

Klaus MÃ¼ller-Dethlefs

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/11254991/publications.pdf>

Version: 2024-02-01

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	Noncovalent Interactions: A Challenge for Experiment and Theory. <i>Chemical Reviews</i> , 2000, 100, 143-168.	47.7	1,572
2	Two-colour photoionization resonance spectroscopy of NO: Complete separation of rotational levels of NO+ at the ionization threshold. <i>Chemical Physics Letters</i> , 1984, 112, 291-294.	2.6	330
3	The ionization energy of nitric oxide. <i>Chemical Physics Letters</i> , 1988, 152, 119-123.	2.6	324
4	A Novel Method Capable of Resolving Rotational Ionic States by the Detection of Threshold Photoelectrons with a Resolution of 1.2 cm^{-1} . <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1984, 39, 1089-1091.	1.5	223
5	Hydrogen-Bonding and van der Waals Complexes Studied by ZEKE and REMPI Spectroscopy. <i>Chemical Reviews</i> , 2000, 100, 3999-4022.	47.7	198
6	The World of Non-Covalent Interactions: 2006. <i>Collection of Czechoslovak Chemical Communications</i> , 2006, 71, 443-531.	1.0	184
7	Chemical Applications of Zero Kinetic Energy (ZEKE) Photoelectron Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 1998, 37, 1346-1374.	13.8	120
8	A new detection scheme for synchronous, high resolution ZEKE and MATI spectroscopy demonstrated on the Phenol-Ar complex. <i>Chemical Physics Letters</i> , 1999, 315, 103-108.	2.6	108
9	Determination of the ionization energy of the benzene-argon complex by zero kinetic energy photoelectron spectroscopy. <i>Chemical Physics Letters</i> , 1987, 135, 219-222.	2.6	85
10	A new approach to vibrational spectroscopy of ion clusters: the "zero kinetic energy (ZEKE) photoelectron spectrum of the phenol-water complex. <i>Chemical Physics Letters</i> , 1991, 181, 1-4.	2.6	72
11	Real-Time Observation of Ionization-Induced Hydrophobic-Hydrophilic Switching. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6149-6151.	13.8	72
12	Fractional Stark State Selective Electric Field Ionization of Very High-n Rydberg States of Molecules. <i>Physical Review Letters</i> , 1996, 76, 3530-3533.	7.8	71
13	The Use of Multidimensional Franck-Condon Simulations to Assess Model Chemistries: A Case Study on Phenol. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4657-4667.	2.5	68
14	Mass analyzed threshold ionization of phenol...CO: Intermolecular binding energies of a hydrogen-bonded complex. <i>Journal of Chemical Physics</i> , 1999, 111, 1947-1954.	3.0	67
15	State-to-state photoionisation dynamics probed by zero kinetic energy (ZEKE) photoelectron spectroscopy. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994, 90, 2425-2442.	1.7	61
16	IR signature of the photoionization-induced hydrophobic-hydrophilic site switching in phenol-Ar _n clusters. <i>Journal of Chemical Physics</i> , 2007, 127, 114307.	3.0	58
17	The non-resonant two-photon zero kinetic energy photoelectron spectrum of CS ₂ . <i>Chemical Physics Letters</i> , 1993, 202, 542-548.	2.6	55
18	Basic principles of ZEKE spectroscopy. Optimized resolution and accurate ionization energy. <i>Chemical Physics Letters</i> , 1994, 228, 417-425.	2.6	54

#	ARTICLE	IF	CITATIONS
19	Rotational band contour analysis in REMPI and ZEKE spectroscopy: elucidating the structures of phenol-X (X=N ₂ , CO and Ar) complexes. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2000, 112, 231-239.	1.7	54
20	Is the phenol-Ar complex van der Waals or hydrogen-bonded? A REMPI and ZEKE spectroscopic study. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2000, 108, 1-11.	1.7	50
21	ZEKE Photoelectron Spectroscopy of the cis and trans Isomers of Formanilide. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 166-168.	13.8	45
22	Dissociation energetics of the phenol+Ar ₂ cluster ion: The role of H isomerization. <i>Journal of Chemical Physics</i> , 2010, 133, 154308.	3.0	42
23	Zero-kinetic-energy (ZEKE) photoelectron spectroscopy of the hydrogen-bonded phenol-methanol complex. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 1609-1621.	1.7	41
24	Calculations on the Jahn-Teller configurations of the benzene cation. <i>Journal of Chemical Physics</i> , 1999, 111, 10550-10554.	3.0	41
25	Hole-Burning Spectra of Phenol-Ar _n (n= 1, 2) Clusters: Resolution of the Isomer Issue. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7569-7575.	2.5	40
26	The structure of phenol-Ar _n (n=1,2) clusters in their S and S ₁ states. <i>Journal of Chemical Physics</i> , 2009, 130, 224303.	3.0	38
27	Ionization-induced conformational changes: REMPI and ZEKE spectroscopy of salicyl and benzyl alcohol. <i>Chemical Physics Letters</i> , 2000, 319, 375-384.	2.6	37
28	Observation of Rotational Isomers I: A ZEKE and Hole-Burning Spectroscopy Study of 3-Methoxyphenol. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11864-11869.	2.5	36
29	A ZEKE photoelectron spectroscopy and ab initio study of the cis- and trans-isomers of formanilide: Characterizing the cationic amide bond ?. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5450-5458.	2.8	35
30	Selective fragmentation of nitrous oxide by site-specific N (1s) excitation using soft X-ray synchrotron radiation. <i>Physica Scripta</i> , 1990, 41, 814-818.	2.5	34
31	Structure and Symmetry of the Benzene Cation. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 603-606.	4.4	34
32	A comparison of hydrogen-bonded and van der Waals isomers of phenol...nitrogen and phenol...carbon monoxide: An ab initio study. <i>Journal of Chemical Physics</i> , 1999, 111, 1955-1963.	3.0	34
33	State of the art theoretical study and comparison to experiment for the phenol-argon complex. <i>Journal of Chemical Physics</i> , 2008, 128, 114319.	3.0	33
34	A Resonance-Enhanced Multiphoton Ionization and Zero Kinetic Energy Photoelectron Study of the Phenol-Kr and Phenol-Xe van der Waals Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1496-1503.	2.5	32
35	The PFI-ZEKE photoelectron spectrum of m-fluorophenol and its aqueous complexes: Comparing intermolecular vibrations in rotational isomers. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2534-2538.	2.8	30
36	Theory of rotational line strengths in coherent anti-Stokes Raman spectroscopy. <i>Molecular Physics</i> , 1991, 73, 1257-1293.	1.7	27

#	ARTICLE	IF	CITATIONS
37	Fully rotationally resolved ZEKE photoelectron spectroscopy of C ₆ H ₆ and C ₆ D ₆ : photoionization dynamics and geometry of the benzene cation. <i>Molecular Physics</i> , 2003, 101, 705-716.	1.7	27
38	The Dynamic Jahn-Teller Effect in the Benzene Cation: Rotationally Resolved ZEKE Photoelectron Spectra of the v ₆ (e _{2g}) Mode. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 1364-1366.	4.4	26
39	Competition between stacking and hydrogen bonding: theoretical study of the phenol ⁺ Ar cation and neutral complex and comparison to experiment. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2780.	2.8	26
40	The S ₁ neutral and D ₀ cationic states of fluorobenzene and fluorobenzene-argon probed by ZEKE spectroscopy with partial rotational resolution. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 23-31.	2.8	25
41	Zeke Spectroscopy: High-Resolution Spectroscopy with Photoelectrons. <i>Advances in Chemical Physics</i> , 2007, , 1-104.	0.3	25
42	Struktur und Symmetrie des Benzol ⁺ Kations. <i>Angewandte Chemie</i> , 1993, 105, 631-634.	2.0	24
43	Excited-State Ab Initio Calculations and Multidimensional Franck-Condon Simulations on Guanine. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13045-13057.	2.5	24
44	Zero kinetic energy photoelectron (ZEKE) spectroscopy of the heterotrimer phenol-water-argon: Interaction between a hydrogen bond and a van der Waals bond. <i>Chemical Physics</i> , 1996, 207, 437-449.	1.9	23
45	A REMPI and ZEKE Spectroscopic Study of trans-Acetanilide·H ₂ O and Comparison to Ab Initio CASSCF Calculations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9188-9195.	2.5	22
46	Applications of ZEKE spectroscopy. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1995, 75, 35-46.	1.7	21
47	A REMPI and ZEKE Spectroscopic Study of a Secondary Amide Group in Acetanilide. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9181-9187.	2.5	21
48	The effect of conformation on the ionization energetics of n-butylbenzene. II. A zero electron kinetic energy photoelectron spectroscopy study with partial rotational resolution. <i>Journal of Chemical Physics</i> , 2003, 119, 12914-12920.	3.0	20
49	The effect of conformation on the ionization energetics of n-butylbenzene. I. A threshold ionization study. <i>Journal of Chemical Physics</i> , 2003, 119, 12908-12913.	3.0	18
50	Binding Energies of the π -Stacked Anisole Dimer: New Molecular Beam Laser Spectroscopy Experiments and CCSD(T) Calculations. <i>Chemistry - A European Journal</i> , 2015, 21, 6740-6746.	3.3	18
51	Zero-kinetic-energy photoelectron-photoion coincidence measurements of Ar in the 2p and N ₂ in the 1s region. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1990, 52, 697-710.	1.7	17
52	Observation of Hydrogen-Bonded Rotational Isomers of the Resorcinol·Water Complex. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7186-7191.	2.5	17
53	Fragmentation Energetics of the Phenol ⁺ Ar ₃ Cation Cluster. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11139-11143.	2.5	17
54	The ZEKE Spectrum of the Phenol·Water Cluster. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1992, 96, 1259-1261.	0.9	16

#	ARTICLE	IF	CITATIONS
55	Chapter 9. Recent applications and developments in ZEKE spectroscopy. Annual Reports on the Progress of Chemistry Section C, 1998, 94, 327.	4.4	16
56	A complete active space self-consistent field (CASSCF) ab initio study of phenol-H ₂ O: the properties of a weak hydrogen-bonded system in its S ₁ excited state. Physical Chemistry Chemical Physics, 2000, 2, 5528-5537.	2.8	16
57	Effect of Noncovalent Interactions on Conformers of the <i>n</i> -Butylbenzene Monomer Studied by Mass Analyzed Threshold Ionization Spectroscopy and Basis-set Convergent <i>ab initio</i> Computations. Journal of Physical Chemistry A, 2008, 112, 5866-5871.	2.5	14
58	Angular distribution of near-zero kinetic energy photoelectrons from the lowest rotational states of the NO A $2\tilde{\Sigma}^+$ state. Chemical Physics Letters, 1991, 183, 239-244.	2.6	13
59	Hydration of a cationic amide group: a ZEKE spectroscopic study of trans-formanilide-H ₂ O. Electronic supplementary information (ESI) available: Ab initio CASSCF/cc-pVDZ geometry parameters of t-FA-H ₂ O-NH in the S ₀ , S ₁ and D ₀ states (Table S1), CASSCF/cc-pVDZ charges of t-FA-H ₂ O-NH in the S ₀ , S ₁ and D ₀ states (Table S2), CASSCF/cc-pVDZ harmonic frequencies for the S ₀ , S ₁ and D ₀ of t-FA-H ₂ O-NH up to 1000 cm ⁻¹ (Table S3). See http://www.rsc.org/suppdata/cp/b2/b200125j/ . Physical Chemistry Chemical Physics, 2002, 4, 2897-2903.	2.8	13
60	Ionization-induced I ⁺ H site-switching in phenol-CH ₄ complexes studied using IR dip spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 110-116.	2.8	13
61	Observation of Rotational Isomers II: A ZEKE and Hole-Burning Spectroscopy Study of Hydrogen-Bonded 3-Methoxyphenol-Water Clusters. Journal of Physical Chemistry A, 2000, 104, 11870-11876.	2.5	12
62	Mass analyzed threshold ionization detected infrared spectroscopy: isomerization activity of the phenol-Ar cluster near the ionization threshold. Physical Chemistry Chemical Physics, 2015, 17, 2494-2503.	2.8	12
63	Dynamischer Jahn-Teller-Effekt im Benzol-Kation: Rotationsaufgelöste ZEKE Photoelektronenspektren der <i>v</i> ₆ (<i>e</i> _{2g})-Mode. Angewandte Chemie, 1993, 105, 1384-1387.	2.0	11
64	ZEKE and Hole-Burning Spectroscopy of the Rotational Isomers of Resorcinol-CO. Journal of Physical Chemistry A, 1999, 103, 9687-9692.	2.5	11
65	Resonance CARS Rotational Line-Strengths. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1985, 89, 318-319.	0.9	9
66	Structure and dynamics of the phenol-water-argon cation radical. Chemical Physics, 1998, 239, 417-428.	1.9	9
67	Spectral shifts and structures of phenol-Ar _n clusters. Physical Chemistry Chemical Physics, 2011, 13, 6077.	2.8	9
68	Bond-selective Photoion Correlations (Memory Effects) in Molecules from Site-Specific 1s Excitation Using Synchrotron Radiation. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1990, 94, 1318-1322.	0.9	8
69	Intermolecular vibration and internal rotation of a methyl group in acetanilide-Ar: a ZEKE photoelectron spectroscopy study. Physical Chemistry Chemical Physics, 2002, 4, 3578-3582.	2.8	8
70	A REMPI and ZEKE spectroscopic study of the trans-formanilide-Ar van der Waals cluster. Chemical Physics Letters, 2002, 351, 121-127.	2.6	8
71	Microsolvation of the chlorine oxide anion and chlorine oxide radical: Structures and energetics of the ClO ⁻ -(H ₂ O) _n and ClO·-(H ₂ O) _n (n = 1-4) clusters. Chemical Physics Letters, 2006, 429, 32-37.	2.6	8
72	Structure and energetics of the anisole-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

#	ARTICLE	IF	CITATIONS
73	ZEKE spectroscopy of hydrogen-bonded phenol complexes. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1994, 68, 247-254.	1.7	7
74	Nonresonant two-photon mass analyzed threshold ionization and zero kinetic energy photoelectron investigation of the $X^1\Sigma^+$ ground state of CH_2CO^+ and CD_2CO^+ . <i>Journal of Chemical Physics</i> , 2002, 117, 6546-6555.	3.0	6
75	Franck-Condon Simulations of Clusters: Phenol-Nitrogen. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4668-4677.	2.5	6
76	A novel experimental system of high stability and lifetime for the laser-desorption of biomolecules. <i>Review of Scientific Instruments</i> , 2010, 81, 063101.	1.3	6
77	Rotationally Resolved ZEKE Photoelectron Spectrum of Benzene. Dynamic Jahn-Teller Effect in the $\tilde{v}_{1/2}(e_2g)$ Mode. <i>Chemistry Letters</i> , 1993, 22, 485-488.	1.3	5
78	Rotational Analysis for the Doppler-Free Photoelectron Spectrum of Water Using the Spectator Model. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11133-11138.	2.5	5
79	Binding Energies of the π -Stacked Anisole Dimer: New Molecular Beam-Laser Spectroscopy Experiments and CCSD(T) Calculations. <i>Chemistry - A European Journal</i> , 2015, 21, 6637-6637.	3.3	3
80	Multidimensional Franck-Condon simulations of photodetachment spectra for the formate-water cluster anion: Investigating H atom transfer along the $\text{HCOOH}+\text{OH}$ reaction coordinate. <i>Journal of Chemical Physics</i> , 2007, 127, 234308.	3.0	2
81	Effect of Noncovalent Interactions on the n-Butylbenzene-Ar Cluster Studied by Mass Analyzed Threshold Ionization Spectroscopy and ab initio Computations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5872-5877.	2.5	2
82	An improved experimental scheme for simultaneous measurement of high-resolution zero electron kinetic energy (ZEKE) photoelectron and threshold photoion (MATI) spectra. <i>Chemical Physics Letters</i> , 2017, 685, 477-481.	2.6	2
83	Chemical Applications of Zero Kinetic Energy (ZEKE) Photoelectron Spectroscopy. , 1998, 37, 1346.		2
84	Threshold ionization spectroscopic investigation of supersonic jet-cooled, laser-desorbed Tryptophan. <i>Chemical Physics Letters</i> , 2016, 657, 142-147.	2.6	1
85	Bond-Selective Memory Effects for 1s-Level Excitation of Molecules: Zero Kinetic Energy (Zeke) Electron-Photoion Coincidence Measurements. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 1991, , 371-392.	0.2	0