and H. F. Schaefer, "On the Electron Affinities of Polycyclic Aromatic Hydrocarbons", Feature Article, *J. Phys. Chem. A* **105**, 524 (2001).
905. L. Sari, J. M. Gonzales, Y. Yamaguchi, and H. F. Schaefer, "The  $\tilde{X}^2\Pi$  and  $\tilde{A}^2\Sigma^+$  Electronic States of the HCSi Radical: Characterization of the Renner-Teller Effect in the Ground State", *J. Chem. Phys.* **114**, 4472 (2001).
906. E. F. Valeev, A. G. Csaszar, W. D. Allen, and H. F. Schaefer, "MP2 Limit for the Barrier to Linearity of Water", *J. Chem. Phys.* **114**, 2875 (2001).
907. A. Y. Timoshkin, H. F. Bettinger, and H. F. Schaefer, "DFT Modeling of Chemical Vapor Deposition of GaN from Organogallium Precursors. I. Thermodynamics of Elimination Reactions", *J. Phys. Chem. A* **105**, 3240 (2001).
908. A. Y. Timoshkin, H. F. Bettinger, and H. F. Schaefer, "DFT Modeling of Chemical Vapor Deposition of GaN from Organogallium Precursors. II. Structures of the Oligomers and Thermodynamics of the Association Processes", *J. Phys. Chem. A* **105**, 3249 (2001).
909. N. R. Brinkman, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "Electron Affinities of Cyano-Substituted Ethylenes", *Mol. Phys.* **99**, 663 (2001).
910. E. F. Valeev, W. D. Allen, H. F. Schaefer, A. G. Csaszar, and A. L. L. East, "Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics", *J. Phys. Chem. A* (William H. Miller Issue) **105**, 2716 (2001).
911. I. S. Ignatyev, H. F. Schaefer, and P. R. Schleyer, "Triplet States of Carbenium and Silylium Cations", *Chem. Phys. Lett.* **337**, 158 (2001).
912. Q. Li, G. Li, W. Xu, Y. Xie, and H. F. Schaefer, "Structures, Thermochemistry, and Electron Affinities of the Disilicon Fluorides, Si<sub>2</sub>F<sub>n</sub>/Si<sub>2</sub>F<sub>n</sub><sup>-</sup> (n = 1-6)", *Mol. Phys.* **99**, 1053 (2001).
913. H. L. Woodcock, D. Moran, P. R. Schleyer, and H. F. Schaefer, "The Almost Bottleable Triplet Carbene: 2,6-dibromo-4-tert-butyl-2',6'-bis(trifluoromethyl)-4'-isopropylidiphenylcarbene", *J. Am. Chem. Soc.* **123**, 4331 (2001).
914. S. S. Wesolowski, M. L. Leininger, P. S. Pentchev, and H. F. Schaefer, "The Electron Affinities of the DNA and RNA Bases", *J. Am. Chem. Soc.* **123**, 4023 (2001).
915. K. W. Sattelmeyer, H. F. Schaefer, and J. F. Stanton, "The Equilibrium Structure of the Ammonium Radical Rydberg Ground State", *J. Chem. Phys.* **114**, 9863 (2001).
916. H. L. Woodcock, S. S. Wesolowski, Y. Yamaguchi, and H. F. Schaefer, "A Systematic Study of the  $\tilde{X}^2B_1$ ,  $\tilde{A}^2A_1$ , and  $\tilde{B}^2B_2$  States of the Neutral Radical PH<sub>2</sub>", *J. Phys. Chem. A* **105**, 5037 (2001).
917. M. L. Leininger, C. D. Sherrill, W. D. Allen, and H. F. Schaefer, "Systematic Study of Diagonalization Methods for Configuration Interaction Matrixes", *J. Comput. Chem.* (Paul von Rague Schleyer Issue) **22**, 1574 (2001).
918. H. F. Schaefer, "Computers and Molecular Quantum Mechanics: 1965-2001, A Personal Perspective", *J. Mol. Struct.* **573**, 129 (2001).
919. I. S. Ignatyev and H. F. Schaefer, "The Role of Hexacoordinated Silicon Intermediates in the Hydrolysis and Racemization Reactions of Silyl Halides", *Organometallics* **20**, 3113 (2001).
920. C. Pak, S. S. Wesolowski, J. C. Rienstra-Kiracofe, Y. Yamaguchi, and H. F. Schaefer, "What is the True Electronic Ground State of the Disilaethynyl Radical (SiSiH):  $^2B_1$  or  $^2A_1$ ?", *J. Chem. Phys.* **115**, 2157 (2001).
921. I. Ignatyev and H. F. Schaefer, "Stable Hexacoordinated Neutral Complexes Between Silyl Halides and Two Water or Two Ammonia Molecules: SiX<sub>4</sub>Y<sub>2</sub> (X = H, F, Cl; Y = H<sub>2</sub>O, NH<sub>3</sub>)", *J. Phys. Chem. A* **105**, 7665 (2001).
922. M. Hofmann and H. F. Schaefer, "Computational Chemistry", *The Encyclopedia of Physical Science and Technology* Vol. 3 (Academic Press, New York, 2001). Pages 487-506.
923. J. P. Kenny, K. M. Krueger, J. C. Rienstra-Kiracofe, and H. F. Schaefer, "C<sub>5</sub>H<sub>4</sub>: Pyramidane and Its Low Lying Isomers", *J. Phys. Chem. A* **105**, 7745 (2001).
924. L. Sari, Y. Yamaguchi, and H. F. Schaefer, "Coupled Cluster Study of the  $\tilde{X}^2\Pi$  and  $\tilde{A}^2\Sigma^+$  Electronic States of the HCGe Radical: Renner-Teller Splitting and the Effects of Relativistic Corrections", *J. Chem. Phys.* **115**, 5934 (2001).
925. Q. Li, G. Li, W. Xu, Y. Xie, and H. F. Schaefer, "Molecules for Materials: Structures, Thermochemistry, and Electron Affinities of the Digermanium Fluorides, Ge<sub>2</sub>F<sub>n</sub>/Ge<sub>2</sub>F<sub>n</sub><sup>-</sup> (n = 1-6)", *Chem. Phys. Chem.* **3**, 179 (2002).
926. B. G. Rocque, J. M. Gonzales, and H. F. Schaefer, "An Analysis of the Conformers of 1,5-Hexadiene", *Mol. Phys.* (Ernest R. Davidson Issue) **100**, 441 (2002).
927. G. S. Tschumper, M. Quack, M. L. Leininger, B. C. Hoffman, E. F. Valeev, and H. F. Schaefer, "Anchoring the Water Dimer Potential Energy Surface with Explicitly Correlated Computations and Focal Point Analyses", *J. Chem. Phys.* **116**, 690 (2002).
928. Q. Li, Y. Liu, Y. Xie, R. B. King, and H. F. Schaefer, "Binuclear Homoleptic Copper Carbonyls Cu<sub>2</sub>(CO)<sub>x</sub> (x = 1-6): Remarkable Structures Contrasting Metal-Metal Multiple Bonding with Low-Dimensional Copper Bonding Manifolds", *Inorg. Chem.* **40**, 5842 (2001).
929. H. F. Schaefer and R. B. King, "Unsaturated Binuclear Homoleptic Metal Carbonyls M<sub>2</sub>(CO)<sub>x</sub> (M = Fe, Co, Ni; x = 5, 6, 7, 8): Are Multiple Bonds Between Transition Metals Possible for These Molecules?" *Pure Appl. Chem.* **73**, 1059 (2001).
930. S. S. Wesolowski, N. R. Brinkmann, E. F. Valeev, H. F. Schaefer, M. P. Repasky, and W. L. Jorgensen, "Three vs. Four Coordinate Phosphorus in the Gas Phase and in Solution: Treacherous Relative Energies for Phosphine Oxide and Phosphinous Acid", *J. Chem. Phys.* **116**, 112 (2002).
931. A. Y. Timoshkin, H. F. Bettinger, and H. F. Schaefer, "Ring, Chain, and Cluster Compounds in the Cl-Ga-N-H System", *Inorg. Chem.* **41**, 738 (2002).
932. R. I. Kaiser, T. N. Le, T. L. Nguyen, A. M. Mebel, N. Balucani, Y. T. Lee, F. Stahl, P. R. Schleyer, and H. F. Schaefer, "A Combined Crossed Molecular Beam and

- Ab Initio* Investigation of C<sub>2</sub> and C<sub>3</sub> Elementary Reactions with Unsaturated Hydrocarbons – Pathways to Hydrogen Deficient Radicals in Combustion Flames”, *Faraday Discuss. Chem. Soc.* **119**, 51 (2001).
933. I. Hahndorf, Y. T. Lee, R. I. Kaiser, L. Vereecken, J. Peeters, H. F. Bettinger, P. R. Schreiner, P. R. Schleyer, W. D. Allen, and H. F. Schaefer, “A Combined Crossed Beam, *Ab Initio*, and Rice-Ramsperger-Kassel-Marcus Investigation of the Reaction of Carbon Atoms C(<sup>3</sup>P<sub>2</sub>) with Benzene, C<sub>6</sub>H<sub>6</sub> (X <sup>1</sup>A<sub>1g</sub>) and d<sub>6</sub>-Benzene, C<sub>6</sub>D<sub>6</sub> (X <sup>1</sup>A<sub>1g</sub>)”, *J. Chem. Phys.* **116**, 3248 (2002).
934. J. C. Rienstra-Kiracofe, G. S. Tschumper, H. F. Schaefer, S. Nandi, and G. B. Ellison, “Atomic and Molecular Electron Affinities: Photoelectron Experiments and Theoretical Computations”, *Chem. Rev.* **102**, 231 (2002). The editor named this paper as one of the six most outstanding papers appearing in *Chemical Reviews* in 2002.
935. J. M. Gonzales, R. S. Cox, S. T. Brown, W. D. Allen, and H. F. Schaefer, “Assessment of Density Functional Theory for Model S<sub>N</sub>2 Reactions: CH<sub>3</sub>X + F<sup>-</sup> (X = F, Cl, CN, OH, SH, NH<sub>2</sub>, PH<sub>2</sub>)”, *J. Phys. Chem. A* **105**, 11327 (2001).
936. N. A. Richardson, Y. Xie, R. B. King, and H. F. Schaefer, “The Flat Potential Energy Surface of the Saturated Binuclear Homoleptic Chromium Carbonyl: Cr<sub>2</sub>(CO)<sub>11</sub> with One, Two and Three Bridging Carbonyls. Comparison with the Well Known HCr<sub>2</sub>(CO)<sub>10</sub><sup>-</sup> Species and the Unobserved H<sub>2</sub>Cr<sub>2</sub>(CO)<sub>9</sub>”, *J. Phys. Chem. A* **105**, 11134 (2001).
937. P. Jensen, S. S. Wesolowski, N. R. Brinkmann, N. A. Richardson, Y. Yamaguchi, H. F. Schaefer, and P. R. Bunker, “A Theoretical Study of  $\tilde{a}$  <sup>4</sup>A<sub>2</sub> CH<sub>2</sub><sup>+</sup>”, *J. Mol. Spectrosc.* **211**, 254 (2002).
938. N. H. Martin, J. D. Brown, K. H. Nance, H. F. Schaefer, P. R. Schleyer, Z.-X. Wang, and H. Lee Woodcock, “Analysis of the Origin of Through-Space Proton NMR Deshielding by Selected Organic Functional Groups”, *Org. Lett.* **3**, 3823 (2001).
939. N. R. Brinkmann, N. A. Richardson, S. S. Wesolowski, Y. Yamaguchi, and H. F. Schaefer, “Characterization of the  $\tilde{X}$  <sup>2</sup>A<sub>1</sub> and  $\tilde{a}$  <sup>4</sup>A<sub>2</sub> Electronic States of CH<sub>2</sub><sup>+</sup>”, *Chem. Phys. Lett.* **352**, 505 (2002).
940. N. R. Brinkmann, H. F. Schaefer, C. T. Sanderson and C. Kutal, “Can the Radical Anion of Alkyl-2-Cyanoacrylates Initiate Anionic Polymerization of these Instant Adhesive Monomers?” *J. Phys. Chem. A* **106**, 847 (2002).
941. B. Galabov, Y. Yamaguchi, R. B. Remington, and H. F. Schaefer, “High Level *Ab Initio* Quantum Mechanical Predictions of Infrared Intensities”, *J. Phys. Chem. A* **106**, 819 (2002).
942. L. Vereecken, J. Peeters, H. F. Bettinger, R. I. Kaiser, P. R. Schleyer, and H. F. Schaefer, “Reaction of Phenyl Radicals with Propyne”, *J. Am. Chem. Soc.* **124**, 2781 (2002).
943. S. T. Brown, N. D. K. Petraco, Y. Yamaguchi, and H. F. Schaefer, “ $\tilde{X}$  <sup>3</sup>Σ<sup>-</sup> and  $\tilde{A}$  <sup>3</sup>Π Electronic States of Linear Disilaketenyliene (SiSiO): Analysis of the Renner Effect in the  $\tilde{A}$  <sup>3</sup>Π State. Comparison with the Analogous Multiple Bonded Systems SiCO, CSiO, and CCO”, *Polyhedron* (Issue on Subvalent and Multiply Bonded Compounds of the p-Block Elements) **21**, 599 (2002).
944. L. Horny, N. D. K. Petraco, C. Pak, and H. F. Schaefer, “What Is the Nature of Polyacetylene Neutral and Anionic Chains HC<sub>2n</sub>H and HC<sub>2n</sub>H<sup>-</sup> (n = 6–12) That Have Been Recently Observed in Neon Matrixes?”, *J. Am. Chem. Soc.* **124**, 5861 (2002).
945. M. R. Hoffmann, C. D. Sherrill, M. L. Leininger, and H. F. Schaefer, “Optimization of MCSCF Excited States Using Directions of Negative Curvature”, *Chem. Phys. Lett.* **355**, 183 (2002).
946. D. Moran, F. Stahl, E. D. Jemmis, H. F. Schaefer, P. R. Schleyer, “Structures, Stabilities and Ionization Potentials of Dodecahedrane Endohedral Complexes”, *J. Phys. Chem. A* **106**, 5144 (2002).
947. B. Galabov, J. P. Kenny, H. F. Schaefer, and J. R. Durig, “Conformational Stability of 3-Fluoropropene: A Challenging Problem for Both Theory and Experiment”, *J. Phys. Chem. A* **106**, 3625 (2002).
948. R. I. Kaiser, F. Stahl, P. R. Schleyer, and H. F. Schaefer, “Atomic and Molecular Hydrogen Elimination in the Crossed Beam Reaction of d<sub>1</sub>-Ethyne Radicals C<sub>2</sub>D(X <sup>2</sup>Σ<sup>+</sup>) with Acetylene, C<sub>2</sub>H<sub>2</sub>(X <sup>1</sup>Σ<sup>+</sup><sub>g</sub>): Dynamics of d<sub>1</sub>-Diacetylene (HCCCCD) and d<sub>1</sub>-Butadiynyl (DCCCC) Formation”, *Phys. Chem. Chem. Phys.* **4**, 2950 (2002).
949. N. D. K. Petraco, W. D. Allen, and H. F. Schaefer, “The Fragmentation Path for Hydrogen Dissociation from Methoxy Radical”, *J. Chem. Phys.* **116**, 10229 (2002).
950. F. Stahl, P. R. Schleyer, H. F. Schaefer, and R. I. Kaiser, “The Reactions of Ethynyl Radicals as a Source of C<sub>4</sub> and C<sub>5</sub> Hydrocarbons in Titan’s Atmosphere”, *Planet. Space Sci.* **50**, 685 (2002).
951. K. W. Sattelmeyer, H. F. Schaefer, and J. F. Stanton, “The Global Minimum Structure of SiC<sub>3</sub>: The Controversy Continues”, *J. Chem. Phys.* **116**, 9151 (2002).
952. H. F. Schaefer, “Quantum Chemistry”, *Encyclopedia of Science and Technology*, 9th ed., Vol. 14 (McGraw-Hill, New York, 2002). Pages 676–681.
953. A. Y. Timoshkin, E. I. Davydova, T. N. Sevastianova, A. V. Suvorov, and H. F. Schaefer, “Relationship Between the Energy of the Donor–Acceptor Bond and the Reorganization Energy in Molecular Complexes”, *Int. J. Quantum Chem.* **88**, 436 (2002).
954. Q. Li, R. Lü, Y. Xie, and H. F. Schaefer, “Molecules for Materials: Germanium Hydride Radicals and Anions. Molecular Structures, Electron Affinities, and Thermochemistry of GeH<sub>n</sub>/GeH<sub>n</sub><sup>-</sup> (n = 0–4) and Ge<sub>2</sub>H<sub>n</sub>/Ge<sub>2</sub>H<sub>n</sub><sup>-</sup> (n = 0–6)”, *J. Comput. Chem.* (Peter Kollman Memorial Issue) **23**, 1642 (2002).
955. C. Pak, Y. Xie, and H. F. Schaefer, “Electron Affinities of the Dibromine Oxides”, *Mol. Phys.* (Megumu Yoshimine Memorial Issue) **101**, 211 (2003).
956. N. A. Richardson, S. S. Wesolowski, and H. F. Schaefer, “Electron Affinity of the Guanine-Cytosine Base Pair and Neutral-Anion Structural Perturbations”, *J. Am. Chem. Soc.* **124**, 10163 (2002).
957. C. J. Barden, P. Charbonneau, and H. F. Schaefer, “Group 13–Group 16 Heterocubanes [RM(μ<sub>3</sub>-E)]<sub>4</sub> (R = H, CH<sub>3</sub>; M = Al, Ga, In; E = O, S, Se, Te) and Group 13 Cubanes [RM(μ<sub>3</sub>-M)]<sub>4</sub> (R = F, Cl, CH<sub>3</sub>, NO<sub>2</sub>; M = Al, Ga, In): A Structural Study”, *Organometallics* **21**, 3605 (2002).
958. F. Stahl, P. R. Schleyer, H. Jiao, H. F. Schaefer, K.-H. Cheu, and N. L. Allinger, “The Resurrection of Neutral Tris-Homoaromaticity”, *J. Org. Chem.* **67**, 6599 (2002).

959. A. Y. Timoshkin and H. F. Schaefer, "From 'Parasitic' Association Toward the Stoichiometry Controlled Gas Phase Synthesis of Nanoparticles: A Theoretically Driven Challenge for Experimentalists", *The Chemical Record* **2**, 319 (2002).
960. M. S. Schuurman, C. Pak, and H. F. Schaefer, "What to Do About Unpaired Electrons? A Hydrocarbon Hexaradical with Three Closs Diradicals Linked by 1,3,5 - Trimethylbenzene as Ferromagnetic Coupler, with Comparison to Successively Ring-Closed Structures", *J. Chem. Phys.* **117**, 7147 (2002).
961. Q. Li, J. F. Zhao, Y. Xie, and H. F. Schaefer, "Electron Affinities, Molecular Structures, and Thermochemistry of the Fluorine, Chlorine, and Bromine Substituted Methyl Radicals", Invited Article, *Mol. Phys.* **100**, 3615 (2002).
962. K. W. Sattelmeyer and H. F. Schaefer, "The  $\nu_5$  Vibrational Frequency of the Vinyl Radical: Conflict Between Theory and Experiment", *J. Chem. Phys.* **117**, 7914 (2002).
963. N. D. K. Petraco, L. Horny, I. Hubac, and H. F. Schaefer, "Brillouin-Wigner Coupled Cluster Theory. Fock Space Approach", *J. Chem. Phys.* **117**, 9580 (2002).
964. Y. Xie, W. Wang, K. Fan, and H. F. Schaefer, "The Ring Structure of the NO Dimer Radical Cation: A Possible New Assignment of the Mysterious IR Absorption at  $1424\text{ cm}^{-1}$ ", *J. Chem. Phys.* **117**, 9727 (2002).
965. Z.-F. Xu, Y. Xie, W.-L. Feng, and H. F. Schaefer, "Systematic Investigation of Electronic and Molecular Structures of the First Transition Metal Series Metallocenes  $M(C_5H_5)_2$ , ( $M = V, Cr, Mn, Fe, Co, \text{ and } Ni$ )", *J. Phys. Chem. A* **107**, 2716 (2003).
966. Y. Xie and H. F. Schaefer, "The Characterization of Metal-Metal Bonds in Binuclear Homoleptic Transition Metal Carbonyls. The Compliance Matrix", *Z. Phys. Chem.* (Sigrid Peyerimhoff Issue) **217**, 189 (2003).
967. H. L. Woodcock, M. Hodoscek, P. Sherwood, Y. S. Lee, H. F. Schaefer, and B. R. Brooks, "Exploring the QM/MM Replica Path Method: A Pathway Optimization of the Chorismate to Prephenate Claisen Rearrangement Catalyzed by Chorismate Mutase", *Theor. Chem. Acc.* **109**, 140 (2003).
968. L. Sari, K. A. Peterson, Y. Yamaguchi, and H. F. Schaefer, "An L-Shaped Equilibrium Geometry for Germanium Dicarbide ( $GeC_2$ )? Interesting Effects of Zero-Point Vibration, Scalar Relativity, and Core-Valence Correlation", *J. Chem. Phys.* **117**, 10008 (2002).
969. S. Lu, W. Xe, Q. Li, Y. Xie, and H. F. Schaefer, "Molecular Structures and Electron Affinities for the Chlorine Oxides  $ClOO$ ,  $ClOOO$ , and  $ClO_3(C_{3v})$ ", *J. Phys. Chem. A* **106**, 12324 (2002).
970. L. Horny, N. D. K. Petraco, and H. F. Schaefer, "Odd Carbon Long Linear Chains  $HC_{2n+1}H$  ( $n = 4-11$ ): Properties of the Neutrals and Radical Anions", *J. Am. Chem. Soc.* **124**, 14716 (2002).
971. P. R. Schreiner, A. A. Fokin, P. R. Schleyer, and H. F. Schaefer, "Model Studies on the Electrophilic Substitution of Methane with Various Electrophiles E ( $E = NO^+_2, F^+, Cl^+, Cl^+_3, HBr^+_2, HCO^+, OH^+, H_2O-OH^+$ , and  $Li^+$ )", *Fundamental World of Quantum Chemistry: A Tribute Volume to the Memory of Per-Olov Löwdin*, Vol. 2, editors E. J. Brändas and E. S. Kryachko (Kluwar, Dordrecht, Holland, 2003). Pages 359-386.
972. G. Gregoire, N. R. Brinkmann, D. van Heijnsbergen, H. F. Schaefer, and M. A. Duncan, "Infrared Photodissociation Spectroscopy of  $Mg^+(CO_2)_n$  and  $Mg^+(CO_2)_n$  Ar Clusters", *J. Phys. Chem. A* **107**, 218 (2003).
973. W. Xu, G. Li, G. Yu, Y. Zhao, Q. Li, and H. F. Schaefer, "The Arsenic Fluorides  $AsF_n$  ( $n = 1-6$ ) and their Anions: Structures, Thermochemistry, and Electron Affinities", *J. Phys. Chem. A* **107**, 258 (2003).
974. J. M. Gonzales, C. J. Barden, S. T. Brown, P. R. Schleyer, and H. F. Schaefer, "Cyclopentadiene Annulated Polycyclic Aromatic Hydrocarbons: Investigations of Electron Affinities", *J. Am. Chem. Soc.* **125**, 1064 (2003).
975. Y. Yamaguchi, L. Sari, S. S. Wesolowski, K. W. Sattelmeyer, and H. F. Schaefer, "Characterization of the  $\tilde{X}^1\Sigma^+$ ,  $\tilde{a}^3\Pi$ , and  $\tilde{A}^1\Pi$  Electronic States of BBO", *Mol. Phys.* (Graham Richards Issue) **101**, 1273 (2003).
976. Y. Xie, H. F. Schaefer, and F. A. Cotton, "The Radical Anions and the Electron Affinities of Perfluorinated Benzene, Naphthalene, and Anthracene", *J. Chem. Soc., Chem. Commun.* 102 (2003).
977. H. L. Woodcock, H. F. Schaefer, and P. R. Schreiner, "The Problematic Energy Differences Between Cumulenes and Poly-yenes: Does this Point to a Systematic Improvement of Density Functional Theory?" *J. Phys. Chem. A* **106**, 11923 (2002).
978. N. A. Richardson, S. S. Wesolowski, and H. F. Schaefer, "The Adenine-Thymine Base Pair Radical Anion: Adding an Electron Results in Major Structural Changes", *J. Phys. Chem. B* **107**, 848 (2003).
979. S. Ilieva, B. Galabov, D. G. Musaev, K. Morokuma, and H. F. Schaefer, "Computational Study of the Aminolysis of Esters. The Reaction of Methylformate with Ammonia", *J. Org. Chem.* **68**, 1496 (2003).
980. J. P. Kenny, W. D. Allen, and H. F. Schaefer, "Complete Basis Set Limit Studies of Conventional and R12 Correlation Methods: The Silicon Dicarbide ( $SiC_2$ ) Barrier to Linearity", *J. Chem. Phys.* **118**, 7353 (2003).
981. S. Li, N. A. Richardson, Y. Xie, R. B. King, and H. F. Schaefer, "The Rule Breaking  $Cr_2(CO)_{10}$ . A 17 Electron System or a  $Cr=Cr$  Double Bond?" *Faraday Discuss. Chem. Soc.* **124**, 315, 347 (2003).
982. A. A. Fokin, P. R. Schreiner, S. I. Kozhushkov, K. Sattelmeyer, H. F. Schaefer, and A. de Meijere, "Delocalization in Sigma Radical Cations: The Intriguing Structures of Ionized [n] Rotanes", *Org. Lett.* **5**, 697 (2003).
983. C. Pak, L. Sari, J. C. Rienstra-Kiracofe, S. S. Wesolowski, L. Horny, Y. Yamaguchi, and H. F. Schaefer, "Theoretical Characterization of the Disilaethynyl Anion ( $Si_2H^-$ )", *J. Chem. Phys.* **118**, 7256 (2003).
984. E. F. Valeev, W. D. Allen, R. Hernandez, C. D. Sherrill, and H. F. Schaefer, "On the Accuracy of Atomic Orbital Expansion Methods: Explicit Effects of k Functions on Atomic and Molecular Energies", *J. Chem. Phys.* **118**, 8594 (2003).
985. D. Moran K. Sukcharoenphon, R. Puchta, H. F. Schaefer, P. R. Schleyer, and C. D. Hoff, "The 2-Pyridinethiol/2-Pyridinethione Tautomeric Equilibrium. A Comparative Experimental and Computational Study", *J. Org. Chem.* **67**, 9061 (2002).

986. R. Guo, K. Balasubramanian, and H. F. Schaefer, "The Treacherous Potential Energy Hypersurface of AgSiO", *J. Chem. Phys.* **118**, 10623 (2003).
987. J. M. Gonzales, C. Pak, R. S. Cox, W. D. Allen, and H. F. Schaefer, "Definitive *Ab Initio* Studies of Model S<sub>N</sub>2 Reactions CH<sub>3</sub>X + F<sup>-</sup> (X = F, Cl, CN, OH, SH, NH<sub>2</sub>, PH<sub>2</sub>)", *Chem. Eur. J.* **9**, 2173 (2003).
988. D. Moran, F. Stahl, H. F. Bettinger, H. F. Schaefer, and P. R. Schleyer, "Toward Graphite: Magnetic Properties of Large Polybenzenoid Hydrocarbons", *J. Am. Chem. Soc.* **125**, 6746 (2003).
989. B. Papas, S. Wang, N. DeYonker, and H. F. Schaefer, "The Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals, and their Anions", *J. Phys. Chem. A* **107**, 6311 (2003).
990. A. Y. Timoshkin and H. F. Schaefer, "Fascinating Transformations of Donor–Acceptor Complexes of Group 13 Metal (Al, Ga, In) Derivatives with Nitriles and Isonitriles: From Monomeric Cyanides to Rings and Cages", *J. Am. Chem. Soc.* **125**, 9998 (2003).
991. R. I. Kaiser, L. Vereecken, J. Peeters, H. F. Bettinger, P. R. Schleyer, and H. F. Schaefer, "Elementary Reactions of the Phenyl Radical, C<sub>6</sub>H<sub>5</sub>, with C<sub>3</sub>H<sub>4</sub> Isomers, and of Benzene, C<sub>6</sub>H<sub>6</sub>, with Atomic Carbon in Extraterrestrial Environments", *Astron. Astrophys.* **406**, 385 (2003).
992. H. F. Schaefer, *Science and Christianity: Conflict or Coherence?* (The University of Georgia, Athens, Georgia, 2004). 204 pages.
993. Y. Xie, J. H. Jang, R. B. King, and H. F. Schaefer, "Binuclear Homoleptic Manganese Carbonyls: Mn<sub>2</sub>(CO)<sub>x</sub> (x = 10, 9, 8, 7)", *Inorg. Chem.* **42**, 5219 (2003).
994. L. Sari, M. C. McCarthy, H. F. Schaefer, and P. Thaddeus, "Mono- and Di-Bridged Isomers of Si<sub>2</sub>H<sub>3</sub> and Si<sub>2</sub>H<sub>4</sub>: the True Ground-State Global Minima. Theory and Experiment in Concert," *J. Am. Chem. Soc.* **125**, 11409 (2003).
995. J. D. Larkin, D. Moran, and H. F. Schaefer, "Molecular Structures and Energetics of the Neutral Aluminum-Trimethylaluminum Complex: An Al–Al Global Minimum?" *Chem. Phys. Lett.* **378**, 65 (2003).
996. K. Sattelmeyer, H. F. Schaefer, and J. F. Stanton, "Use of 2h and 3h–p-like Coupled-Cluster Tamm-Dancoff Approaches for the Equilibrium Properties of Ozone", *Chem. Phys. Lett.* **378**, 42 (2003).
997. R. S. Walters, N. R. Brinkmann, H. F. Schaefer, and M. A. Duncan, "Infrared Spectroscopy of Mass-Selected Al<sup>+</sup>(CO<sub>2</sub>)<sub>n</sub> and Al<sup>+</sup>(CO<sub>2</sub>)<sub>n</sub> Ar Clusters", *J. Phys. Chem. A* **107**, 7396 (2003).
998. L. Sari, Y. Yamaguchi, and H. F. Schaefer, "The <sup>3</sup>Σ<sup>-</sup> and <sup>3</sup>Π States of GeC and GeSi: The Problematic Dissociation Energy of GeC", *J. Chem. Phys.* **119**, 8266 (2003).
999. G. Yan, N. R. Brinkmann, and H. F. Schaefer, "Energetics and Structures of Adamantane and the 1- and 2-Adamantyl Radicals, Cations, and Anions", *J. Phys. Chem.* **107**, 9479 (2003).
1000. D. Moran, H. L. Woodcock, Z. Chen, H. F. Schaefer, and P. R. Schleyer, "On the Viability of Small Endohedral Hydrocarbon Cage Complexes: X@C<sub>4</sub>H<sub>4</sub>, X@C<sub>8</sub>H<sub>8</sub>, X@C<sub>8</sub>H<sub>4</sub>, X@C<sub>10</sub>H<sub>16</sub>, X@C<sub>12</sub>H<sub>12</sub>, and X@C<sub>16</sub>H<sub>16</sub>", *J. Am. Chem. Soc.* **125**, 11442 (2003).
1001. N. R. Brinkmann and H. F. Schaefer, "The SF<sub>6</sub><sup>-</sup> Enigma for Density Functional Theory: Is the KMLYP Functional a Reasonable Solution for this Problematic Anion?" *Chem. Phys. Lett.* **381**, 123 (2003).
1002. Q. Li, S. Lü, Y. Xie, P. R. Schleyer, and H. F. Schaefer, "Molecular Structures, Thermochemistry, and Electron Affinities for the Dichlorine Oxides: Cl<sub>2</sub>O<sub>n</sub>/Cl<sub>2</sub>O<sub>n</sub><sup>-</sup> (n = 1–4)", *Int. J. Quantum Chem.* (Leland C. Allen Issue) **95**, 731 (2003).
1003. L. Horny, K. W. Sattelmeyer, and H. F. Schaefer, "The Elusive Electron Affinity of ClF", *J. Chem. Phys.* **119**, 11615 (2003).
1004. S. Li, N. A. Richardson, R. B. King, and H. F. Schaefer, "Chromium–Chromium Multiple Bonding in Cr<sub>2</sub>(CO)<sub>9</sub>", *J. Phys. Chem.* **107**, 10118 (2003).
1005. L. T. M. Profeta, J. D. Larkin, and H. F. Schaefer, "The Thymine Radicals and their Respective Anions: Molecular Structures and Electron Affinities", *Mol. Phys.* **101**, 3277 (2003).
1006. N. R. Brinkmann, G. S. Tschumper, G. Yan, and H. F. Schaefer, "An Alternate Mechanism for the Dimerization of Formic Acid", *J. Phys. Chem.* **107**, 10208 (2003).
1007. S. Li, K. W. Sattelmeyer, Y. Yamaguchi, and H. F. Schaefer, "Characterization of the Three Lowest-Lying Singlet Electronic States of AlOH", *J. Chem. Phys.* **119**, 10208 (2003).
1008. G. N. Srinivas, A. Anoop, E. D. Jemmis, T. P. Hamilton, K. Lammertsma, J. Leszczynski, and H. F. Schaefer, "Non-Planarity at Tri-Coordinated Aluminum and Gallium! Novel Structures for X<sub>3</sub>H<sup>m</sup><sub>n</sub> (X = B, Al, Ga; n = 3, m = -2; n = 4, m = -1; n = 5, m = 0; n = 6, m = +1)", *J. Am. Chem. Soc.* **125**, 16397 (2003).
1009. C. J. Barden and H. F. Schaefer, "Accuracy and Applicability of Quantum Chemical Methods for Computational Medicinal Chemistry", in *Computational Medicinal Chemistry and Drug Discovery*, editors P. Bultinck, H. DeWinter, W. Langenaeker, and J. P. Tollenaere (Marcel Dekker, New York, 2004). Pages 133–151.
1010. N. A. Richardson, Y. Yamaguchi, and H. F. Schaefer, "Isomerization of the Newly Discovered Interstellar Molecule SiCN to SiNC Through Two Transition States", *J. Chem. Phys.* **119**, 12946 (2003).
1011. N. J. DeYonker, Y. Yamaguchi, W. D. Allen, C. Pak, and H. F. Schaefer "Low-Lying Electronic States of FeCN and FeNC: A Theoretical Journey into Isomerization and Quartet/Sextet Competition", *J. Chem. Phys.* **120**, 4726 (2004).
1012. K. W. Sattelmeyer, Y. Yamaguchi, and H. F. Schaefer, "Energetics of the Low-Lying Isomers of HCCO", *Chem. Phys. Lett.* **383**, 266 (2004).
1013. A. C. Simmonett, S. E. Wheeler, and H. F. Schaefer, "The Vinyl Radical and Fluorinated Vinyl Radicals, C<sub>2</sub>H<sub>3–n</sub>F<sub>n</sub> (n = 0–3), and Corresponding Anions: Comparison with the Isoelectronic Complexes [X···YC≡CZ]<sup>-</sup>", *J. Phys. Chem. A* **108**, 1608 (2004).
1014. L. D. Speakman, B. N. Papas, H. L. Woodcock, and H. F. Schaefer, "A Reinterpretation of Microwave and Infrared Spectroscopic Studies of Benzaldehyde", *J. Chem. Phys.* **120**, 4247 (2004).



1015. S. E. Wheeler, K. W. Sattelmeyer, P. R. Schleyer, and H. F. Schaefer, "Geometries and Atomization Energies of Small Lithium Clusters and Hydrogenated Lithium Clusters", *J. Chem. Phys.* **120**, 4683 (2004).
1016. Y. Zhao, W. Xu, Q. Li, Y. Xie, and H. F. Schaefer, "The Arsenic Clusters  $As_n$  ( $n = 1-5$ ) and their Anions: Structures, Thermochemistry, and Electron Affinities", *J. Comput. Chem.*
1017. L. Gong, Q. Li, W. Xu, Y. Xie, and H. F. Schaefer, "Novel Interhalogen Molecules: Structures, Thermochemistry, and Electron Affinities of the Dibromine Fluorides  $Br_2F_n/Br_2F_n^-$  ( $n = 1-6$ )", *J. Phys. Chem. A* **108**, 3598 (2004).
1018. R. D. DeKock, M. J. McGuire, P. Piecuch, W. D. Allen, H. F. Schaefer, K. Kowalski, S. A. Spronk, D. B. Lawson, and S. L. Laursen, "The Electronic Structure and Vibrational Spectrum of *trans*-HNOO", *J. Phys. Chem. A* **108**, 2893 (2004).
1019. M. Schuurman, S. Muir, W. D. Allen, and H. F. Schaefer, "Toward Subchemical Accuracy in Computational Thermochemistry: Focal Point Analysis of the Heat of Formation of NCO and [H, N, C, O] Isomers", *J. Chem. Phys.*
1020. N. A. Richardson, S. Wang, and H. F. Schaefer, "DNA Nucleosides and their Radical Anions: Molecular Structures and Electron Affinities", *J. Am. Chem. Soc.* **126**, 4404 (2004).