

List of Publications by Wolfram Koch

1984

1. Francis Maquin, Daniel Stahl, Andrzej Sawaryn, Paul v.R. Schleyer, Wolfram Koch, Gernot Frenking, and Helmut Schwarz: "**Experimental and Theoretical Studies of the Charge Stripping from CH_3X^+ and CH_2XH^+ Ions**", *J. Chem. Soc., Chem. Commun.*, 504 (1984).
2. Wolfram Koch, Gernot Frenking, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Theoretical and Experimental Studies on the Tetrafluoroethylene Dication**", *J. Chem. Soc., Chem. Commun.*, 1187 (1984).
3. Gernot Frenking, Nikolaus Heinrich, Wolfram Koch, and Helmut Schwarz: "**On the Origin of the Different Activation Energies for Hydrogen Additions at the C and O Centers of R-CO^+ Ions**", *Chem. Phys. Lett.*, **105**, 490 (1984).
4. Gernot Frenking and Wolfram Koch: "**Neutral and Cationic HOF Structures**", *Chem. Phys. Lett.*, **105**, 659 (1984).
5. Wolfram Koch, Gernot Frenking, and Helmut Schwarz: "**On the Barrier and Nature of [1,2]-Hydrogen Migrations in HCN/HNC and Their Cation Radicals**", *Naturwissenschaften*, **71**, 473 (1984).
6. Wolfram Koch, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Experimental and Theoretical Evidence for a Stable Ketene Dication in the Gas Phase**", *J. Chem. Soc., Chem. Commun.*, 1679 (1984).
7. Gernot Frenking and Wolfram Koch: "**Structures and Stabilities of Ion/Dipole Complexes**", *J. Mol. Struct. THEOCHEM*, **110**, 49 (1984).

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8. Gernot Frenking, Wolfram Koch, Michael Schaale, and Hans Baumgärtel: "**The Unimolecular Decay of Difluoroethylene Cations. An Experimental and Quantum Chemical Study**", *Int. J. Mass Spectrom. Ion Proc.*, **61**, 305 (1985).
9. Wolfram Koch, Gernot Frenking, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Theoretical and Experimental Studies on the Ground State Potential Energy Surface of the $\text{C}_2\text{H}_4\text{O}_2^{2+}$ Dications**", *Int. J. Mass Spectrom. Ion Proc.*, **63**, 59 (1985).
10. C. Guenat, F. Maquin, D. Stahl, W. Koch, and H. Schwarz: "**Experimental and *ab initio* Molecular Orbital Studies on CCl_4^{2+} Dications**", *Int. J. Mass Spectrom. Ion Proc.*, **63**, 265 (1985).
11. Wolfram Koch and Helmut Schwarz: "**Structures and Stabilities of $\text{C}_6\text{H}_6^{3+}$ Isomers. An *ab initio* Molecular Orbital Study**", *Chem. Phys. Lett.*, **113**, 145 (1985).
12. Wolfram Koch and Gernot Frenking: " **CF^{2+} and CF_2^{2+} : Two Unusually Stable Dications with Carbon-Fluorine Double Bonding**", *Chem. Phys. Lett.*, **114**, 178 (1985).
13. Gernot Frenking, Wolfram Koch, Michael Schaale: "***Ab initio* Investigation of the Potential Energy Surface of $\text{C}_2\text{H}_2\text{F}_2$ and $\text{C}_2\text{H}_2\text{F}_2^+$** ", *J. Comput. Chem.*, **6**, 189 (1985).

14. Wolfram Koch, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Experimental and *ab initio* Molecular Orbital Studies on CH₃O²⁺ Dications**", *J. Am. Chem. Soc.*, **107**, 2256 (1985).
15. Wolfram Koch, Gernot Frenking, and Helmut Schwarz: "**The Structures and Energies of SiH_n²⁺ Dications (n=1-5)**", *J. Chem. Soc., Chem. Commun.*, 1119 (1985).
16. Wolfram Koch, Helmut Schwarz, Francis Maquin, and Daniel Stahl: "**On the Formation of Doubly Charged Cation Radical from Acetyl and 1-Hydroxy Cations in the Gas Phase**", *Int. J. Mass Spectrom. Ion Proc.*, **67**, 171 (1985).
17. Eugen Illenberger, Paul B. Comita, John.I. Braumann, Heinz P. Fenzlaff, Martin Heni, Nikolaus Heinrich, Wolfram Koch, and Gernot Frenking: "**Experimental and Theoretical Investigation of the Azide Anion in the Gas Phase**", *Ber. Bunsenges. Phys. Chem.*, **89**, 1026 (1985).
18. Wolfram Koch, Nikolaus Heinrich, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Combined Experimental and *ab initio* Molecular Orbital Studies on Gaseous OH_n²⁺ Species (n=1-4)**", *Int. J. Mass Spectrom. Ion Proc.*, **67**, 305 (1985).
19. Wolfram Koch, Francis Maquin, Daniel Stahl, and Helmut Schwarz: "**Gaseous Organic Dications: Species with Remarkable Properties**", *Chimia*, **39**, 376 (1985).

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20. Nikolaus Heinrich, Wolfram Koch, and Gernot Frenking: "**On the Use of Koopmans' Theorem to Estimate Negative Electron Affinities**", *Chem. Phys. Lett.*, **124**, 20 (1986).
21. Wolfram Koch and Helmut Schwarz: "**The NH_n²⁺ Dications. A Theoretical Investigation**", *Int. J. Mass Spectrom. Ion Proc.*, **68**, 49 (1986).
22. Wolfram Koch, Gernot Frenking, and Christian C. Chang: "**Theoretical Investigations of Small, Multiply Charged Cations. I SiH²⁺**", *J. Chem. Phys.*, **84**, 2703 (1986).
23. Gernot Frenking and Wolfram Koch: "**A Møller-Plesset Study of the Electron Affinities of the Diatomic Hydrides XH (X=Li, Be, B, C, N, O, F)**", *J. Chem. Phys.*, **84**, 3224 (1986).
24. Nikolaus Heinrich, Gernot Frenking, Wolfram Koch, and Helmut Schwarz: "**Substituent Effects on Neutral and Ionized C-C and C-O Double Bonds and Their Implications for the Stability Order of Keto/Enol Tautomers**", *J. Am. Chem. Soc.*, **108**, 593 (1986).
25. Wolfram Koch and Helmut Schwarz: "***Ab initio* Molecular Orbital Studies on CH₂O₂²⁺ Isomers**", *Chem. Phys. Lett.*, **125**, 443 (1986).
26. Herman Halim, Nikolaus Heinrich, Wolfram Koch, Jochen Schmidt, and Gernot Frenking: "**MINDO/3 and MNDO Calculations of Closed and Open Shell Cations**", *J. Comput. Chem.*, **7**, 93 (1986).
27. Wolfram Koch, Gernot Frenking, Helmut Schwarz, Francis Maquin, and Daniel Stahl: "**Experimental and Theoretical Studies on SiH_n²⁺ Dications (n=1-5)**", *J. Chem. Soc., Perkin II*, 757 (1986).

28. Gernot Frenking, Wolfram Koch, and Helmut Schwarz: "**Theoretical Investigations of Fluorine Substituted Ethene Dications**", *J. Comput. Chem.*, **7**, 406 (1986).
29. Wolfram Koch, Nikolaus Heinrich, and Helmut Schwarz: "**Ab initio Molecular Orbital Study of the CNH_3^{2+} Potential Energy Surface**", *J. Am. Chem. Soc.*, **108**, 5400 (1986).
30. Wolfram Koch and Gernot Frenking: "**Hydrogen Substitution by He^+ : Theoretical Investigations on the Structure and Stabilities of He_2O^{2+} , He_2N^{2+} , and HeC_2^{2+}** ", *J. Chem. Soc., Chem. Commun.*, 1095 (1986).
31. Wolfram Koch, Gernot Frenking, Jürgen Gauss, and Dieter Cremer: "**Donor-Acceptor Interaction and the Peculiar Structures of Dications**", *J. Am. Chem. Soc.*, **108**, 5505 (1986).
32. Wolfram Koch, Gernot Frenking, Dieter Cremer, Jürgen Gauss, Andrzej Sawaryn, and Paul v.R. Schleyer: "**Structures, Stabilities and Bonding in C_2Be , CBe_2 , and C_2Be_2** ", *J. Am. Chem. Soc.*, **108**, 5732 (1986).
33. Thomas Drewello, Wolfram Koch, Helmut Schwarz, and Daniel Stahl: "**The CCl_4^{2+} Dication Revisited**", *Int J. Mass Spectrom. Ion Proc.*, **72**, 313 (1986).
34. Ben van Baar, Wolfram Koch, Carlito B. Lebrilla, Johan K. Terlouw, Thomas Weiske, and Helmut Schwarz: "**Aminoacetylene and its Radical Cation - Identification of Potentially Interstellar Molecules**", *Angew. Chem.*, **98**, 834 (1986); *Angew. Chem. Int. Ed. Engl.*, **25**, 827 (1986).
35. Einar Uggerud, Wolfram Koch, and Helmut Schwarz: "**A Quantum Chemical Investigation of the Unimolecular Chemistry of Formic Acid Radical Cation and Some of its Isomers**", *Int J. Mass Spectrom. Ion Proc.*, **73**, 187 (1986).
36. Wolfram Koch and Gernot Frenking: "**Theoretical Predictions of Metastable Ions with Short Carbon-Helium Bonds**", *Int J. Mass Spectrom. Ion Proc.*, **74**, 133 (1986).
37. Wolfram Koch, Jack Collins, and Gernot Frenking: "**Are There Neutral Helium Compounds Which are Stable in Their Ground States? A Theoretical Investigation of HeBCH and HeBeO** ", *Chem. Phys. Lett.*, **132**, 330 (1986).
38. Bernd Giese, Nikolaus Heinrich, Hans Horler, Wolfram Koch, and Helmut Schwarz: "**Experimental and Theoretical Studies of the Mechanism of 1,2-Migration of Vinyl and Formyl Substituents in Free Radicals**", *Chem. Ber.*, **119**, 3528 (1986).

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39. Wolfram Koch and Gernot Frenking: "**Theoretical Investigations of the Structures and Electron Affinities of NCO, NCS Isomers, CH_2N , and CHNH** ", *J. Phys. Chem.*, **91**, 49 (1986).
40. Wolfram Koch and Helmut Schwarz: "**Experimental and Theoretical Studies of Small Organic Dications, Molecules with Remarkable Properties**", in *Structure/Reactivity and Thermochemistry of Ions*, S.G. Lias and P. Ausloos (eds.), D. Reidel, Dordrecht (1987).
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43. Wolfram Koch and Gernot Frenking: **"Theoretical Investigations of Small, Multiply Charged Cations. II CNe^{n+} ($n=1-4$)"**, *J. Chem. Phys.*, **86**, 5617 (1987).
44. Gernot Frenking and Wolfram Koch: **"The Singlet-Triplet Splitting of the Low-Lying Electronic States H_2O^{2+} and a Comparison with Isoelectronic CH_2 and CHe_2^{2+} "**, *Chem. Phys. Lett.*, **138**, 503 (1987).
45. Wolfram Koch, Gernot Frenking, and Brian T. Luke: **"Theoretical Investigations of the Low-Lying Electronic States of the HeC^{2+} Dication"**, *Chem. Phys. Lett.*, **139**, 149 (1987).
46. Wolfram Koch, Gernot Frenking, Jürgen Gauss, Dieter Cremer, and Jack R. Collins: **"Helium-Organic Chemistry: Theoretical Predictions and Experimental Challenge"**, *J. Am. Chem. Soc.*, **109**, 5917 (1987).
47. Wolfram Koch, Bowen Liu, Thomas Weiske, Carlito B. Lebrilla, Thomas Drewello, and Helmut Schwarz: **"The CH^{2+} Dication. Metastable or Not? A Combined Theoretical and Experimental Investigation"**, *Chem. Phys. Lett.*, **142**, 147 (1987).
48. Paul v.R. Schleyer, T. William Bentley, Wolfram Koch, Alexander J. Kos, and Helmut Schwarz: **"Structures and Energies of Isomeric Cyclopentenyl Cations. Resolution of the Question of Anchimeric Assistance in Cyclopenten-4-yl Solvolysis"**, *J. Am. Chem. Soc.*, **109**, 6953 (1987).

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50. Nikolaus Heinrich, Wolfram Koch, Charles J. Morrow, and Helmut Schwarz: **"A Theoretical Study of the Reaction of Ketene Radical Cation with Ethylene: Stepwise versus Concerted 2+1 Cycloaddition"**, *J. Am. Chem. Soc.*, **110**, 6332 (1988).
51. Wolfram Koch, Bowen Liu, and Douglas J. DeFrees: **"The C_4H_7^+ Cation. A Theoretical Investigation"**, *J. Am. Chem. Soc.*, **110**, 7325 (1988).
52. Gernot Frenking, Wolfram Koch, and Jack R. Collins: **"Fixation of N_2 and CO by BeO . A Theoretical Investigation of the Structures and the Stabilities of NNBeO , OCBeO and COBeO "**, *J. Chem. Soc., Chem. Commun.*, 1147 (1988).
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55. Wolfram Koch, Bowen Liu, Douglas J. DeFrees: "**Structure of the 2-Norbornyl Cation**", *J. Am. Chem. Soc.*, **111**, 1527 (1989).
56. Wolfram Koch: "**Structure, Stability and Vibrational Spectrum of HCNKrF⁺**", *J. Chem. Soc., Chem. Commun.*, 215 (1989).
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69. Carol A. Deakyne, Joel F. Liebman, Gernot Frenking, and Wolfram Koch: "**A Comparative Study of Isoelectronic and Isogyric Reactions: Molecular Orbital Calculations of Diatomic Hydrides and Halides**", *J. Phys. Chem.*, **94**, 2306 (1990).
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