Karl K Irikura

List of Publications by Year
in descending order

86	3,429	186254	144002
papers	citations	28 h-index	57 g-index

94	94	94	3120
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermochemical spinâ€orbit corrections for platinum cation (Pt +). International Journal of Quantum Chemistry, 2021, 121, e26448.	2.0	2
2	Polarizability of atomic Pt, Pt+, and Ptâ^'. Journal of Chemical Physics, 2021, 154, 174302.	3.0	2
3	Thermochemical spinâ€orbit corrections for atomic platinum (Pt). International Journal of Quantum Chemistry, 2020, 120, e26074.	2.0	6
4	Multireaction Approach to Quantum Thermochemistry. Journal of Physical Chemistry A, 2020, 124, 8088-8099.	2.5	3
5	Electron impact total ionization cross sections of diboranes - B2H4 and B2H6. International Journal of Mass Spectrometry, 2019, 440, 4-9.	1.5	1
6	Ab Initio Computation of Energy Deposition During Electron Ionization of Molecules. Journal of Physical Chemistry A, 2017, 121, 7751-7760.	2.5	10
7	N-Protonated Isomers and Coulombic Barriers to Dissociation of Doubly Protonated Ala₈Arg. Journal of the American Society for Mass Spectrometry, 2017, 28, 2170-2180.	2.8	2
8	Partial Ionization Cross Sections of Organic Molecules. Journal of Research of the National Institute of Standards and Technology, 2017, 122, 1-67.	1.2	8
9	Semi-empirical estimation of ion-specific cross sections in electron ionization of molecules. Journal of Chemical Physics, 2016, 145, 224102.	3.0	16
10	Thermochemistry of HO₂ + HO₂ â†' H₂O₄: Does HO₂ Dimerization Affect Laboratory Studies?. Journal of Physical Chemistry A, 2015, 119, 7052-7062.	2.5	10
11	High-resolution, vacuum-ultraviolet absorption spectrum of boron trifluoride. Journal of Chemical Physics, 2014, 141, 194301.	3.0	4
12	Facile Smilesâ€type rearrangement in radical cations of Nâ€acyl arylsulfonamides and analogs. Rapid Communications in Mass Spectrometry, 2014, 28, 829-834.	1.5	8
13	Quantitative estimation of uncertainties from wavefunction diagnostics. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	18
14	Anharmonic partition functions for polyatomic thermochemistry. Journal of Chemical Thermodynamics, 2014, 73, 183-189.	2.0	11
15	Aminoxyl (Nitroxyl) Radicals in the Early Decomposition of the Nitramine RDX. Journal of Physical Chemistry A, 2013, 117, 2233-2241.	2.5	25
16	Anharmonic Vibrational Frequency Calculations Are Not Worthwhile for Small Basis Sets. Journal of Chemical Theory and Computation, 2013, 9, 951-954.	5.3	47
17	Gas-Phase Energetics of Thorium Fluorides and Their Ions. Journal of Physical Chemistry A, 2013, 117, 1276-1282.	2.5	9
18	Tryptic y ++ Fragment Ion Distributions Are Guided by Coulombic Repulsion. Journal of the American Society for Mass Spectrometry, 2012, 23, 483-488.	2.8	1

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19	N-Protonated Isomers as Gateways to Peptide Ion Fragmentation. Journal of the American Society for Mass Spectrometry, 2011, 22, 2222-2231.	2.8	15
20	Electron ionization and gas-phase ion molecule reactions of methylcyclohexane. International Journal of Mass Spectrometry, 2011, 300, 2-11.	1.5	3
21	Response to â€œComment on â€˜Uncertainties in scaling factors for ab initio vibrational zero-point energiesâ€™ and â€˜Calibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functionalâ€™â€•[J. Chem. Phys. 134, 167101 (2011)]. Journal of Chemical Physics, 2011, 134, 167102.	3.0	5
22	Symmetry Numbers for Rigid, Flexible, and Fluxional Molecules: Theory and Applications. Journal of Physical Chemistry B, 2010, 114, 16304-16317.	2.6	65
23	Scaling Factors and Uncertainties for ab Initio Anharmonic Vibrational Frequencies. Journal of Chemical Theory and Computation, 2010, 6, 2822-2828.	5.3	64
24	Thermochemistry of Ammonium Nitrate, NH4NO3, in the Gas Phase. Journal of Physical Chemistry A, 2010, 114, 11651-11653.	2.5	7
25	Uncertainties in scaling factors forab initiovibrational zero-point energies. Journal of Chemical Physics, 2009, 130, 114102.	3.0	74
26	Unimolecular Decomposition of 5-Aminotetrazole and its Tautomer 5-Iminotetrazole: New Insight from Isopotential Searching. Journal of Physical Chemistry A, 2009, 113, 2483-2490.	2.5	34
27	Sigma Stellation:â€‰ A Design Strategy for Electron Boxes. Journal of Physical Chemistry A, 2008, 112, 983-988.	2.5	29
28	In-Adamantane, a Small Inside-Out Molecule. Journal of Organic Chemistry, 2008, 73, 7906-7908.	3.2	6
29	chapter 2 Obtaining Molecular Thermochemistry from Calculations. Comprehensive Chemical Kinetics, 2007, , 7-42.	2.3	2
30	Competition between Hydrogen Abstraction and Halogen Displacement in the Reaction of Br with CH3I, CH3Br, and CH3Clâ€. Journal of Physical Chemistry A, 2007, 111, 6852-6859.	2.5	5
31	Experimental Vibrational Zero-Point Energies: Diatomic Molecules. Journal of Physical and Chemical Reference Data, 2007, 36, 389-397.	4.2	336
32	Is NO3Formed during the Decomposition of Nitramine Explosives?. Journal of Physical Chemistry A, 2006, 110, 13974-13978.	2.5	24
33	Multi-determinant trial functions in the determination of the dissociation energy of the beryllium dimer: Quantum Monte Carlo study. International Journal of Quantum Chemistry, 2006, 106, 2373-2378.	2.0	26
34	Mass scaling for vibrational frequencies from ab initio calculations. Chemical Physics Letters, 2005, 403, 275-279.	2.6	5
35	Performance of binary-encounter-Bethe (BEB) theory for electron-impact ionization cross sections of molecules containing heavy elements (Z > 10). Surface and Interface Analysis, 2005, 37, 973-977.	1.8	20
36	Uncertainties in Scaling Factors for ab Initio Vibrational Frequencies. Journal of Physical Chemistry A, 2005, 109, 8430-8437.	2.5	431

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37	Electron-Impact Ionization Cross Sections of Molecules Containing Heavy Elements (Z> 10). Journal of Chemical Theory and Computation, 2005, 1, 1153-1161.	5.3	16
38	Uncertainty associated with virtual measurements from computational quantum chemistry models. Metrologia, 2004, 41, 369-375.	1.2	37
39	Electron-impact total ionization cross-sections of the chlorofluoromethanes. International Journal of Mass Spectrometry, 2003, 222, 189-200.	1.5	31
40	Ab initio characterization of the weakly bound anions ClOOâ¯ and ArClâ¯. International Journal of Mass Spectrometry, 2003, 228, 667-676.	1.5	8
41	New Empirical Procedures for Improving ab Initio Energeticsâ€. Journal of Physical Chemistry A, 2002, 106, 9910-9917.	2.5	8
42	Electron-impact total ionization cross sections of hydrocarbon ions. Journal of Research of the National Institute of Standards and Technology, 2002, 107, 63.	1.2	22
43	Electron-impact ionization cross sections for polyatomic molecules, radicals, and ions. AIP Conference Proceedings, 2000, , .	0.4	32
44	Electron-impact total ionization cross sections of SFx(x = 1â€“5). International Journal of Mass Spectrometry, 2000, 201, 187-195.	1.5	44
45	Electronic Structure of BCl Determined by Ab Initio Calculations and Resonance-Enhanced Multiphoton Ionization Spectroscopyâ€. Journal of Physical Chemistry A, 2000, 104, 3800-3805.	2.5	17
46	Predicting Unexpected Chemical Reactions by Isopotential Searching. Journal of Physical Chemistry A, 2000, 104, 2191-2194.	2.5	37
47	The reaction of BF3 with H2O: Infrared spectrum of BF2OH trapped in solid neon. Journal of Chemical Physics, 2000, 113, 5705-5715.	3.0	32
48	Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies. International Journal of Mass Spectrometry, 1999, 185-187, 577-587.	1.5	6
49	Gas-Phase Thermochemistry of Iron Oxides and Hydroxides:â€‰ Portrait of a Super-Efficient Flame Suppressant. Journal of Physical Chemistry A, 1999, 103, 1150-1159.	2.5	52
50	The Ionization Energy of CF3:â€‰ When Does Entropy Matter in Gas-Phase Reactions?. Journal of the American Chemical Society, 1999, 121, 7689-7695.	13.7	30
51	Extracting Thermochemical Information from Ab Initio Data. , 1999, , 353-372.		8
52	Inexpensive vibrational anharmonicities from estimated derivatives: Diatomic molecules. Journal of Computational Chemistry, 1998, 19, 1315-1324.	3.3	7
53	Infrared spectra of molecular ions derived from the hydrogen and methyl halides trapped in solid neon. Journal of Molecular Structure, 1998, 449, 111-118.	3.6	3
54	Systematic Errors in ab Initio Bond Dissociation Energies. Journal of Physical Chemistry A, 1998, 102, 9031-9039.	2.5	13

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55	Computational Thermochemistry. ACS Symposium Series, 1998, , 2-18.	0.5	21
56	Experimental and ab initio study of the infrared spectra of ionic species derived from PF5, PF3, and F3PO and trapped in solid neon. Journal of Chemical Physics, 1998, 108, 8381-8393.	3.0	21
57	The vibrational spectra of molecular ions isolated in solid neon. XIV. CH3F+, CH3Cl+, CH3Br+, and their ylidion isomers. Journal of Chemical Physics, 1997, 106, 489-503.	3.0	24
58	Rotational and Vibrational Spectroscopy and Ideal Gas Heat Capacity of HFC 134a (CF3CFH2). Journal of Physical Chemistry A, 1997, 101, 2288-2297.	2.5	34
59	Nearly ab Initio Thermochemistry:â€‰ The Use of Reaction Schemes. Application to IO and HOI. Journal of Physical Chemistry A, 1997, 101, 1580-1587.	2.5	42
60	Ab Initio Ionization and Excitation Spectra Involving IO(X2Î) and IO+(X3Î£-, a1Î”, b1Î£+). Journal of Physical Chemistry A, 1997, 101, 6897-6902.	2.5	13
61	Electronic Structure of the BF2Radical Determined byab InitioCalculations and Resonance-Enhanced Multiphoton Ionization Spectroscopy. Journal of Physical Chemistry A, 1997, 101, 2045-2049.	2.5	11
62	Protonatedp-Benzoquinone. Journal of Organic Chemistry, 1996, 61, 3167-3171.	3.2	7
63	Matrix isolation study of the interaction of excited neon atoms with BCl3: Infrared spectra of BCl+3, BCl+2, and BClâ‚‚. Journal of Chemical Physics, 1996, 104, 8871-8878.	3.0	19
64	Thermochemistry of disulfur decafluoride, S2F10. Journal of Chemical Physics, 1995, 103, 10162-10168.	3.0	5
65	Spectroscopy of the fluoromethylene radicals HCF and DCF by 2+1 resonance enhanced multiphoton ionization spectroscopy and by ab initio calculation. Journal of Chemical Physics, 1995, 103, 1303-1308.	3.0	21
66	Structure and thermochemistry of sulfur fluorides SFn(n=1â€“5) and their ions SF+n(n=1â€“5). Journal of Chemical Physics, 1995, 102, 5357-5367.	3.0	80
67	Matrix isolation study of the interaction of excited neon atoms with SiF4: Infrared spectra of SiF+3 and SiFâ‚‚. Journal of Chemical Physics, 1995, 103, 5308-5314.	3.0	16
68	<title>New spectroscopy of free radicals produced by the reactions of fluorine and chlorine with diborane</title>. , 1994, , .		2
69	Matrix isolation study of the interaction of excited neon atoms with CF4. Infrared spectra of CF+3 and CFâ‚‚. Journal of Chemical Physics, 1994, 101, 8290-8296.	3.0	41
70	Excited electronic states of PF2. Chemical Physics Letters, 1994, 228, 273-278.	2.6	11
71	Postionization Chemical Separation: A Mass Spectrometric Technique for Isotopic Analysis of Mixtures. Analytical Chemistry, 1994, 66, 3447-3448.	6.5	11
72	Energetics of Third-Row Transition Metal Methylidene Ions MCH2+ (M = La, Hf, Ta, W, Re, Os, Ir, Pt, Au). Journal of the American Chemical Society, 1994, 116, 8733-8740.	13.7	119

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73	Two-photon Rydberg series in atomic boron. Journal of the Optical Society of America B: Optical Physics, 1993, 10, 763.	2.1	8
74	Detection of11BF and10BF by resonanceâ€enhanced multiphoton ionization spectroscopy. Applied Physics Letters, 1993, 62, 1697-1698.	3.3	4
75	<title>New ways to optically detect CH2 and HCF radicals using resonance-enhanced multiphoton ionization spectroscopy</title>. , 1993, , .		0
76	Detection of methylene (~X 3B1) radicals by 3 + 1 resonance-enhanced multiphoton ionization spectroscopy. The Journal of Physical Chemistry, 1992, 96, 518-519.	2.9	23
77	Electronic spectrum of the trichlorosilyl radical. The Journal of Physical Chemistry, 1992, 96, 4306-4310.	2.9	7
78	Two new electronic states of methylene. The Journal of Physical Chemistry, 1992, 96, 6131-6133.	2.9	23
79	Singlet-triplet gaps in substituted carbenes CXY (X, Y = H, fluoro, chloro, bromo, iodo, silyl). Journal of the American Chemical Society, 1992, 114, 48-51.	13.7	153
80	Gas-phase synthesis of metalloporphyrin ions. Journal of the American Chemical Society, 1991, 113, 2767-2768.	13.7	35
81	Methane oligomerization in the gas phase by third-row transition-metal ions. Journal of the American Chemical Society, 1991, 113, 2769-2770.	13.7	165
82	Electronic structure considerations for methane activation by third-row transition-metal ions. The Journal of Physical Chemistry, 1991, 95, 8344-8351.	2.9	257
83	Prospects for the involvement of transition metals in the chemistry of diffuse interstellar clouds: formation of FeH+ by radiative association. International Journal of Mass Spectrometry and Ion Processes, 1990, 99, 213-222.	1.8	12
84	Osmium tetroxide and its fragment ions in the gas phase: reactivity with hydrocarbons and small molecules. Journal of the American Chemical Society, 1989, 111, 75-85.	13.7	232
85	Thermochemistry of silaethylene and methylsilylene from experiment and theory. Journal of the American Chemical Society, 1988, 110, 24-30.	13.7	50
86	Dynamics of DNA Oligomers. Journal of Biomolecular Structure and Dynamics, 1983, 1, 231-252.	3.5	188