

STEVE SCHEINER
PAPERS PUBLISHED

1. Charge Relay System and Tetrahedral Intermediates in Acylation of Serine Proteinases
S. Scheiner, D. A. Kleier, and W. N. Lipscomb
Proc. Natl. Acad. Sci., USA, **1975** 72, 2606-2610.
2. Catalytic Mechanism of Serine Proteinases
S. Scheiner and W. N. Lipscomb
Proc. Natl. Acad. Sci., USA, **1976** 73, 432-436.
3. Nucleophilic Attack on Carbonyl Systems with Comments on Orbital Steering
S. Scheiner, W. N. Lipscomb, and D. A. Kleier
J. Am. Chem. Soc., **1976** 98, 4770-4777.
4. Comments on Orbital Steering
D. A. Kleier, S. Scheiner, and W. N. Lipscomb
Int. J. Quantum Chem: Quantum Biology Symp. No. 3, **1976** 161-169.
5. Hydrolysis of Peptides by Carboxypeptidase A
S. Scheiner and W. N. Lipscomb
J. Am. Chem. Soc., **1977** 99, 3466-3472.
6. Theoretical Studies of Environmental Effects on Protein Conformation: Flexibility of the Peptide Bond
S. Scheiner and C. W. Kern
J. Am. Chem. Soc., **1977** 99, 7042-7050.
7. Energies of Polypeptides: Theoretical Conformational Study of Polyglycine Using Quantum Mechanical Partitioning
S. Scheiner and C. W. Kern
Proc. Natl. Acad. Sci., USA, **1978** 75, 2071-2075.
8. Quantum Mechanical Partitioning of the Energies of Polypeptides: Conformational Study of Polyglycine
S. Scheiner and C. W. Kern
J. Am. Chem. Soc., **1978** 100, 7539-7548.
9. Theoretical Study of Proton Transfers between Base Pairs of DNA
S. Scheiner and C. W. Kern
Chem. Phys. Letters, **1978** 57, 331-333.
10. Molecular Orbital Study of Multiply Hydrogen Bonded Systems: Formic Acid Dimer and DNA Base Pairs
S. Scheiner and C. W. Kern
J. Am. Chem. Soc., **1979** 101, 4081-4085.

11. Internal Rotations in Aliphatic Molecules: n-Butane and 2,2,3,3-Tetrafluorobutane
S. Scheiner
J. Am. Chem. Soc., **1980** 102, 3723-3728.
12. Molecular Orbital Treatments of Hydrogen Bonded Systems. 2. Dimers of Water and HCN
S. Scheiner
Theor. Chim. Acta, **1980** 57, 71-80.
13. Proton Transfer Potentials in Hydrogen-Bonded Systems. $(\text{H}_5\text{O}_2)^+$
S. Scheiner
Int. J. Quantum Chem., Quantum Biol. Symp. No. 7, **1980** 199-206.
14. Influence of Intramolecular Hydrogen Bonding on the Electronic Structure of Oxymorphone
S. Scheiner and V. M. Kolb
Proc. Natl. Acad. Sci., USA, **1980** 77, 5602-5605.
15. Proton Transfers in Hydrogen Bonded Systems. Cationic Oligomers of Water
S. Scheiner
J. Am. Chem. Soc., **1981** 103, 315-320.
16. Quantum Chemical Studies of Proton Transport in Biomembranes
S. Scheiner
Ann. N. Y. Acad. Sci., **1981** 367, 493-509.
17. Proton Transfers in Hydrogen Bonded Systems. 2. Electron Correlation Effects in $(\text{N}_2\text{H}_7)^+$
S. Scheiner and L. B. Harding
J. Am. Chem. Soc., **1981** 103, 2169-2173.
18. Proton Transfers in Hydrogen Bonded Systems. 3. Electron Correlation Effects in $(\text{H}_3\text{NHOH})^+$
S. Scheiner and L. B. Harding
Chem. Phys. Letters, **1981** 79, 39-43.
19. Proton Transfers in Hydrogen Bonded Systems. 5. Analysis of Electronic Redistributions in $(\text{N}_2\text{H}_7)^+$
S. Scheiner
Int. J. Quantum Chem., Quantum Biology Symp. No. 8, **1981** 221-229.
20. Proton Transfers in Hydrogen Bonded Systems. 6. Electronic Redistributions in $(\text{N}_2\text{H}_7)^+$ and $(\text{O}_2\text{H}_5)^+$
S. Scheiner
J. Chem. Phys., **1981** 75, 5791-5801.
21. Proton Transfers in Hydrogen Bonded Systems. 4. Cationic Dimers of NH_3 and OH_2
S. Scheiner
J. Phys. Chem., **1982** 86, 376-382.

22. Comparison of Proton Transfers in Cationic Heterodimers and Homodimers of NH_3 and OH_2
S. Scheiner
J. Chem. Phys., **1982** 77, 4039-4050.
23. Møller-Plesset Treatment of Electron Correlation in $(\text{HOHOH})^-$
M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1982** 77, 4586-4593.
24. Basis Set Dependence of Protonation Reactions of NH_3 , OH_2 , and SH_2
S. Scheiner
Chem. Phys. Lett., **1982** 93, 540-544.
25. Role of d Functions in Ab Initio Calculation of the Equilibrium Structure of $\text{H}_2\text{S-HF}$
S. Scheiner
J. Chem. Phys., **1983** 78, 599-600.
26. Ab Initio Study of Proton Transfers Including Effects of Electron Correlation
S. Scheiner, M. M. Szczesniak and L. D. Bigham
Int. J. Quantum Chem., **1983** 23, 739-751.
27. Energetics and Electronic Rearrangements of Proton Transfer in $(\text{H}_3\text{NHOH}_2)^+$
S. Scheiner
Int. J. Quantum Chem., **1983** 23, 753-764).
28. Hydrogen Bonding of the Carbonyl Groups of Uridine Nucleosides
S. Scheiner
Biopolymers, **1983** 22, 731-745.
29. Molecular Orbital Study of Proton Transfer in $(\text{H}_3\text{NHOH}_2)^+$
S. Scheiner and L. B. Harding
J. Phys. Chem., **1983** 87, 1145-1153.
30. Ab Initio Molecular Orbital Estimates of Charge Partitioning between Bjerrum and Ionic Defects in Ice
S. Scheiner and J. F. Nagle
J. Phys. Chem., **1983** 87, 4267-4272.
31. Angular Dependence of the Interaction between the N-Lone Pair of Amines and a Proton: Relevance to Drug-Receptor Systems
V. M. Kolb and S. Scheiner
J. Pharm. Sci., **1984** 73, 389-392.
32. Interactions between Aromatic Systems: Dimers of Benzene and s-Tetrazine
J. B. Pawliszyn, M. M. Szczesniak and S. Scheiner
J. Phys. Chem., **1984** 88, 1726-1730.

33. Studies of Dispersion Energy in Hydrogen-Bonded Systems. H₂O-HOH, H₂O-HF, H₃N-HF, HF-HF
M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1984** *80*, 1535-1542.
34. Proton Transfers between First and Second-Row Atoms: (H₂OHS₂)⁺ and (H₃NHS₂)⁺
S. Scheiner
J. Chem. Phys., **1984** *80*, 1982-1987
35. Improvement of Polarized Double-Zeta Basis Sets for Molecular Interactions. Complexes of NH₃, OH₂ and FH with H⁺ and Li⁺
Z. Latajka and S. Scheiner
Chem. Phys. Lett., **1984** *105*, 435-439.
36. New Insights in the Clastic Binding Hypothesis for Opiate-Receptor Interactions. II. Proton-Transfer Mechanism
V. M. Kolb and S. Scheiner
J. Pharm. Sci., **1984** *73*, 719-723.
37. Effects of Basis Set and Electron Correlation on the Calculated Properties of the Ammonia Dimer
Z. Latajka and S. Scheiner
J. Chem. Phys., **1984** *81*, 407-409.
38. Theoretical Study of Internal Rotation in Perfluorobutadiene
T. Choudhury and S. Scheiner
J. Mol. Struct., Theochem., **1984** *18*, 373-379.
39. Ab Initio Study of FH-PH₃ and ClH-PH₃ including the Effects of Electron Correlation
Z. Latajka and S. Scheiner
J. Chem. Phys., **1984** *81*, 2713-2716.
40. Effects of Molecular Charge and Methyl Substitution on Proton Transfers between Oxygen Atoms
E. A. Hillenbrand and S. Scheiner
J. Am. Chem. Soc., **1984** *106*, 6266-6273.
41. Ab Initio Comparison of H-bonds and Li-bonds: Complexes of LiF, LiCl, HF, and HCl with NH₃
Z. Latajka and S. Scheiner
J. Chem. Phys., **1984** *81*, 4014-4017
42. Theoretical Study of H₂O-HF and H₂O-HCl: Comparison with Experiment
M. M. Szczesniak, S. Scheiner and Y. Bouteiller
J. Chem. Phys., **1984** *81*, 5024-5030

43. Interactions Involving Aromatic Systems: Benzene + Acetylene
S. Scheiner and M. M. Szczesniak
Int. J. Quantum Chem., Quantum Biology Symp. No. 11, **1984** 201-208 .
44. Effects of External Ions on the Energetics of Proton Transfers across Hydrogen Bonds
S. Scheiner, P. Redfern and M. M. Szczesniak
J. Phys. Chem., **1985** 89, 262-266.
45. Interactions between Benzene and DNA Bases. A Model of Intercalation.
S. Scheiner and M. M. Szczesniak
In 'Molecular Basis of Cancer, Part B: Macromolecular Recognition, Chemotherapy, and Immunology', Ed. R. Rein, Alan R. Liss, Inc., New York, 1985, pp. 53-63.
46. Analysis of Proton Translocation through Hydrogen-Bonded Chains using Molecular Orbital Methods
S. Scheiner and E. Hillenbrand
In "Water and Ions in Biological Systems", Eds. A. Pullman, V. Vasilescu & L. Packer, Plenum, New York, 1985, pp. 571-584.
47. Comparison of Proton Transfers between First and Second Row Atoms: $(\text{H}_2\text{SHSH}_2)^+$ and $(\text{H}_2\text{OHOH}_2)^+$
L. Bigham and S. Scheiner
J. Chem. Phys., **1985** 82, 3316-3321.
48. Effects of External Ions on the Dynamics of Proton Transfer in a Hydrogen Bond
M. M. Szczesniak and S. Scheiner
J. Phys. Chem., **1985** 89, 1835-1840.
49. Modification of pK Values Caused by Change in H-Bond Geometry
S. Scheiner and E. A. Hillenbrand
Proc. Natl. Acad. Sci., USA, **1985** 82, 2741-2745.
50. Influence of Basis Set on the Calculated Properties of $(\text{H}_3\text{N-HCl})$
Z. Latajka and S. Scheiner
J. Chem. Phys., **1985** 82, 4131-4134.
51. Effects of Alkylation upon the Proton Affinities of Nitrogen and Oxygen Bases
P. Redfern and S. Scheiner
J. Comput. Chem., **1985** 6, 168-172.
52. Comparison between Proton Transfers involving Carbonyl and Hydroxyl Oxygens
S. Scheiner and E. A. Hillenbrand
J. Phys. Chem., **1985** 89, 3053-3060.

53. Contribution of Dispersion to the Properties of H₂S--HF and H₂S--HCl
M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1985** 83, 1778-1783
54. Theoretical Studies of Proton Transfers
S. Scheiner
Acc. Chem. Res., **1985** 18, 174-180.
55. Role of Polarization Functions in Cation Binding. H₃N-Li⁺ and H₂O-Li⁺
Z. Latajka and S. Scheiner
Chem. Phys., **1985** 98, 59-70.
56. Analysis of the Principles Governing Proton Transfer Reactions. Comparison of the Imine and Amine Groups
E. A. Hillenbrand and S. Scheiner
J. Am. Chem. Soc., **1985** 107, 7690-7696.
57. The Potential Energy Surface of (NH₃)₂
Z. Latajka and S. Scheiner
J. Chem. Phys., **1986** 84, 341-347.
58. Contribution of Dispersion to the Properties of H-Bonded Systems. Complexes of HF and HCl with NH₃, PH₃, H₂O, and H₂S
S. Scheiner, M. M. Szczesniak and Z. Latajka
J. Mol. Struct., Theochem, **1986** 135, 179-188.
59. Energetics of Proton Transfer between Carbon Atoms. (H₃CH--CH₃)⁻
Z. Latajka and S. Scheiner
Int. J. Quantum Chem., **1986** 29, 285-292.
60. Factors Influencing Proton Positions in Biomolecules
S. Scheiner, P. Redfern and E. A. Hillenbrand
Int. J. Quantum Chem., **1986** 29, 817-827.
61. The Basis Set Dependence of Structures and Energies of Various States of Cyclodisiloxane
R. Brenstein and S. Scheiner
Int. J. Quantum Chem., **1986** 29, 1191-1208.
62. Correction of the Basis Set Superposition Error in SCF and MP2 Interaction Energies. The Water Dimer
M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1986** 84, 6328-6335.
63. Quantum Mechanical Test of Marcus Theory. Effects of Alkylation upon Proton Transfer
S. Scheiner and P. Redfern
J. Phys. Chem., **1986** 90, 2969-2974.

64. Ab Initio Study of Structure and Cooperativity in $\text{H}_3\text{N-HF-HF}$ and $\text{H}_3\text{P-HF-HF}$
I. J. Kurnig, M. M. Szczesniak and S. Scheiner
J. Phys. Chem., **1986** 90, 4253-4258.
65. Effect of Secondary Basis Set Superposition Error upon Calculated Vibrational Intensities
M. M. Szczesniak and S. Scheiner
Chem. Phys. Letters, **1986** 131, 230-236.
66. Additivity of the Effects of External Ions and Dipoles upon the Energetics of Proton Transfer
I. J. Kurnig and S. Scheiner
Int. J. Quantum Chem., Quantum Biology Symposium 13, **1986** 71-79.
67. Analysis of the Principles Governing Proton-Transfer Reactions. Carboxyl Group
E. A. Hillenbrand and S. Scheiner
J. Am. Chem. Soc., **1986** 108, 7178-7186.
68. Kinetics of Proton Transfer in $(\text{H}_3\text{CH}\cdots\text{CH}_3)^-$
S. Scheiner and Z. Latajka
J. Phys. Chem., **1987** 91, 724-730.
69. The Proton Position in Hydrogen Halide - Amine Complexes. BrH-NH_3 and $\text{BrH-NH}_2\text{CH}_3$
Z. Latajka, S. Scheiner and H. Ratajczak
Chem. Phys. Lett., **1987** 135, 367-372; *Err.* **1987** 138, 384.
70. Basis Sets for Molecular Interactions. 1. Construction and Tests on $(\text{HF})_2$ and $(\text{H}_2\text{O})_2$
Z. Latajka and S. Scheiner
J. Comput. Chem., **1987** 8, 663-673.
71. Basis Sets for Molecular Interactions. 2. Application to $\text{H}_3\text{N-HF}$, $\text{H}_3\text{N-HOH}$, $\text{H}_2\text{O-HF}$, $(\text{NH}_3)_2$,
and $\text{H}_3\text{CH-OH}_2$
Z. Latajka and S. Scheiner
J. Comput. Chem., **1987** 8, 674-682.
72. Hydrogen Bonding and Proton Transfers Involving Triply Bonded Atoms. $\text{HC}\equiv\text{N}$ and $\text{HC}\equiv\text{CH}$
S. Cybulski and S. Scheiner
J. Am. Chem. Soc., **1987** 109, 4199-4206.
73. Primary and Secondary Basis Set Superposition Error at the SCF and MP2 Levels.
 $\text{H}_3\text{N--Li}^+$ and $\text{H}_2\text{O--Li}^+$
Z. Latajka and S. Scheiner
J. Chem. Phys., **1987** 87, 1194-1204.
74. Vibrational Frequencies and Intensities of H-Bonded Systems. 1:1 and 1:2 Complexes of NH_3
and PH_3 with HF
I. J. Kurnig, M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1987** 87, 2214-2224.

75. Three Dimensional Spatial Characteristics of Primary and Secondary Basis Set Superposition Error
Z. Latajka and S. Scheiner
Chem. Phys. Lett., **1987** 140, 338-343.
76. Structure, Energetics, and Vibrational Spectrum of H₂O··HCl
Z. Latajka and S. Scheiner
J. Chem. Phys., **1987** 87, 5928-5936.
77. Ab Initio Investigation of the Structure of Hydrogen Halide - Amine Complexes in the Gas Phase and in a Polarizable Medium
I. J. Kurnig and S. Scheiner
Int. J. Quantum Chem., Quantum Biology Symposium 14, **1987** 47-56.
78. Theoretical Vibrational Study of the FX..O(CH₃)₂ Hydrogen-Bonded Complex
Y. Bouteiller, C. Mijoule, M. M. Szczesniak and S. Scheiner
J. Chem. Phys., **1988** 88, 4861-4866.
79. Ab Initio Investigation of Interactions between Local Anesthetics and Receptor. Complexes Involving Amine, Phosphate, Amide, Na⁺, K⁺, Ca²⁺ and Cl⁻
M. Remko and S. Scheiner
J. Pharm. Sci., **1988** 77, 304-308.
80. Is CN⁻ Significantly Anisotropic? Comparison of CN⁻ vs. Cl⁻: Clustering with HCN and Condensed Phase Thermochemistry
M. Meot-Ner, S. M. Cybulski, S. Scheiner and J. F. Liebman
J. Phys. Chem., **1988** 92, 2738-2745.
81. Structure, Energetics, and Vibrational Spectra of H-Bonded Systems. Dimers and Trimers of HF and HCl
Z. Latajka and S. Scheiner
Chem. Phys., **1988** 122, 413-430.
82. Vibrational Frequencies and Intensities of H-bonded and Li-bonded Complexes. H₃N..HCl and H₃N..LiCl
M. M. Szczesniak, I. J. Kurnig and S. Scheiner
J. Chem. Phys., **1988** 89, 3131-3138.
83. Effects of Electron Correlation upon Molecular Interactions. Correction of the Electrostatic Interaction between DNA Bases
M. M. Szczesniak, S. Scheiner and P. Hobza
J. Mol. Struct., Theochem, **1988** 179, 177-184.

84. Accurate Evaluation of SCF and MP2 Components of Interaction Energies. Complexes of HF, OH₂ and NH₃ with Li⁺
M. M. Szczesniak and S. Scheiner
Coll. Czech. Chem. Commun., **1988** 53, 2214-2229.
85. Relationship between the Angular Characteristics of a H-bond and the Energetics of Proton Transfer Occurring Within
S. Scheiner
J. Mol. Struct., **1988** 177, 79-91.
86. The Geometry and Internal Rotational Barrier of Carbamic Acid and Several Derivatives
M. Remko and S. Scheiner
J. Mol. Struct., Theochem, **1988** 180, 175-188.
87. Effects of External Ions upon Proton Transfer Reactions. H-Bonded Systems Containing HCOOH
S. Scheiner and T. Das
Int. J. Quantum Chem., Quantum Biology Symposium 15, **1988** 137-147.
88. Ab Initio Investigation of Hydrogen Bonding by Carbamates. Complexes including N-methyl methylcarbamate, N-phenyl methylcarbamate, dimethyl ether, and methyl acetate
M. Remko and S. Scheiner
J. Mol. Struct., Theochem, **1988** 181, 19-24.
89. Hydrogen Bonding and Proton Transfers Involving the Carboxylate Group
S. M. Cybulski and S. Scheiner
J. Am. Chem. Soc., **1989** 111, 23-31.
90. Factors Contributing to Distortion Energies of Bent H-Bonds. Implications for Proton Transfer Potentials
S. M. Cybulski and S. Scheiner
J. Phys. Chem., **1989** 93, 6565-6574.
91. The Potential Energy Surface and Equilibrium Geometry of Ar··PH₃
Z. Latajka and S. Scheiner
J. Mol. Struct., **1989** 198, 205-213.
92. Dissection of Basis Set Superposition Error at SCF and Correlated Levels. HF Dimer
Z. Latajka and S. Scheiner
J. Mol. Struct., Theochem, **1989** 199, 9-22.
93. Structure and Energetics of Weakly Bound Complexes. Systems Incorporating NH₃ and PH₃
S. Scheiner
J. Mol. Struct. **1989** 200, 117-129.

94. Nonadditive effects in HF and HCl trimers.
G. Chalasinski, S. M. Cybulski, M. M. Szczesniak, S. Scheiner
J. Chem. Phys. **1989** *91*, 7048-7056.
95. Analysis of the Potential Energy Surface of Ar...NH₃
G. Chalasinski, S. M. Cybulski, M. M. Szczesniak and S. Scheiner
J. Chem. Phys. **1989** *91*, 7809-7817.
96. Ab Initio Studies of the Structure, Energetics, and Vibrational Spectra of Hydrogen-Bonded Systems
S. Scheiner
J. Mol. Struct., Theochem, **1989** *202*, 177-192.
97. Perturbations of Proton Transfer Potentials Caused by Polar Molecules
S. Scheiner, R. Wang, L. Wang
Int. J. Quantum Chem., Quantum Biology Symposium 16, **1989** 211-217.
98. Structure, Energetics, and Vibrational Spectrum of H₃N··HOH
Z. Latajka and S. Scheiner
J. Phys. Chem. **1990** *94*, 217-221.
99. Ab Initio Investigations of the Hydrolysis of the Carbamate Bond
M. Remko and S. Scheiner
J. Mol. Struct., (Theochem) **1990** *204*, 331-335.
100. Comparison of Morokuma and Perturbation Theory Approaches to Decomposition of Molecular Interaction Energy. (NH₄)⁺···NH₃
S. M. Cybulski, S. Scheiner
Chem. Phys. Lett. **1990** *166*, 57-64.
101. Potential Energy Surface for Dispersion Interaction in (H₂O)₂ and (HF)₂
M. M. Szczesniak, R. J. Brenstein, S. M. Cybulski, S. Scheiner
J. Phys. Chem. **1990** *94*, 1781-1788.
102. Factors Contributing to Distortion Energies of Bent H-Bonds. 2. Imine, Carbonyl, Carboxyl and Carboxylate Groups
S. M. Cybulski and S. Scheiner
J. Phys. Chem., **1990** *94*, 6106-6116.
103. Intermolecular Potential of the Methane Dimer and Trimer
M. M. Szczesniak, G. Chalasinski, S. M. Cybulski, and S. Scheiner
J. Chem. Phys. **1990** *93*, 4243-4253.
104. Correlation between Interaction Energy and Shift of the Carbonyl Stretching Frequency
Z. Latajka, S. Scheiner
Chem. Phys. Lett. **1990** *174*, 179-184.

105. Isotropy in Ionic Interactions. 2. How Spherical is the Ammonium Ion? Comparison of the Gas-Phase Clustering Energies and Condensed-Phase Thermochemistry of K^+ and NH_4^+
J. F. Liebman, M. J. Romm, M. Meot-Ner, S. M. Cybulski, S. Scheiner
J. Phys. Chem. **1991** 95, 1112-1119.
106. Ab Initio Study of the Intermolecular Potential of Ar--H₂O
G. Chalasinski, M. M. Szczesniak, S. Scheiner
J. Chem. Phys. **1991** 94, 2807-2816.
107. Theoretical Vibrational Study of FX··NH₃ (X=H,D,Li) Complexes
Y. Bouteiller, Z. Latajka, H. Ratajczak, S. Scheiner
J. Chem. Phys. **1991** 94, 2956-2960.
108. Ab Initio Study of Intermolecular Potential of H₂O Trimer
G. Chalasinski, M. M. Szczesniak, P. Cieplak, S. Scheiner
J. Chem. Phys. **1991** 94, 2873-2883.
109. Ab Initio Investigation of Interactions between Models of Membrane-Active Compounds and Polar Groups of Membranes: Complexes involving Amine, Ether, Amide, Phosphate, and Carboxylate
M. Remko, S. Scheiner
J. Pharm. Sci. **1991** 80, 328-332.
110. Correlated Proton Transfer Potentials. (HO-H-OH)⁻ and (H₂O-H-OH₂)⁺
Z. Latajka, S. Scheiner
J. Mol. Struct., Theochem **1991** 234, 373-385.
111. Effect of Intermolecular Orientation upon Proton Transfer within a Polarizable Medium
S. Scheiner, X. Duan
Biophys. J. **1991** 60, 874-883.
112. AM1 and Ab Initio Studies of Aminomethylphosphonic Acid
Z. Latajka, H. Ratajczak, S. Scheiner, J. Barycki
J. Mol. Struct., Theochem **1991** 235, 417-422.
113. Ab Initio Studies of Hydrogen-Bonded Complexes between Uracil and HCl
Z. Latajka, H. Ratajczak, Th. Zeegers-Huyskens, S. Scheiner
J. Mol. Struct., Theochem **1991** 235, 409-415.
114. Effect of Proton Transfer on Neighboring Hydrogen Bond Strength
S. Scheiner, W. O. Yu
Int. J. Quantum Chem., Quantum Biology Symposium 18, **1991** 37-48.
115. Deprotonation Energies of Ground and Excited States of HCN
V. Marudharajan, S. Scheiner
Chem. Phys. Lett. **1991** 186, 356-362.

116. Deprotonation Energy and Charge Redistribution in Excited States of Acetylene
V. Marudharajan, S. Scheiner
J. Phys. Chem. **1991** *95*, 10280-10284.
117. On the Underlying Source of Energetics of Bending of Hydrogen Bonds
S. Scheiner
J. Mol. Struct., Theochem **1992** *256*, 1-16.
118. Effect of Bond Multiplicity upon Hydrogen Bonding and Proton Transfers. Double Bonded Atoms
S. Scheiner, L. Wang
J. Am. Chem. Soc. **1992** *114*, 3650-3655.
119. Energetics, Proton Transfer Rates, and Kinetic Isotope Effects in Bent Hydrogen Bonds
X. Duan, S. Scheiner
J. Am. Chem. Soc. **1992** *114*, 5849-5856.
120. Analytic Functions Fit to Proton Transfer Potentials
X. Duan, S. Scheiner
J. Mol. Struct. **1992** *270*, 173-185.
121. Basis Set Superposition Error in Proton Transfer Potentials
Z. Latajka, S. Scheiner, G. Chalasinski
Chem. Phys. Lett. **1992** *196*, 384-389.
122. Fundamental Aspects of Lithium Ion Transfer
X. Duan, S. Scheiner
J. Phys. Chem. **1992** *96*, 7971-7975.
123. The Proton Position in Amine-HX (X=Br, I) Complexes
Z. Latajka, S. Scheiner, H. Ratajczak
Chem. Phys. **1992** *166*, 85-96.
124. Modeling of Coupled Proton Transfers by Analytic Functions
X. Duan, S. Scheiner
Int. J. Quantum Chem. **1992** *QBS19*, 109-124.
125. Calculation of Barriers to Proton Transfer Using a Variety of Electron Correlation Methods
K. Luth, S. Scheiner
Int. J. Quantum Chem. **1992** *QCS19*, 817-835.
126. Calculation of Barriers to Proton Transfer Using Variations of Multi-Configuration Self-Consistent Field Methods. I. Combinations of Orbitals
K. Luth, S. Scheiner
J. Chem. Phys. **1992** *97*, 7507-7518.

127. Calculation of Barriers to Proton Transfer Using Variations of Multi-Configuration Self-Consistent Field Methods. II. Configuration Interaction
K. Luth, S. Scheiner
J. Chem. Phys. **1992** 97, 7519-7527.
128. Proton Transfer in the Ground and First Excited Triplet States of Malonaldehyde
Z. Latajka, S. Scheiner
J. Phys. Chem. **1992** 96, 9764-9767.
129. Proton-Donor Properties of Water and Ammonia in van der Waals Complexes with Rare Gas Atoms. Kr-H₂O and Kr-NH₃
G. Chalasinski, M.M. Szczesniak, S. Scheiner
J. Chem. Phys. **1992** 97, 8181-8187.
130. Variational Transition State Theory Calculation of Proton Transfer Dynamics in (H₃CH··CH₃)⁻
A. D. Isaacson, L. Wang, S. Scheiner
J. Phys. Chem. **1993** 97, 1765-1769.
131. Hydrogen Bonding and Proton Transfers of the Amide Group
S. Scheiner, L. Wang
J. Am. Chem. Soc. **1993** 115, 1958-1963.
132. Ground and Excited State Intramolecular Proton Transfer in OCCNN Ring
X. Duan, S. Scheiner
Chem. Phys. Lett. **1993** 204, 36-44.
133. Proton-Donor Properties of Water and Ammonia in van der Waals Complexes. Be-H₂O and Be-NH₃
G. Chalasinski, M.M. Szczesniak, S. Scheiner
J. Chem. Phys. **1993** 98, 7020-7028.
134. Applicability of the Marcus Equation to Proton Transfer in Symmetric and Unsymmetric Systems
S. Scheiner, X. Duan
J. Mol. Struct., Theochem **1993** 285, 27-32.
135. Behavior of Interaction Energy and Intramolecular Bond Stretch in Linear and Bifurcated Hydrogen Bonds
X. Duan, S. Scheiner
Int. J. Quantum Chem.: QBS20 **1993** 181-190.
136. Modeling Proton Transfer Potentials in Angularly Deformed Hydrogen Bonds
X. Duan, S. Scheiner, R. Wang
Int. J. Quantum Chem.: QBS20 **1993** 77-87.

137. Comparison of Ground and Triplet State Geometries of Malonaldehyde
K. Luth, S. Scheiner
Int. J. Quantum Chem. QCS27 **1993** 419-429.
138. Relationship between Strength of Hydrogen Bond and Barrier to Proton Transfer
S. Scheiner
J. Mol. Struct., Theochem **1994** 307, 65-71.
139. Molecular Modeling of the Antiarrhythmic - Receptor Interaction
M. Remko, S. Scheiner, B. M. Rode
J. Mol. Struct. **1994** 307, 35-46.
140. Variation of Atomic Charges during Proton Transfer in Hydrogen Bonds
J. Florian, S. Scheiner
J. Comput. Chem. **1994** 15, 553-560.
141. Excited State Energetics and Proton Transfer Barriers in Malonaldehyde
K. Luth, S. Scheiner
J. Phys. Chem. **1994** 98, 3582-3587.
142. Calculation of Deuterium Isotope Effects in Proton Transfer Reactions
S. Scheiner
J. Mol. Struct. **1994** 321, 1-10.
143. The Ionic Hydrogen Bond. 5. Polydentate and Solvent-Bridged Structures. Complexing of the Proton and the Hydronium Ion by Polyethers
M. Meot-Ner, L. W. Sieck, S. Scheiner, X. Duan
J. Am. Chem. Soc. **1994** 116, 7848-7856.
144. Ab Initio Study of $\text{He}(^1S) + \text{Cl}_2(X \ ^1\Sigma_g, \ ^3\Pi_u)$ Potential Energy Surfaces
G. Chalasinski, M. Gutowski, M. M. Szczesniak, J. Sadlej, S. Scheiner
J. Chem. Phys. **1994** 101, 6800-6809.
145. Theoretical Study of Hydrogen Bonding and Proton Transfer in the Ground and Lowest Excited Singlet States of Tropolone
M.V. Vener, S. Scheiner, N.D. Sokolov
J. Chem. Phys. **1994** 101, 9755-9765.
146. Bent Hydrogen Bonds and Proton Transfers
S. Scheiner
Acc. Chem. Res. **1994** 27, 402-408
147. Theoretical-Study On The Analytic-Functions Fitting To Proton-Transfer Potentials In Water-System
R.S. Wang, Z.M. Su, S. Scheiner
Acta Chimica Sinica, **1994**, 52, 1150-1154

148. Ab Initio Study of the Structure of Guanine-Cytosine Base Pair Conformers in Gas Phase and Polar Solvents
J. Florian, J. Leszczynski, S. Scheiner
Mol. Phys. **1995** *84*, 469-480.
149. Critical Assessment of Density Functional Methods for Study of Proton Transfer Processes. (FHF)⁻
Z. Latajka, Y. Bouteiller, S. Scheiner
Chem. Phys. Lett. **1995** *234*, 159-164.
150. Proton and Lithium Ion Transfer between Two Water Molecules with an External Restraining Force
T. Kar, S. Scheiner
J. Am. Chem. Soc. **1995** *117*, 1344-1351.
151. Hydrogen Bonding and Proton Transfer in the Ground and Lowest Excited Singlet States of o-Hydroxyacetophenone
M.V. Vener, S. Scheiner
J. Phys. Chem. **1995** *99*, 642-649.
152. Proton Transfer in Ground and Excited Electronic States of Glyoxalmonohydrazine
K. Luth, S. Scheiner
J. Phys. Chem. **1995** *99*, 7352-7359.
153. Hardness Profiles of Some 1,2-Hydrogen Shift Reactions
T. Kar, S. Scheiner
J. Phys. Chem. **1995** *99*, 8121-8124.
154. Transfer of a Proton between N atoms in Excited Electronic States of 1,5-diaza-1,3-pentadiene
C. Rovira, S. Scheiner
J. Phys. Chem. **1995** *99*, 9854-9861.
155. Site-Site Function and Successive Reaction Counterpoise Calculation of Basis Set Superposition Error for Proton Transfer
A. J. Abkowitz, Z. Latajka, S. Scheiner, G. Chalasinski
J. Mol. Struct., Theochem **1995** *342*, 153-159.
156. The Nonexistence of Specially Stabilized Hydrogen Bonds in Enzymes
S. Scheiner, T. Kar
J. Am. Chem. Soc. **1995** *117*, 6970-6975.
157. Proton Transfer in H₅O₂⁺ and H₃O₂⁻ with an External Restraining Force
T. Kar, S. Scheiner
Int. J. Quantum Chem.: QBS29 **1995** 567-575.

158. Relative Stability of Hydrogen and Deuterium Bonds
S. Scheiner, M. Cuma
J. Am. Chem. Soc. **1996** *118* 1511-1521.
159. Complexing of the Ammonium Ion by Polyethers. Comparative Complexing Thermochemistry of Ammonium, Hydronium and Alkali Ions
M. Meot-Ner, L. W. Sieck, J. F. Liebman, S. Scheiner
J. Phys. Chem. **1996** *100* 6445-6450.
160. The Proton Transfer Properties of Imidazole
S. Scheiner, M. Yi
J. Phys. Chem. **1996** *100* 9235-9241.
161. Influence of Electron Correlation Effects on Calculated Properties and Vibrational Spectra of $\text{FF}\cdots\text{NH}_3$ and $\text{FCI}\cdots\text{NH}_3$ charge transfer complexes
Z. Latajka, S. Scheiner, Y. Bouteiller, H. Ratajczak
J. Mol. Struct., **1996** *376* 343-351.
162. Characterization of Ground and Excited Electronic State Deprotonation Energies of Systems Containing Double Bonds using Natural Bond Orbital Analysis
J. K. Badenhoop, S. Scheiner
J. Chem. Phys. **1996** *105* 4675-4691.
163. Proton Transfer between Phenol and Ammonia in Ground and Excited Electronic States
M. Yi and S. Scheiner
Chem. Phys. Lett. **1996** *262* 567-572.
164. Three-Center Bond Index Profiles
T. Kar, S. Scheiner
J. Mol. Struct., Theochem **1996** *370* 45-49.
165. Structure, Energetics and Vibrational Spectra of Dimers, Trimers, and Tetramers of HX (X = Cl, Br, I)
Z. Latajka and S. Scheiner
Chem. Phys. **1997** *216* 37-52.
166. BN-Naphthalene and Carbon-Containing Derivatives: An Ab Initio Study
T. Kar, D. E. Elmore, S. Scheiner
J. Mol. Struct., Theochem **1997** *392* 65-74.
167. Influence of Isotopic Substitution on Strength of Hydrogen Bonds of Common Organic Groups
M. Cuma and S. Scheiner
J. Phys. Org. Chem. **1997** *10* 383-395.

168. Excited State Intramolecular Proton Transfer in Anionic Analogues of Malonaldehyde
S. Scheiner, T. Kar, M. Cuma
J. Phys. Chem. A **1997** 101 5901-5909.
169. Intermolecular MH...HF Bonding in Monohydride Mo and W Complexes
G. Orlova, S. Scheiner
J. Phys. Chem. A **1998** 102 260-269.
170. Effect of Nonproximate Atomic Substitution on Excited State Intramolecular Proton Transfer
M. Cuma, C. Thompson, S. Scheiner
J. Comput. Chem. **1998** 19 129-138.
171. Ab Initio Calculations of Hardness and Chemical Potential of Open Shell Systems Using SCF, MP2, and MP4 Methods
T. Kar, S. Scheiner, A.B. Sannigrahi
Theochem. **1998** 427 79-85.
172. Intermolecular H...H Bonding and Proton Transfer in Semisandwich Re and Ru Complexes
G. Orlova, S. Scheiner
J. Phys. Chem. A **1998** 102 4813-4818.
173. Hardness and Chemical Potential Profiles for Some Open Shell HAB → HBA Type Reactions. Ab Initio and Density Functional Study
T. Kar, S. Scheiner, A.B. Sannigrahi
J. Phys. Chem. A **1998** 102 5967-5973.
174. Ionic Hydrogen Bonds in Bioenergetics. 3. Proton Transport in Membranes, Modeled by Ketone/Water Clusters
M. Meot-Ner, S. Scheiner, W. O. Yu
J. Am. Chem. Soc. **1998** 120 6980-6990.
175. Competition between Rotamerization and Proton Transfer in o-Hydroxybenzaldehyde
M. Cuma, S. Scheiner, T. Kar
J. Am. Chem. Soc. **1998** 120 10497-10503.
176. Inter- and Intramolecular Hydrogen Bonds with Transition Metal Atoms in Metallocenes of the Iron Subgroup
G. Orlova, S. Scheiner
Organometallics **1998** 17 4362-4367.
177. Structure, Stability, and Bonding of BC₂N: An Ab Initio Study
T. Kar, M. Cuma, S. Scheiner
J. Phys. Chem. A **1998** 102 10134-10141.

178. Activation and Cleavage of H-R Bonds through Intermolecular H \cdots H Bonding upon Reaction of Proton Donors HR with 18-Electron Transition Metal Hydrides
G. Orlova, S. Scheiner, T. Kar
J. Phys. Chem. A **1999** 103 514-520.
179. Effect of Adjoining Aromatic Ring upon Excited State Proton Transfer. o-Hydroxybenzaldehyde.
M. Cuma, S. Scheiner, T. Kar
Theochem. **1999** 467 37-49.
180. Comparison of Methods for Calculating the Properties of Intramolecular Hydrogen Bonds. Excited State Proton Transfer
T. Kar, S. Scheiner, M. Cuma
J. Chem. Phys. **1999** 111 849-858.
181. Effects of Chemical Substitution upon Excited State Proton Transfer. Fluoroderivatives of Salicylaldehyde
M. Forés and S. Scheiner
Chem. Phys. **1999** 246 65-74
182. Ionic Hydrogen Bond Effects on the Acidities, Basicities, Solvation, Solvent Bridging, and Self-Assembly of Carboxylic Groups
M. Meot-Ner, D. Elmore, S. Scheiner
J. Am. Chem. Soc. **1999** 121 7625-7635
183. Fundamental Properties of the CH \cdots O Interaction: Is It a True Hydrogen Bond?
Y. Gu, T. Kar, S. Scheiner
J. Am. Chem. Soc. **1999** 121 9411-9422
184. Does Thermochemical Mimicry Extend to Gibbs Energies? The Differences of K $^+$ and NH $_4^+$, and of Na $^+$ and H $_3$ O $^+$
J.F. Liebman, S. Scheiner
Struct. Chem. **1999** 10 391-392
185. Calculation of Isotope Effects from First Principles
S. Scheiner
Biochim. Biophys. Acta **2000** 1458 28-42
186. Evaluation of the H-Bonding Properties of CH \cdots O Interactions Based upon NMR Spectra
S. Scheiner, Y. Gu, T. Kar
J. Mol. Struct. (Theochem) **2000** 500 441-452
187. Theoretical Studies of Excited State Proton Transfer in Small Model Systems
(Invited Feature Article)
S. Scheiner
J. Phys. Chem. A **2000** 104 5898-5909

188. Comparison of the CH \cdots N and CH \cdots O Interactions Involving Substituted Alkanes
Y. Gu, T. Kar, S. Scheiner
J. Mol. Struct. **2000** 552 17-31
189. Structure, Stability and Bonding of (BC $_2$ N) $_n$, n=2,3: An Ab Initio Study
T. Kar, M. Cuma, S. Scheiner
J. Mol. Struct. **2000** 556 275-281
190. Strength of the C $^\alpha$ H \cdots O Hydrogen Bond of Amino Acid Residues
S. Scheiner, T. Kar, Y. Gu
J. Biol. Chem. **2001** 276 9832-9837
191. Electronic Structure and Bonding in Metal Phthalocyanines, Metal = Fe, Co, Ni, Cu, Zn, Mg
M.-S. Liao, S. Scheiner
J. Chem. Phys. **2001** 114 9780-9791
192. Proton Conduction by a Chain of Water Molecules in Carbonic Anhydrase
A. Isaev, S. Scheiner
J. Phys. Chem. B **2001** 105 6420-6426
193. Boron-Nitrogen (BN) Substitution Patterns in C/BN Hybrid Fullerenes: C $_{60-2x}$ (BN) $_x$ (x=1-7)
J. Pattanayak, T. Kar, S. Scheiner
J. Phys. Chem. **2001** 105 8376-8384
194. Insertion of Lithium Ions into Carbon Nanotubes: An Ab Initio Study
T. Kar, J. Pattanayak, S. Scheiner
J. Phys. Chem. A **2001** 105 10397-10403
195. Influence of Hybridization and Substitution upon the Properties of the CH \cdots O Hydrogen Bond
S. Scheiner, S. J. Grabowski, T. Kar
J. Phys. Chem. A **2001** 105 10607-10612
196. Analytic function fit of potential energy of proton transfer in N $_2$ H $_7^+$
Rong-Shun Wang, Xiu-Mei Pan, Zhong-Min Su and Steve Scheiner
Huaxue Xuebao **2001** 59 2056-2062
197. Substituent Effects upon Protonation-Induced Red Shift of Phenyl-Pyridine Copolymers
S. Scheiner, T. Kar
J. Phys. Chem. B **2002** 106 534-539
198. Electronic Structure and Bonding in Unligated and Ligated Fe II Porphyrins
M.-S. Liao, S. Scheiner
J. Chem. Phys. **2002** 116 3635-3645

199. Red versus Blue-Shifting Hydrogen Bonds: Are There Fundamental Distinctions?
S. Scheiner, T. Kar
J. Phys. Chem. A **2002** 106 1784-1789.
200. Boron-Nitrogen (BN) Substitution of Fullerenes: C₆₀ to C₁₂B₂₄N₂₄ CBN ball
J. Pattanayak, T. Kar, S. Scheiner
J. Phys. Chem. A **2002** 106 2970-2978
201. Electronic Structure and Bonding in Metal Porphyrins, Metal = Fe, Co, Ni, Cu, Zn
M.-S. Liao, S. Scheiner
J. Chem. Phys. **2002** 117 205-219
202. Acetylene as Potential Hydrogen-Bond Proton Acceptor
S. Scheiner, S. J. Grabowski
J. Mol. Struct. **2002** 615 209-218
203. A Comparative Study of Metal-Porphyrins, -Porphyrazines, and -Phthalocyanines
M.-S. Liao, S. Scheiner
J. Comput. Chem. **2002** 23 1391-1403
204. Comparison of Various Types of Hydrogen Bonds Involving Aromatic Amino Acids
S. Scheiner, T. Kar, J. Pattanayak
J. Am. Chem. Soc. **2002** 124 13257-13264
205. Relativistic Effects in Iron-, Ruthenium-, and Osmium Porphyrins
M.-S. Liao, S. Scheiner
Chem. Phys. **2002** 285 195-206
206. Substituent effects upon protonation-induced red shift of phenyl-pyridine copolymers
S. Scheiner, T. Kar
Polym. Prepr. (Am. Chem. Soc., Div. Polym. Chem.) **2002** 43 50-51
207. Electronic structure and bonding in metal porphyrins and phthalocyanines
S. Scheiner and M.-S. Liao
Polym. Prepr. (Am. Chem. Soc., Div. Polym. Chem.) **2002** 43 96-97
208. β -Substituted Copper Porphyrin Cations: A_{2u} or A_{1u} Radicals?
M.-S. Liao, S. Scheiner
Chem. Phys. Lett. **2003** 367 199-206
209. Performance Assessment of Density-Functional Methods for Study of Charge-Transfer Complexes
M.-S. Liao, Y. Lu, S. Scheiner
J. Comput. Chem. **2003** 24 623-631

210. Comparison of BN and AlN Substitution on the Structure and Properties of C₆₀ Fullerene
J. Pattanayak, T. Kar, S. Scheiner
J. Phys. Chem. A **2003** *107* 4056-4065
211. A DFT/TDDFT Study of Group 4A Metal Porphyrins
M.-S. Liao, S. Scheiner
Mol. Phys. **2003** *101* 1227-1238
212. Comparison between Hydrogen and Dihydrogen Bonds among H₃BNH₃, H₂BNH₂, and NH₃
T. Kar, S. Scheiner
J. Chem. Phys. **2003** *119* 1473-1482
213. Rules for BN-Substitution in BCN-Fullerenes. Separation of BN and C Domains
T. Kar, J. Pattanayak, S. Scheiner
J. Phys. Chem. A **2003** *107* 8630-8637
214. DFT Calculations and Spectral Measurements of Charge-Transfer Complexes Formed by Aromatic Amines and Nitrogen Heterocycles with Tetracyanoethylene and with Chloranil
M.-S. Liao, Y. Lu, V. D. Parker, S. Scheiner
J. Phys. Chem. A **2003** *107* 8939-8948
215. CH··F Hydrogen Bonds. Dimers of Fluoromethanes
E. Kryachko, S. Scheiner
J. Phys. Chem. A **2004** *108* 2527-2535
216. Actinyls in Expanded Porphyrin. A Relativistic Density Functional Study
M.-S. Liao, T. Kar, S. Scheiner
J. Phys. Chem. A **2004** *108* 3056-3063
217. Substitution Patterns in Mono BN-Fullerenes: C_n (n = 20, 24, 28, 32, 36 and 40)
J. Pattanayak, T. Kar, S. Scheiner
J. Phys. Chem. A **2004** *108* 7681-7685
218. Comparison of Cooperativity in CH··O and OH··O Hydrogen Bonds
T. Kar, S. Scheiner
J. Phys. Chem. A **2004** *108* 9161-9168
219. Effects of Peripheral Substituents and Axial Ligands on the Electronic Structure and Properties of Iron Phthalocyanine
M.-S. Liao, T. Kar, S. M. Gorun, S. Scheiner
Inorg. Chem. **2004** *43* 7151-7161
220. Effect of Solvent upon CH··O Hydrogen Bonds with Implications for Protein Folding
S. Scheiner, T. Kar
J. Phys. Chem. B **2005** *109* 3681-3689

221. Stepwise Hydration of Ionized Aromatics. Energies and Structures of the Hydrated Benzene Cation, and the Mechanism of Deprotonation Reactions
Y. Ibrahim, M. Meot-Ner, E. H. Alshraeh, M. S. El-Shall, S. Scheiner
J. Am. Chem. Soc. **2005** *127* 7053-7064
222. Theoretical Investigation of the Weakly Dihydrogen Bonded Complexes FArCCH $\cdot\cdot$ HBeX (X = H, F, Cl, Br)
M. Solimannejad, S. Scheiner
J. Phys. Chem. A (Letter) **2005** *109* 6137-6139
223. Effects of Peripheral Substituents on the Electronic Structure and Properties of Unligated and Ligated Metal Phthalocyanines, Metal = Fe, Co, Zn
M.-S. Liao, J. D. Watts, M.-J. Huang, S. M. Gorun, T. Kar, S. Scheiner
J. Chem. Theory Comp. **2005** *1* 1201-1210
224. Relative Strengths of NH $\cdot\cdot$ O and CH $\cdot\cdot$ O Hydrogen Bonds between Polypeptide Chain Segments
S. Scheiner
J. Phys. Chem. B **2005** *109* 16132-16141
225. Theoretical Investigation of the Dihydrogen Bond Linking MH₂ with HCCRgF (M=Zn,Cd; Rg=Ar,Kr)
M. Solimannejad, S. Scheiner
J. Phys. Chem. A **2005** *109* 11933-11935.
226. Cooperativity of Conventional and Unconventional Hydrogen Bonds involving Imidazole
T. Kar, S. Scheiner
Int. J. Quantum Chem. **2006** *106* 843-851
227. Stabilities and Properties of Complexes Pairing Hydroperoxyl Radical with Monohalomethanes
M. Solimannejad, S. Scheiner
J. Phys. Chem. A **2006** *110* 5948-5951.
228. Weak Hydrogen Bonds in Complexes Pairing Monohalomethanes with Neutral Formic Acid
M. Solimannejad, S. Scheiner
Chem. Phys. Lett. **2006** *424* 1-6
229. Hydrogen Bonding of Radicals: Interaction of Dimethyl Ether with OOH, HOOH, and OOH \cdot
M. Solimannejad, S. Scheiner
Chem. Phys. Lett. **2006** *429* 38-42
230. Contributions of NH $\cdot\cdot$ O and CH $\cdot\cdot$ O H-Bonds to the Stability of β -Sheets in Proteins
S. Scheiner
J. Phys. Chem. B **2006** *110* 18670-18679

231. Theoretical Evidence for a NH··XC Blue Shifting Hydrogen Bond: Complexes Pairing Monohalomethanes with HNO
M. Solimannejad, S. Scheiner
J. Phys. Chem. A **2007** *111* 4431-4435
232. Minimum Energy Pathways for Proton-Transfer between Adjacent Sites Exposed to Water
R. Friedman, S. Fischer, E. Nachliel, S. Scheiner, M. Gutman
J. Phys. Chem. B **2007** *111* 6059-6070
233. Underlying Source of the Relation between Polypeptide Conformation and Strength of NH··O Hydrogen Bonds
S. Scheiner, T. Kar
J. Mol. Struct. **2007** (in press)
234. The Strength with Which a Peptide Group Can Form a Hydrogen Bond Varies with the Internal Conformation of the Polypeptide Chain
S. Scheiner
J. Phys. Chem. B **2007** *111* (in press)
235. Periodicity in Proton Conduction along a H-bonded Chain. Application to Biomolecules
A. Isaev, T. Kar, S. Scheiner
Int. J. Quantum Chem. (in press)
236. Analysis of Complexes Pairing Hydroperoxyl Radical with Peroxyformic Acid
M. Solimannejad, S. Gh. Shirazi, S. Scheiner
J. Phys. Chem. A (in press)
237. Theoretical Investigation of the Mechanism of $\text{LiH} + \text{NH}_3 \rightarrow \text{LiNH}_2 + \text{H}_2$
T. Kar, S. Scheiner, L. Li
Chem. Phys. Lett. (submitted)
238. Analysis of Catalytic Mechanism of Serine Proteases. Viability of Ring-Flip Hypothesis
S. Scheiner
Biochem. (submitted)
239. Bonding Rearrangements of Hydrogen Bonded Complexes involving Alkynes
E. S. Kryachko, S. Scheiner
J. Phys. Chem. A (submitted)
240. Structure and Properties of Perfluoroalkylated Phthalocyanines. A Theoretical Study
M.S. Liao, J. D. Watts, M.-J. Huang, S. M. Gorun, S. Scheiner
(in preparation)