

Publications

- 70 T_1 , T_1 state energies and electron affinities of small α,ω -diphenylpolyenes investigated by anion photodetachment photoelectron spectroscopy and excited state theory.
F. Vogeler, S. Siegert, C.M. Marian, R. Weinkauff, Chem. Phys. Chem. 12 (2011) 1948-1956
- 69 Direct access to the dipole-forbidden $n\pi^*$ T_1 state of p-benzoquinone by photodetachment photoelectron spectroscopy
S. Siegert, F. Vogeler, R. Weinkauff, Z. Phys. Chem. 225 (2011) 507
- 68 Throwing light on dark states of α -oligothiophenes of chain lengths 2 to 6: radical anion photoelectron spectroscopy and excited state theory.
S. Siegert, F. Vogeler, C.M. Marian, R. Weinkauff, Phys. Chem. Chem. Phys. 13, (2011) 10350-10363
- 67 Rotationally resolved electronic spectroscopy of 5-methoxyindole, Ch. Brand, O. Oeltermann, D. Pratt, R. Weinkauff, W. L. Meerts, W. van der Zande, K. Kleinermanns, M. Schmitt, J. Chem. Phys. 133 (2010) 024303.
- 66 Direct spectroscopy of contact charge transfer states: Possible consequences for tryptophan excited-state deactivation pathways by O_2 and formation of reactive oxygen species. S. Siegert, F. Vogeler, J. Schiedt, R. Weinkauff, Phys. Chem. Chem. Phys. 12 (2010) 4996-5006.
- 65 The Conformational Landscape of 5-Methoxytryptamine Studied by Rotationally Resolved Fluorescence Spectroscopy and Resonant Ionization Spectroscopy.
T.B. Chau Vu, I. Kalkman, W.L. Meerts, C. Brand, Y.N. Svartsov, S. Wiedemann, R. Weinkauff, M. Schmitt, Phys. Chem. Chem. Phys. 11 (2009) 2433-2440.
64. Excited States of Thiophene: Ring Opening as Deactivation Mechanism.
S. Salzmann, M. Kleinschmidt, R. Weinkauff, C.M. Marian, Phys. Chem. Chem. Phys. 10 (2008) 380.
63. Ultrafast Dynamics in Thiophene Investigated by Femtosecond Pump Probe Photoelectron Spectroscopy and Theory.
R. Weinkauff, L. Lehr, E.W. Schlag, R. Weinkauff, S. Salzmann, C.M. Marian Phys. Chem. Chem. Phys. 10 (2008) 393.
- 62 Anion Photoelectron Imaging of Deprotonated Thymine and Cytosine
B.F. Parsons, S.M. Sheehan, T.A. Yen, D.M. Neumark, N. Wehres, R. Weinkauff Phys. Chem. Chem. Phys. 9 (2007) 3291.
- 61 Comparison of Photoelectron-Spectroscopy Results to *ab initio* and Density Functional Calculations: The Ethylbenzene Cation.
F. Lehrer, R. Weinkauff, A. Metsala. Z. Phys. Chem. 221 (2007) 723.

- 60 **Charge Distribution in 3'-Deoxythymidine - Fullerene: Mass Spectrometry, Laser Excitation and Computational Studies.**
J.-F. Greisch, R. Weinkauff, E. DePauw, E. S. Kryachko, F. Remacle
Isr. J. Chem. 47 (2007) 25.
- 59 Excited State Dynamics of Protonated and Isolated Adenine.
D. Nolting, Th. Schultz, I.V. Hertel, R. Weinkauff, Chem. Phys. Chem. 8 (2007) 751.
- 58 Double Resonance Spectroscopy of Different Conformers of the Neurotransmitter Amphetamine and its Clusters with Water.
R. Brause, H. Fricke, M. Gerhards, R. Weinkauff, K. Kleinermanns, J. Phys. Chem. 327 (2006) 43.
- 57 Excited state dynamics and fragmentation channels of the protonated dipeptide H₂N-Leu-Trp-COOH
D. Nolting, Th. Schultz, I.V. Hertel, R. Weinkauff, Phys. Chem. Chem. Phys. 8 (2006) 5247.
- 56 Dissociation Kinetics of Peptide Ions
E.W. Schlag, H.L. Selzle, P. Schanen, R. Weinkauff, R.D. Levine J. Phys. Chem. A 110 (2006) 8497.
- 55 **Molecule-Based Photonically-Switched Half and Full Adder.**
F. Remacle, R. Weinkauff, R. D. Levine, J. Phys. Chem. A, 110 (2006) 177.
- 54 The Electronic Spectrum of Protonated Adenine: Theory and Experiment.
C. Marian, D. Nolting, R. Weinkauff, Phys. Chem. Chem. Phys. 7 (2005) 3306.
- 53 Fs Dynamics after Local Photoionization: 2-Phenylethyl-N,N-dimethylamine as a Model System for Non-Resonant Downhill Charge Transfer in Peptides.
L. Lehr, T. Horneff, R. Weinkauff, E.W. Schlag, J. Phys. Chem. A 109 (2005) 8074.
- 52 Control of Local Ionization and Charge Transfer in the Bifunctional Molecule 2-Phenyl-N,N-dimethylamine Using Rydberg Fingerprint Spectroscopy.
W. Cheng, N. Kuthirummal, J.L. Gosselin, T. I. Sølling, R. Weinkauff, P.M. Weber, J. Phys. Chem. A 109 (2005) 1920.
- 51 Protonation Effect on the Electronic Spectrum of Tryptophan in the Gas Phase
D. Nolting, Ch. Marian, R. Weinkauff, Phys. Chem. Chem. Phys. 6 (2004) 2633.
- 50 The Dipeptide Cyclic(Glycyltryptophanyl) in the Gas Phase: A concerted Action of Density functional Calculations, S₀-S₁- Two-photon Ionization, Spectral UV/UV Hole Burning and Laser Photoelectron Spectroscopy.
S. Wiedemann, A. Metsala, D. Nolting, R. Weinkauff, Phys. Chem. Chem. Phys. 6 (2004) 641.
49. Local Ionization in 2-Phenylethyl-N,N-dimethylamine: Dissociation Directly After Ionization
R. Weinkauff, L. Lehr, A. Metsala, J. Phys. Chem. A 107 (2003) 2787.

48. Molecular Physics of Building Blocks of Life under Isolated or Defined Conditions
R. Weinkauff, J-P. Schermann, M.S. de Vries, K. Kleinermanns, Eur. Phys. J. D 20 (2002) 309
47. Molecular Logic Machines by Optical Spectroscopy and Charge Migration Along a Molecular Wire Realized as a Peptide.
F. Remacle, R. Weinkauff, D. Steinitz, K.L. Kompa, R.D. Levine, Chem. Phys. 281 (2002) 363.
46. Microsolvation of Small Anions by Aromatic Molecules: An Exploratory Study.
K. Le Barbu, J. Schiedt, R. Weinkauff, E.W. Schlag, J.M. Nilles, S.-J. Xu, O.C. Thomas, K.H. Bowen, J. Chem Phys. 116 (2002) 9663.
45. Comment on "Iodine Effect on the Relaxation Pathway of Photoexcited Iodide-(Water)_n Anion Clusters.
A.V. Davis, M.T. Zanni, R. Weinkauff, D. Neumark, Chem. Phys. Lett. 353 (2002) 455.
44. Separation of Neutral Versus Cation Dissociation Processes in an Ultracompact double Time-of-Flight Spectrometer: First Results on CH₃I.
L. Lehr, R. Weinkauff, E.W. Schlag, Int. J. Mass Spectrom. 206 (2001) 191.
43. Microsolvation of Similar-sized Aromatic Molecules: Photoelectron Spectroscopy of Bithiophene-, Azulene, and Naphthalene-Water Anion Clusters.
J. Schiedt, W.J. Knott, K. LeBarbu, R. Weinkauff, E.W. Schlag, J. Chem. Phys. 113 (2000) 9470.
42. Investigation of Charge Localization and Charge Delocalization in Model Molecules by Multiphoton Ionization Photoelectron Spectroscopy and DFT Calculations.
R. Weinkauff, F. Lehrer, E.W. Schlag, A. Metsala, Faraday Discuss, 115 (2000) 363.
41. Electronic Control of Site Selective Reactivity: A Model Combining Charge Migration and Dissociation.
F. Remacle, R.D. Levine, E.W. Schlag, R. Weinkauff, J. Phys. Chem. A 103 (1999) 10149.
40. Efficient and Robust Anion Source Based on a Micro-Cannel Plate Electron Gun.
J. Schiedt, R. Weinkauff, Rev. Sci. Instrum. 70 (1999) 1.
39. Electron Solvation Dynamics in Finite Systems: A Femtosecond Study of Iodide-(Water)_n Anion Clusters.
L. Lehr, M.T. Zanni, B.J. Greenblatt, R. Weinkauff, D.M. Neumark, Science 284 (1999) 635.
38. Size Dependence of Triplet and Singlet States of α -Oligothiophenes.
S. Rentsch, J.P. Yang, W. Paa, E. Birkner, J. Schiedt, R. Weinkauff, Phys. Chem. chem. Phys. 1 (1999) 1707.
37. Resonant Photodetachment via Shape and Feshbach Resonances: P-Benzoquinone

- Anions as a Model System.
J. Schiedt and R. Weinkauff, *J. Chem. Phys.*, 110 (1999) 304.
36. Anion Spectroscopy of Uracil, Thymine and the Amino-Oxo and the Amino-Hydroxy Tautomers of Cytosine and their Water Clusters.
J. Schiedt, R. Weinkauff, D.M. Neumark, E.W. Schlag, *Chem. Phys.* 239 (1998) 511.
 35. Dynamics of Charge-Transfer-to-Solvent Precursor States in $I(D_2O)_n$ Clusters.
M.T. Zanni, L. Lehr, B.J. Greenblatt, R. Weinkauff, D.M. Neumark, in *Ultrafast Phenomena XI*, Eds: T. Elsaesser, J.G. Fujimoto, D.A. Wiersma, W. Zinth, Springer Verlag, Berlin (1998) 474.
 34. Charge Transfer and Charge Localization in Extended Radical Cations: Investigation of Model Molecules for Peptides.
R. Weinkauff, F. Lehrer, in: *Resonance Ionization Spectroscopy*, Eds.: J. C. Vickerman, I. Lyon, N.P. Lockyer, J.E. Parks, The American Institute of Physics, Bristol (1998), 117
 33. Spectroscopy of Carbendazim in the UV Region by Resonant Multiphoton Ionization.
B. Bescos, J. M. Orea, C. Montero, A. G. Urena, R. Weinkauff, U. Boesl, E.W. Schlag, *Chem. Phys. Lett.*, 287 (1998) 371
 32. Dynamical Principles in Biological Processes.
E.W. Schlag, S.H. Lin, R. Weinkauff, P.M. Rentzepis, *Proc. Natl. Acad. Sci. USA* 95 (1998) 1358
 31. Nonstationary Electronic States and Site-Selective Reactivity.
R. Weinkauff, E. W. Schlag, T. J. Martinez, and R. D. Levine, *J. Phys. Chem. A* 101 (1997), 7702
 30. Energetics of Photoinduced Electron Transfer in the Indole $\square O_2$ Cluster in Gas Phase: Possible Consequences for Photoexcited Tryptophan in Solution.
R. Weinkauff, J. Schiedt, *Photochem. Photobiol.* 66 (1997), 569
 29. Photodetachment Photoelectron Spectroscopy of Perylene and CS_2 : Two Extreme Cases.
J. Schiedt, R. Weinkauff, *Chem. Phys. Lett.* 274 (1997), 18
 28. Efficient Cationization by Cs^+ Adduct Ion Formation in a Supersonic Beam.
P. Schanen, D. Yang, R. Weinkauff, and E. W. Schlag, *Int. J. Mass Spectrom. Ion Processes* 167/168 (1997) 447
 27. Peptides and Biological Relevant Molecules in the Gas Phase.
R. Weinkauff, *International Symposium on Molecular Beams, Conf. Ser. XVII* (1997), 67
 26. Verfahren und Vorrichtung zum Quasi-Ionisieren von Probenmolekülen in der Gasphase.
R. Weinkauff, P. Schanen, and E. W. Schlag; Deutsches Patent, angenommen am 14.02. 1997
 25. Time Multiplexing: A New Single Shot Femtosecond Pump-Probe Technique.
R. Weinkauff, L. Lehr, D. Georgiev, and E. W. Schlag, *Appl. Phys. B* 64 (1997) 515

24. Photodetachment Photoelectron Spectroscopy of Mass Selected Anions: Anthracene and the Anthracene-H₂O Cluster.
J. Schiedt and R. Weinkauf, Chem. Phys. Lett. 266 (1997), 201
23. Highly Efficient Charge Transfer in Peptide Cations in the Gas Phase: Threshold Effects and Mechanism.
R. Weinkauf, P. Schanen, A. Metsala, E. W. Schlag, M. Bürgle and H. Kessler
J. Phys. Chem. 100 (1996), 18567
22. Elementary Processes in Peptides: Electron Mobility and Dissociation in Peptide Cations in the Gas Phase.
R. Weinkauf, P. Schanen, D. Yang, S. Soukara, and E. W. Schlag, J. Phys. Chem. 99 (1995), 11255
21. Spin-Orbit Coupling in the O₂⁻ Anion.
J. Schiedt and R. Weinkauf, Z. Naturforsch. 50a (1995), 1041
20. Laser Spectroscopy of Molecular Ions: The A-X Transition of the Acetylene Radical Cation.
Ch. Cha, R. Weinkauf, and U Boesl, J. Chem. Phys. 103 (1995), 5224
19. Femtosecond versus Nanosecond Multiphoton Ionization and Dissociation of Large Molecules.
R. Weinkauf, P. Aicher, G. Wesley, J. Grotemeyer, and E. W. Schlag, J. Phys. Chem. 98 (1994), 8381
18. Laser Spectroscopy of Molecular Ions: The A-X Transition in the OCS Radical Cation.
R. Weinkauf and U. Boesl, J. Chem. Phys. 101 (1994), 8482

17. Laser Ion Sources for Time-of-Flight Mass Spectrometry.
U. Boesl, R. Weinkauff, C. Weickhardt, and E. W. Schlag, *J. Int. Mass Spectrom. Ion Processes*, 131 (1994), 87
16. Rydberg Spectroscopy of OCS: New Assignments in the 70 000- 74 000 cm⁻¹ Energy Region.
R. Weinkauff and U. Boesl, *J. Chem. Phys.* 98 (1993), 4459
15. Reflectron Time-of-Flight Mass Spectrometry and Laser Excitation for the Analysis of Neutrals, Ionized Molecules and Secondary Fragments.
U. Boesl, R. Weinkauff, and E. W. Schlag, *Int. J. Mass Spectrom. Ion Processes* 112 (1992), 121
14. Spectroscopy of Molecular Ions Prepared by Resonant Multiphoton Ionization: The OCS⁺ Ion.
R. Weinkauff, and U. Boesl, in: "Resonance Ionization Spectroscopy" Conf. Ser. 114, ed.: J. E. Parks, N. Omenetto, Institute of Physics, Bristol (1991), 181
13. Laser Tandem Mass Spectrometer with Two Lasers in a Reflectron Time-of-Flight Analyzer.
C. Weickhardt, R. Weinkauff, K. Walter, U. Boesl, in: "Resonance Ionization Spectroscopy" Conf. Ser. 114, ed.: J. E. Parks, N. Omenetto, Institute of Physics, Bristol (1991), 169
12. MS-MS Time-of-Flight Mass Spectrometer.
United States Patent 6,032,722, date of patent: July 16 (1991)
U. Boesl, R. Weinkauff, K. Walter, and E. W. Schlag
11. Multiphoton Dissociation of Organic Molecules: Step by Step Investigation with Laser Tandem Mass Spectrometry.
U. Boesl, R. Weinkauff, K. Walter, C. Weickhardt, and E. W. Schlag, *Ber. Bunsenges. Phys. Chem.* 94 (1990), 1357-1362
10. Tandem Time-of-Flight Techniques and Multiphoton Mass Spectrometry: The Ladder Switching in Benzene.
U. Boesl, R. Weinkauff, K. Walter, C. Weickhardt, and E. W. Schlag, *J. Phys. Chem.* 94 (1990), 8567-8573
9. Tandem Massenspektroskopie im Flugzeit-Massenspektrometer.
U. Boesl, R. Weinkauff, K. Walter, E. W. Schlag
Deutsches Patent, Nr.: DE3920566 CS, eingereicht am 23.06.89, erteilt am 01.04.93
8. Laser Tandem Mass Spectrometry in a Time-of-Flight Instrument.
R. Weinkauff, K. Walter, C. Weickhardt, U. Boesl, and E. W. Schlag, *Z. Naturforsch.* 44a (1989), 1219

7. Resonant Enhanced Multiphoton Dissociation Spectroscopy of Molecular Ions: Technique and Application to $\text{CH}_3\text{I}^+/\text{CD}_3\text{I}^+$.
U. Boesl, R. Weinkauff, K. Walter, *Advances in Laser Science IV*, ed.: J. L. Gole, D. F. Heller, M. Lapp. W. C. Stwalley, American Institute of Physics, New York (1989), 488
6. Spectroscopy of the Benzene Cation: Resonance-Enhanced Multiphoton Dissociation Spectra of the $\text{B}(\text{E}_{2g})\text{-X}(\text{E}_{1g})$ Transition.
K. Walter, R. Weinkauff, U. Boesl, and E. W. Schlag, *Chem. Phys. Lett.* 155 (1989), 8
5. Molecular Ion Spectroscopy: Mass Selected, Resonant Two-Photon Dissociation Spectra of CH_3I^+ and CD_3I^+ .
K. Walter, R. Weinkauff, U. Boesl, and E. W. Schlag, *J. Chem. Phys.* 89 (1988) 1914
4. Mass-Selected Molecular Ion Spectra: (1+1)-Photodissociation Spectroscopy of CH_3I^+ and CD_3I^+ .
R. Weinkauff, K. Walter, U. Boesl, and E. W. Schlag, *Chem. Phys. Lett.* 141 (1987), 267
3. High-Resolution Laser Mass Spectrometry.
H. J. Neusser, U. Boesl, R. Weinkauff, and E. W. Schlag, *Int. J. Mass Spectrom. Ion Processes* 60 (1984), 147
2. Multiphoton Mass Spectrometry: Metastables.
H. Kühlewind, U. Boesl, R. Weinkauff, H. J. Neusser, and E. W. Schlag, *Laser Chem.* 3 (1983), 3
1. Multiphoton Mass Spectrometry of Metastables: Direct Observation of Decay in a High-Resolution Time-of-Flight Instrument.
U. Boesl, H. J. Neusser, R. Weinkauff, and E. W. Schlag, *J. Phys. Chem.* 86 (1982), 4857