Klaus MÃ¼ller-Dethlefs

List of Publications by Year
in descending order

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85 papers	5,061 citations	136950 32 h-index	88630 70 g-index
91 all docs	91 docs citations	91 times ranked	3131 citing authors

#	Article	IF	Citations
1	An improved experimental scheme for simultaneous measurement of high-resolution zero electron kinetic energy (ZEKE) photoelectron and threshold photoion (MATI) spectra. Chemical Physics Letters, 2017, 685, 477-481.	2.6	2
2	Threshold ionization spectroscopic investigation of supersonic jet-cooled, laser-desorbed Tryptophan. Chemical Physics Letters, 2016, 657, 142-147.	2.6	1
3	Binding Energies of the Ï€-Stacked Anisole Dimer: New Molecular Beam-Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6637-6637.	3.3	3
4	Mass analyzed threshold ionization detected infrared spectroscopy: isomerization activity of the phenolâ€“Ar cluster near the ionization threshold. Physical Chemistry Chemical Physics, 2015, 17, 2494-2503.	2.8	12
5	Binding Energies of the Ï€â€Stacked Anisole Dimer: New Molecular Beamâ€”Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6740-6746.	3.3	18
6	Structure and energetics of the anisoleâ€“Ar_n (n = 1, 2, 3) complexes: high-resolution resonant two-photon and threshold ionization experiments, and quantum chemical calculations. Physical Chemistry Chemical Physics, 2015, 17, 12530-12537.	2.8	8
7	Ionization-induced Ï€ â†' H site-switching in phenolâ€“CH₄complexes studied using IR dip spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 110-116.	2.8	13
8	Spectral shifts and structures of phenolâ‹¯Arn clusters. Physical Chemistry Chemical Physics, 2011, 13, 6077.	2.8	9
9	A novel experimental system of high stability and lifetime for the laser-desorption of biomolecules. Review of Scientific Instruments, 2010, 81, 063101.	1.3	6
10	Dissociation energetics of the phenol+â‹¯Ar2 cluster ion: The role of Ï€â†'H isomerization. Journal of Chemical Physics, 2010, 133, 154308.	3.0	42
11	Fragmentation Energetics of the Phenol⁺Â·Â·Â·Ar₃ Cation Cluster. Journal of Physical Chemistry A, 2010, 114, 11139-11143.	2.5	17
12	Rotational Analysis for the Doppler-Free Photoelectron Spectrum of Water Using the Spectator Modelâ€. Journal of Physical Chemistry A, 2010, 114, 11133-11138.	2.5	5
13	The structure of phenol-Arnâ€ˆ(n=1,2) clusters in their S and S1 states. Journal of Chemical Physics, 2009, 130, 224303.	3.0	38
14	Competition between stacking and hydrogen bonding: theoretical study of the phenolâ‹¯Ar cation and neutral complex and comparison to experiment. Physical Chemistry Chemical Physics, 2008, 10, 2780.	2.8	26
15	State of the art theoretical study and comparison to experiment for the phenolâ‹¯argon complex. Journal of Chemical Physics, 2008, 128, 114319.	3.0	33
16	Effect of Noncovalent Interactions on the n-ButylbenzeneÂ·Â·Â·Ar Cluster Studied by Mass Analyzed Threshold Ionization Spectroscopy and ab initio Computations. Journal of Physical Chemistry A, 2008, 112, 5872-5877.	2.5	2
17	Effect of Noncovalent Interactions on Conformers of the n-Butylbenzene Monomer Studied by Mass Analyzed Threshold Ionization Spectroscopy and Basis-set Convergent ab initio Computations. Journal of Physical Chemistry A, 2008, 112, 5866-5871.	2.5	14
18	IR signature of the photoionization-induced hydrophobicâ†'hydrophilic site switching in phenol-Arn clusters. Journal of Chemical Physics, 2007, 127, 114307.	3.0	58

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19	Hole-Burning Spectra of Phenolâ^'Arn(n= 1, 2) Clusters:Â Resolution of the Isomer Issueâ€. Journal of Physical Chemistry A, 2007, 111, 7569-7575.	2.5	40
20	Multidimensional Franck-Condon simulations of photodetachment spectra for the formate-water cluster anion: Investigating H atom transfer along the HCOOH+OH reaction coordinate. Journal of Chemical Physics, 2007, 127, 234308.	3.0	2
21	Zeke Spectroscopy: High-Resolution Spectroscopy with Photoelectrons. Advances in Chemical Physics, 2007, , 1-104.	0.3	25
22	The World of Non-Covalent Interactions: 2006. Collection of Czechoslovak Chemical Communications, 2006, 71, 443-531.	1.0	184
23	Excited-State Ab Initio Calculations and Multidimensional Franckâ^'Condon Simulations on Guanine. Journal of Physical Chemistry A, 2006, 110, 13045-13057.	2.5	24
24	The Use of Multidimensional Franckâ^'Condon Simulations to Assess Model Chemistries:Â A Case Study on Phenol. Journal of Physical Chemistry A, 2006, 110, 4657-4667.	2.5	68
25	Franckâ^'Condon Simulations of Clusters:Â Phenolâ^'Nitrogen. Journal of Physical Chemistry A, 2006, 110, 4668-4677.	2.5	6
26	Microsolvation of the chlorine oxide anion and chlorine oxide radical: Structures and energetics of the ClOâ^'Â·(H2O)n and ClOÂ·(H2O)nn=1â€“4 clusters. Chemical Physics Letters, 2006, 429, 32-37.	2.6	8
27	Real-Time Observation of Ionization-Induced Hydrophobicâ†'Hydrophilic Switching. Angewandte Chemie - International Edition, 2005, 44, 6149-6151.	13.8	72
28	The S1neutral and D0cationic states of fluorobenzene and fluorobenzeneâ€“argon probed by ZEKE spectroscopy with partial rotational resolution. Physical Chemistry Chemical Physics, 2004, 6, 23-31.	2.8	25
29	Fully rotationally resolved ZEKE photoelectron spectroscopy of C6H6and C6D6: photoionization dynamics and geometry of the benzene cation. Molecular Physics, 2003, 101, 705-716.	1.7	27
30	The effect of conformation on the ionization energetics ofn-butylbenzene. II. A zero electron kinetic energy photoelectron spectroscopy study with partial rotational resolution. Journal of Chemical Physics, 2003, 119, 12914-12920.	3.0	20
31	The effect of conformation on the ionization energetics of n-butylbenzene. I. A threshold ionization study. Journal of Chemical Physics, 2003, 119, 12908-12913.	3.0	18
32	Nonresonant two-photon mass analyzed threshold ionization and zero kinetic energy photoelectron investigation of the Xl∫â€‰2B1 ground state of CH2CO+ and CD2CO+. Journal of Chemical Physics, 2002, 117, 6546-6555.	3.0	6
33	A REMPI and ZEKE Spectroscopic Study of trans-AcetanilideÂ·H2O and Comparison to Ab Initio CASSCF Calculations. Journal of Physical Chemistry A, 2002, 106, 9188-9195.	2.5	22
34	A REMPI and ZEKE Spectroscopic Study of a Secondary Amide Group in Acetanilide. Journal of Physical Chemistry A, 2002, 106, 9181-9187.	2.5	21
35	A Resonance-Enhanced Multiphoton Ionization and Zero Kinetic Energy Photoelectron Study of the PhenolÂ·Kr and PhenolÂ·Xe van der Waals Complexes. Journal of Physical Chemistry A, 2002, 106, 1496-1503.	2.5	32
36	The PFI-ZEKE photoelectron spectrum of m-fluorophenol and its aqueous complexes: Comparing intermolecular vibrations in rotational isomers. Physical Chemistry Chemical Physics, 2002, 4, 2534-2538.	2.8	30

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37	Intermolecular vibration and internal rotation of a methyl group in acetanilideÂ·Ar: a ZEKE photoelectron spectroscopy study. Physical Chemistry Chemical Physics, 2002, 4, 3578-3582.	2.8	8
38	Hydration of a cationic amide group: a ZEKE spectroscopic study of trans-formanilideâ€“H2OElectronic supplementary information (ESI) available: Ab initio CASSCF/cc-pVDZ geometry parameters of t-FAâ€“H2ONH in the S0, S1 and D0 states (Table S1), CASSCF/cc-pVDZ charges of t-FAâ€“H2ONH in the S0, S1 and D0 states (Table S2), CASSCF/cc-pVDZ harmonic frequencies for the S0, S1 and D0 of t-FAâ€“H2ONH up to 1000 cmâ€“1 (Table S3). See http://www.rsc.org/suppdata/cp/b2/b200125j/. Physical Chemistry Chemical Physics, 2002, 4, 2897-2903.	2.8	13
39	ZEKE Photoelectron Spectroscopy of the cis and trans Isomers of Formanilide. Angewandte Chemie - International Edition, 2002, 41, 166-168.	13.8	45
40	A REMPI and ZEKE spectroscopic study of the trans-formanilideÂ·Ar van der Waals cluster. Chemical Physics Letters, 2002, 351, 121-127.	2.6	8
41	A ZEKE photoelectron spectroscopy and ab initio study of the cis- and trans-isomers of formanilide: Characterizing the cationic amide bond ?. Physical Chemistry Chemical Physics, 2001, 3, 5450-5458.	2.8	35
42	Ionization-induced conformational changes: REMPI and ZEKE spectroscopy of salicyl and benzyl alcohol. Chemical Physics Letters, 2000, 319, 375-384.	2.6	37
43	Is the phenolÂ·Ar complex van der Waals or hydrogen-bonded? A REMPI and ZEKE spectroscopic study. Journal of Electron Spectroscopy and Related Phenomena, 2000, 108, 1-11.	1.7	50
44	Rotational band contour analysis in REMPI and ZEKE spectroscopy: elucidating the structures of phenolÂ·X (X=N2, CO and Ar) complexes. Journal of Electron Spectroscopy and Related Phenomena, 2000, 112, 231-239.	1.7	54
45	Noncovalent Interactions:Â A Challenge for Experiment and Theory. Chemical Reviews, 2000, 100, 143-168.	47.7	1,572
46	Hydrogen-Bonding and van der Waals Complexes Studied by ZEKE and REMPI Spectroscopy. Chemical Reviews, 2000, 100, 3999-4022.	47.7	198
47	A complete active space self-consistent field (CASSCF) ab initio study of phenolâ€“N2: the properties of a weak hydrogen-bonded system in its S1 excited state. Physical Chemistry Chemical Physics, 2000, 2, 5528-5537.	2.8	16
48	Observation of Rotational Isomers I:Â A ZEKE and Hole-Burning Spectroscopy Study of 3-Methoxyphenol. Journal of Physical Chemistry A, 2000, 104, 11864-11869.	2.5	36
49	Observation of Rotational Isomers II:Â A ZEKE and Hole-Burning Spectroscopy Study of Hydrogen-Bonded 3-MethoxyphenolÂ·Water Clusters. Journal of Physical Chemistry A, 2000, 104, 11870-11876.	2.5	12
50	Calculations on the Jahnâ€“Teller configurations of the benzene cation. Journal of Chemical Physics, 1999, 111, 10550-10554.	3.0	41
51	Mass analyzed threshold ionization of phenolâ‹…CO: Intermolecular binding energies of a hydrogen-bonded complex. Journal of Chemical Physics, 1999, 111, 1947-1954.	3.0	67
52	A comparison of hydrogen-bonded and van der Waals isomers of phenolâ‹…â‹…nitrogen and phenolâ‹…â‹…carbon monoxide: An ab initio study. Journal of Chemical Physics, 1999, 111, 1955-1963.	3.0	34
53	A new detection scheme for synchronous, high resolution ZEKE and MATI spectroscopy demonstrated on the PhenolÂ·Ar complex. Chemical Physics Letters, 1999, 315, 103-108.	2.6	108
54	Observation of Hydrogen-Bonded Rotational Isomers of the ResorcinolÂ·Water Complex. Journal of Physical Chemistry A, 1999, 103, 7186-7191.	2.5	17

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55	ZEKE and Hole-Burning Spectroscopy of the Rotational Isomers of ResorcinolÂ·CO. Journal of Physical Chemistry A, 1999, 103, 9687-9692.	2.5	11
56	Chemical Applications of Zero Kinetic Energy (ZEKE) Photoelectron Spectroscopy. Angewandte Chemie - International Edition, 1998, 37, 1346-1374.	13.8	120
57	Structure and dynamics of the phenolâ€“waterâ€“argon cation radical. Chemical Physics, 1998, 239, 417-428.	1.9	9
58	Chapter 9. Recent applications and developments in ZEKE spectroscopy. Annual Reports on the Progress of Chemistry Section C, 1998, 94, 327.	4.4	16
59	Chemical Applications of Zero Kinetic Energy (ZEKE) Photoelectron Spectroscopy. , 1998, 37, 1346.		2
60	Zero kinetic energy photoelectron (ZEKE) spectroscopy of the heterotrimer phenol-water-argon: Interaction between a hydrogen bond and a van der Waals bond. Chemical Physics, 1996, 207, 437-449.	1.9	23
61	Fractional Stark State Selective Electric Field Ionization of Very High-nRydberg States of Molecules. Physical Review Letters, 1996, 76, 3530-3533.	7.8	71
62	Applications of ZEKE spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 1995, 75, 35-46.	1.7	21
63	Basic principles of ZEKE spectroscopy. Optimized resolution and accurate ionization energy. Chemical Physics Letters, 1994, 228, 417-425.	2.6	54
64	ZEKE spectroscopy of hydrogen-bonded phenol complexes. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 247-254.	1.7	7
65	State-to-state photoionisation dynamics probed by zero kinetic energy (ZEKE) photoelectron spectroscopy. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2425-2442.	1.7	61
66	The non-resonant two-photon zero kinetic energy photoelectron spectrum of CS2. Chemical Physics Letters, 1993, 202, 542-548.	2.6	55
67	Structure and Symmetry of the Benzene Cation. Angewandte Chemie International Edition in English, 1993, 32, 603-606.	4.4	34
68	The Dynamic Jahn-Teller Effect in the Benzene Cation: Rotationally Resolved ZEKE Photoelectron Spectra of the ν6(e2g) Mode. Angewandte Chemie International Edition in English, 1993, 32, 1364-1366.	4.4	26
69	Struktur und Symmetrie des Benzolâ€Kations. Angewandte Chemie, 1993, 105, 631-634.	2.0	24
70	Dynamischer Jahnâ€Tellerâ€Effekt im Benzolâ€Kation: RotationsaufgelÃ¶ste ZEKE Photoelektronenspektren der ν₆(e_{2g})â€Mode. Angewandte Chemie, 1993, 105, 1384-1387.	2.0	11
71	Zero-kinetic-energy (ZEKE) photoelectron spectroscopy of the hydrogen-bonded phenolâ€“methanol complex. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1609-1621.	1.7	41
72	Rotationally Resolved ZEKE Photoelectron Spectrum of Benzene. Dynamic Jahn-Teller Effect in the Î½6(e2g) Mode. Chemistry Letters, 1993, 22, 485-488.	1.3	5

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73	The ZEKE Spectrum of the Phenolâ€¦Water Cluster. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 1259-1261.	0.9	16
74	Theory of rotational line strengths in coherent anti-Stokes Raman spectroscopy. Molecular Physics, 1991, 73, 1257-1293.	1.7	27
75	Angular distribution of near-zero kinetic energy photoelectrons from the lowest rotational states of the NO A 2Î£+ state. Chemical Physics Letters, 1991, 183, 239-244.	2.6	13
76	A new approach to vibrational spectroscopy of ion clusters: the â€œzero kinetic energy (ZEKE)â€• photoelectron spectrum of the phenolâ€”water complex. Chemical Physics Letters, 1991, 181, 1-4.	2.6	72
77	Bond-Selective Memory Effects for 1s-Level Excitation of Molecules: Zero Kinetic Energy (Zeke) Electron-Photoion Coincidence Measurements. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1991, , 371-392.	0.2	0
78	Bondâ€selective Photoion Correlations (â€œMemory Effectsâ€) in Molecules from Siteâ€Specific 1s Excitation Using Synchrotron Radiation. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1990, 94, 1318-1322.	0.9	8
79	Zero-kinetic-energy photoelectrom-photoion coincidence measurements of AR in the 2p and N2 in the 1s region. Journal of Electron Spectroscopy and Related Phenomena, 1990, 52, 697-710.	1.7	17
80	Selective fragmentation of nitrous oxide by site-specific N (1s) excitation using soft X-ray synchrotron radiation. Physica Scripta, 1990, 41, 814-818.	2.5	34
81	The ionization energy of nitric oxide. Chemical Physics Letters, 1988, 152, 119-123.	2.6	324
82	Determination of the ionization energy of the benzene-argon complex by zero kinetic energy photoelectron spectroscopy. Chemical Physics Letters, 1987, 135, 219-222.	2.6	85
83	Resonance CARS Rotational Lineâ€Strengths. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1985, 89, 318-319.	0.9	9
84	Two-colour photoionization resonance spectroscopy of NO: Complete separation of rotational levels of NO+ at the ionization threshold. Chemical Physics Letters, 1984, 112, 291-294.	2.6	330
85	A Novel Method Capable of Resolving Rotational Ionic States by the Detection of Threshold Photoelectrons with a Resolution of 1.2 cm⁻¹. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1984, 39, 1089-1091.	1.5	223