Branko Ruscic

List of Publications by Year
in descending order

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141 papers	10,991 citations	34105 52 h-index	30922 102 g-index
164 all docs	164 docs citations	164 times ranked	6369 citing authors

#	Article	IF	Citations
1	Substitution Reactions in the Pyrolysis of Acetone Revealed through a Modeling, Experiment, Theory Paradigm. Journal of the American Chemical Society, 2021, 143, 3124-3142.	13.7	28
2	Adsorbate Partition Functions via Phase Space Integration: Quantifying the Effect of Translational Anharmonicity on Thermodynamic Properties. Journal of Physical Chemistry C, 2021, 125, 20249-20260.	3.1	9
3	Reactions of NO₃ with aromatic aldehydes: gas-phase kinetics and insights into the mechanism of the reaction. Atmospheric Chemistry and Physics, 2021, 21, 13537-13551.	4.9	7
4	Elaborated thermochemical treatment of HF, CO, N2, and H2O: Insight into HEAT and its extensions. Journal of Chemical Physics, 2021, 155, 184109.	3.0	15
5	Toward accurate high temperature anharmonic partition functions. Proceedings of the Combustion Institute, 2019, 37, 315-322.	3.9	10
6	Thermochemistry. Computer Aided Chemical Engineering, 2019, 45, 3-114.	0.5	31
7	An Automated Thermochemistry Protocol Based on Explicitly Correlated Coupled-Cluster Theory: The Methyl and Ethyl Peroxy Families. Journal of Physical Chemistry A, 2019, 123, 5673-5682.	2.5	6
8	High-accuracy extrapolated ab initio thermochemistry. IV. A modified recipe for computational efficiency. Journal of Chemical Physics, 2019, 150, 224102.	3.0	58
9	Active Thermochemical Tables: The Partition Function of Hydroxymethyl (CH2OH) Revisited. Journal of Physical Chemistry A, 2019, 123, 4212-4231.	2.5	13
10	Enthalpy of Formation of C₂H₂O₄ (Oxalic Acid) from High-Level Calculations and the Active Thermochemical Tables Approach. Journal of Physical Chemistry A, 2019, 123, 3481-3496.	2.5	9
11	A master equation simulation for the â€¢OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105.	3.0	42
12	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	31.2	980
13	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538.	4.6	20
14	Bond Dissociation Energies for Diatomic Molecules Containing 3d Transition Metals: Benchmark Scalar-Relativistic Coupled-Cluster Calculations for 20 Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1044-1056.	5.3	81
15	An Experimental and Theoretical Study of the Thermal Decomposition of C₄H₆ Isomers. Journal of Physical Chemistry A, 2017, 121, 3827-3850.	2.5	20
16	Thermal Decomposition of Potential Ester Biofuels. Part I: Methyl Acetate and Methyl Butanoate. Journal of Physical Chemistry A, 2017, 121, 4658-4677.	2.5	31
17	A vacuum ultraviolet laser pulsed field ionization-photoion study of methane (CH₄): determination of the appearance energy of methylium from methane with unprecedented precision and the resulting impact on the bond dissociation energies of CH₄and CH₄⁺. Physical Chemistry Chemical Physics, 2017, 19, 9592-9605.	2.8	21
18	Post-transition state dynamics and product energy partitioning following thermal excitation of the Fâ‹¯HCH2CN transition state: Disagreement with experiment. Journal of Chemical Physics, 2017, 147, 144301.	3.0	14

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19	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806.	2.5	33
20	Enthalpy of Formation of N₂H₄ (Hydrazine) Revisited. Journal of Physical Chemistry A, 2017, 121, 6187-6198.	2.5	31
21	Ab Initio Computations and Active Thermochemical Tables Hand in Hand: Heats of Formation of Core Combustion Species. Journal of Physical Chemistry A, 2017, 121, 6580-6602.	2.5	144
22	Time-Resolved Kinetic Chirped-Pulse Rotational Spectroscopy in a Room-Temperature Flow Reactor. Journal of Physical Chemistry Letters, 2017, 8, 6180-6188.	4.6	18
23	Standard electrode potentials involving radicals in aqueous solution: inorganic radicals (IUPAC) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.9	351
24	Active Thermochemical Tables: Sequential Bond Dissociation Enthalpies of Methane, Ethane, and Methanol and the Related Thermochemistry. Journal of Physical Chemistry A, 2015, 119, 7810-7837.	2.5	180
25	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.5	59
26	High-temperature chemistry of HCl and Cl2. Combustion and Flame, 2015, 162, 2693-2704.	5.2	41
27	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. Highlights in Theoretical Chemistry, 2015, , 31-46.	0.0	1
28	On the HCN â€“ HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934.	2.5	32
29	Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. Highlights in Theoretical Chemistry, 2015, , 191-202.	0.0	2
30	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. Theoretical Chemistry Accounts, 2014, 133, .	1.4	72
31	Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	95
32	Uncertainty quantification in thermochemistry, benchmarking electronic structure computations, and Active Thermochemical Tables. International Journal of Quantum Chemistry, 2014, 114, 1097-1101.	2.0	177
33	Electronic States of the Quasilinear Molecule Propargylene (HCCCH) from Negative Ion Photoelectron Spectroscopy. Journal of the American Chemical Society, 2014, 136, 10361-10372.	13.7	18
34	Active Thermochemical Tables: Water and Water Dimer. Journal of Physical Chemistry A, 2013, 117, 11940-11953.	2.5	99
35	Prompt NO formation in flames: The influence of NCN thermochemistry. Proceedings of the Combustion Institute, 2013, 34, 657-666.	3.9	31
36	Near-threshold shape resonance in the photoionization of 2-butyne. Journal of Chemical Physics, 2012, 136, 154303.	3.0	23

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37	Inhibition of hydrogen oxidation by HBr and Br2. Combustion and Flame, 2012, 159, 528-540.	5.2	31
38	Highâ€temperature rate constants for H/D + C₂H₆ and C₃H₈. International Journal of Chemical Kinetics, 2012, 44, 194-205.	1.6	45
39	Shock Tube and Theoretical Studies on the Thermal Decomposition of Propane: Evidence for a Roaming Radical Channel. Journal of Physical Chemistry A, 2011, 115, 3366-3379.	2.5	57
40	Rate Constants for the Thermal Decomposition of Ethanol and Its Bimolecular Reactions with OH and D: Reflected Shock Tube and Theoretical Studies. Journal of Physical Chemistry A, 2010, 114, 9425-9439.	2.5	139
41	Heats of Formation of C₆H₅^{â€¢}, C₆H₅⁺, and C₆H₅NO by Threshold Photoelectron Photoion Coincidence and Active Thermochemical Tables Analysis. Journal of Physical Chemistry A, 2010, 114, 13134-13145.	2.5	87
42	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. Chemical Physics, 2009, 356, 14-24.	1.9	92
43	Thermal Decomposition of NH₂OH and Subsequent Reactions: Ab Initio Transition State Theory and Reflected Shock Tube Experiments. Journal of Physical Chemistry A, 2009, 113, 10241-10259.	2.5	86
44	IS HO⁺₂A DETECTABLE INTERSTELLAR MOLECULE?. Astrophysical Journal, 2009, 697, 601-609.	4.5	35
45	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	1.9	37
46	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	3.0	367
47	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
48	Kinetics of the Reaction of Methyl Radical with Hydroxyl Radical and Methanol Decompositionâ€. Journal of Physical Chemistry A, 2007, 111, 3932-3950.	2.5	188
49	Portal-based Knowledge Environment for Collaborative Science. Concurrency Computation Practice and Experience, 2007, 19, 1703-1716.	2.2	9
50	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Bornâ€“Oppenheimer corrections for a â€˜simpleâ€™ organic molecule. Computational and Theoretical Chemistry, 2007, 811, 345-353.	1.5	60
51	Active Thermochemical Tables:Â Accurate Enthalpy of Formation of Hydroperoxyl Radical, HO2â€. Journal of Physical Chemistry A, 2006, 110, 6592-6601.	2.5	255
52	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. Journal of Chemical Physics, 2006, 125, 144108.	3.0	646
53	Reflected Shock Tube Studies of High-Temperature Rate Constants for OH + NO2â†’ HO2+ NO and OH + HO2â†’ H2O + O2â€. Journal of Physical Chemistry A, 2006, 110, 6602-6607.	2.5	50
54	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. ChemPhysChem, 2006, 7, 1664-1667.	2.1	45

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55	Direct identification of propargyl radical in combustion flames by vacuum ultraviolet photoionization mass spectrometry. Journal of Chemical Physics, 2006, 124, 074302.	3.0	36
56	Theoretical calculations on the reaction of ethylene with oxygen. Chemical Physics, 2005, 311, 335-341.	1.9	15
57	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part 1.. ChemInform, 2005, 36, no.	0.0	1
58	A Collaborative Informatics Infrastructure for Multi-Scale Science. Cluster Computing, 2005, 8, 243-253.	5.0	18
59	Pulsed field-ionization photoelectron-photoion coincidence study of the process N2+hÎ½â†'N++N+eâ^': Bond dissociation energies of N2 and N2+. Journal of Chemical Physics, 2005, 123, 074330.	3.0	50
60	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	4.2	283
61	Active Thermochemical Tables: thermochemistry for the 21st century. Journal of Physics: Conference Series, 2005, 16, 561-570.	0.4	360
62	Introduction to Active Thermochemical Tables:Â Several â€œKeyâ€•Enthalpies of Formation Revisitedâ€. Journal of Physical Chemistry A, 2004, 108, 9979-9997.	2.5	582
63	Hartreeâ€“Fock and density functional complete basis-set (CBS) predicted nuclear shielding anisotropy and shielding tensor components. Solid State Nuclear Magnetic Resonance, 2003, 23, 145-167.	2.3	25
64	Theoretical investigation of the transition states leading to HCI elimination in 2-chloropropene. Molecular Physics, 2002, 100, 865-874.	1.7	10
65	Toward Hartreeâ^'Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. Journal of Physical Chemistry A, 2002, 106, 10396-10407.	2.5	68
66	On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. Journal of Physical Chemistry A, 2002, 106, 2727-2747.	2.5	466
67	A Grid Service-Based Active Thermochemical Table Framework. Lecture Notes in Computer Science, 2002, , 25-38.	1.3	6
68	Evidence for a Lower Enthalpy of Formation of Hydroxyl Radical and a Lower Gas-Phase Bond Dissociation Energy of Water. Journal of Physical Chemistry A, 2001, 105, 1-4.	2.5	175
69	Photoionization of HOCO revisited: a new upper limit to the adiabatic ionization energy and lower limit to the enthalpy of formation. Chemical Physics Letters, 2000, 316, 45-50.	2.6	58
70	Characterization of nitrogen-containing radical products from the photodissociation of trimethylamine using photoionization detection. Journal of Chemical Physics, 2000, 113, 3088-3097.	3.0	11
71	Ionization Energy of Methylene Revisited:Â Improved Values for the Enthalpy of Formation of CH2and the Bond Dissociation Energy of CH3via Simultaneous Solution of the Local Thermochemical Network. Journal of Physical Chemistry A, 1999, 103, 8625-8633.	2.5	121
72	A photoionization study of the hydroperoxyl radical, HO2, and hydrogen peroxide, H2O2,. Journal of Electron Spectroscopy and Related Phenomena, 1998, 97, 131-146.	1.7	92

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73	Simultaneous Adjustment of Experimentally Based Enthalpies of Formation of CF3X, X = nil, H, Cl, Br, I, CF3, CN, and a Probe of G3 Theory. Journal of Physical Chemistry A, 1998, 102, 10889-10899.	2.5	77
74	Direct observation of the ionization threshold of triplet methylene by photoionization mass spectrometry. Journal of Chemical Physics, 1998, 108, 6748-6755.	3.0	26
75	On the heats of formation of trifluoromethyl radical CF3and its cation CF3+. Journal of Chemical Physics, 1997, 106, 210-221.	3.0	81
76	Evidence of rotational autoionization in the threshold region of the photoionization spectrum of CH3. Journal of Chemical Physics, 1997, 107, 9852-9856.	3.0	34
77	A photoionization study of trifluoromethanol, CF3OH, trifluoromethyl hypofluorite, CF3OF, and trifluoromethyl hypochlorite, CF3OCl. Journal of Chemical Physics, 1997, 106, 9111-9121.	3.0	28
78	On the heat of formation of carbonyl fluoride, CF2O. Journal of Chemical Physics, 1996, 105, 9781-9795.	3.0	42
79	Photoionization of atomic bismuth. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 1743-1759.	1.5	2
80	Experimental determination of Î”H0f(HOBr) and ionization potentials (HOBr): Implications for corresponding properties of HOI. Journal of Chemical Physics, 1994, 101, 7795-7803.	3.0	66
81	Threshold photoelectron spectrum of HOBr. Journal of Chemical Physics, 1994, 101, 9215-9218.	3.0	9
82	The Hâ€“NCO bond energy and Î”H0f (NCO) from photoionization mass spectrometric studies of HNCO and NCO. Journal of Chemical Physics, 1994, 100, 4498-4508.	3.0	59
83	The Hâ€“NCS bond energy, Î”Hâ—‹f (HNCS), Î”Hâ—‹f (NCS), and IP(NCS) from photoionization mass spectrometric studies of HNCS, NCS, and (NCS)2. Journal of Chemical Physics, 1994, 101, 7975-7989.	3.0	33
84	The heats of formation of some C2H5O+ isomers, relevant bond energies in ethanol and PA(CH3CHO). Journal of Chemical Physics, 1994, 101, 10936-10946.	3.0	70
85	Photoionization of Group V trimers and tetramers. Journal of Electron Spectroscopy and Related Phenomena, 1993, 66, 39-54.	1.7	10
86	Heat of formation of hydroxymethyl and methanol D0(H-CH2OH). The Journal of Physical Chemistry, 1993, 97, 11451-11455.	2.9	61
87	Photoionization mass spectrometry of CH2S and HCS. Journal of Chemical Physics, 1993, 98, 2568-2579.	3.0	84
88	Photoionization mass spectrometric studies of Sb2 and Bi2. Journal of Chemical Physics, 1993, 99, 8445-8450.	3.0	11
89	Determination of consecutive bond energies by photoionization of SbHn (n=1â€“3). Journal of Chemical Physics, 1993, 99, 5840-5848.	3.0	4
90	Photoionization mass spectrometric studies of the isomeric transient species CH2SH and CH3S. Journal of Chemical Physics, 1992, 97, 1818-1823.	3.0	61

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91	Photoionization of As2and As4: Implications for group V clusters. Journal of Chemical Physics, 1992, 96, 6696-6709.	3.0	32
92	Vacuum ultraviolet photoionization mass spectrometric study of C60. Journal of Chemical Physics, 1992, 96, 911-918.	3.0	195
93	Three laws for D0 (BiF). Chemical Physics, 1992, 166, 215-227.	1.9	15
94	Photoionization mass spectrometric study of CH3OF. Journal of Chemical Physics, 1991, 95, 7957-7961.	3.0	26
95	Some recent developments in the chemistry of hypofluorites. Journal of Fluorine Chemistry, 1991, 54, 1.	1.7	1
96	Photoionization mass spectrometric study of N2H2and N2H3: Nâ€“H, N=N bond energies and proton affinity of N2. Journal of Chemical Physics, 1991, 95, 4378-4384.	3.0	59
97	Photoionization mass spectrometric studies of the isomeric transient species CD2OH and CD3O. Journal of Chemical Physics, 1991, 95, 4033-4039.	3.0	76
98	Photoionization mass spectrometric study of Si2H6. Journal of Chemical Physics, 1991, 95, 2407-2415.	3.0	28
99	Photoionization mass spectrometric studies of the transient species Si2Hn (n=2â€“5). Journal of Chemical Physics, 1991, 95, 2416-2432.	3.0	72
100	Photoionâ€pair formation and photoelectronâ€induced dissociative attachment in C2H2:D0(HCCâ€“H). Journal of Chemical Physics, 1990, 93, 5586-5593.	3.0	41
101	Photoionization studies of GeHn (n=2â€“4). Journal of Chemical Physics, 1990, 92, 1865-1875.	3.0	94
102	Electric field effects in the photoionization of N2near threshold. Journal of Chemical Physics, 1990, 93, 1741-1746.	3.0	17
103	Photoionization of HBr and DBr near threshold. Journal of Chemical Physics, 1990, 93, 1747-1754.	3.0	12
104	Autoionization in atomic chlorine: Comparison of theories and experiment. Physical Review A, 1989, 40, 6716-6718.	2.5	9
105	A photoionization study of the COOH species. Journal of Chemical Physics, 1989, 91, 6780-6785.	3.0	84
106	Mechanisms of photodissociative ionization of HCOOH: The heat of formation of COOH+. Journal of Chemical Physics, 1989, 91, 6772-6779.	3.0	28
107	The ethyl radical: Photoionization and theoretical studies. Journal of Chemical Physics, 1989, 91, 114-121.	3.0	108
108	Photoelectron spectra, electronic structure and long-range electronic interaction in some steroids. Pure and Applied Chemistry, 1989, 61, 2139-2150.	1.9	22

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109	Bonding and structure in the hydrides of groups III-VI deduced from photoionization studies. Computational and Theoretical Chemistry, 1989, 202, 363-373.	1.5	2
110	Photoion-pair formation in Cl2. Chemical Physics, 1988, 123, 317-328.	1.9	19
111	Electrochemical separation of the inner monolayer in methylene blue/leucomethylene blue conductive films induced by a sulphur-modified gold surface. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1988, 250, 427-442.	0.1	20
112	Photochemical formation and transport of ozone in Athens, Greece. Atmospheric Environment, 1988, 22, 1855-1861.	1.0	79
113	Photoionization studies of (BH3)n(n=1,2). Journal of Chemical Physics, 1988, 88, 5580-5593.	3.0	106
114	A photoionization study of the vinyl radical. Journal of Chemical Physics, 1988, 88, 7396-7404.	3.0	61
115	Photoionization mass spectrometric studies of SiHn (n=1â€“4). Journal of Chemical Physics, 1987, 86, 1235-1248.	3.0	263
116	The ionization potentials of CH4 and CD4. Journal of Chemical Physics, 1987, 86, 674-676.	3.0	86
117	Superstructural ordering in low-temperature phase of superionic Cu2Se. Solid State Ionics, 1987, 23, 37-47.	2.7	53
118	On the empirical correlation schemes for ionization energies in ring compounds. Journal of Electron Spectroscopy and Related Phenomena, 1987, 43, 147-154.	1.7	10
119	Photoelectron spectra of Ga20, In20 and Tl20. Journal of Electron Spectroscopy and Related Phenomena, 1986, 41, 357-384.	1.7	7
120	On the generalized approach to the structure count. Theoretica Chimica Acta, 1986, 69, 107-117.	0.8	10
121	Photoionisation of atomic sulphur. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, 2825-2840.	1.6	36
122	Photoionisation of atomic selenium. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, 2841-2845.	1.6	15
123	Fourier transform photoelectron spectroscopy: The correlation function and the harmonic oscillator approximation. Journal of Chemical Physics, 1986, 85, 3776-3784.	3.0	11
124	Substitution Effects on Electronic Structure of Thiophene. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1985, 40, 1214-1218.	0.7	11
125	Application of photoelectron spectroscopy to biologically active molecules and their constituent parts XI: Steroids. International Journal of Quantum Chemistry, 1985, 28, 161-167.	2.0	3
126	Photoionisation of atomic fluorine. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, L79-L83.	1.6	22

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127	Photoionisation of atomic bromine. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 1503-1514.	1.6	51
128	Application of photoelectron spectroscopy to biologically active molecules and their constituent parts. IX. 1,4-Benzodiazepin-2-ones. International Journal of Quantum Chemistry, 1983, 23, 1667-1676.	2.0	7
129	Photoelectron spectra of the lanthanide trihalides and their interpretation. Journal of Chemical Physics, 1983, 78, 5443-5467.	3.0	50
130	Photoionization of Atomic Chlorine. Physical Review Letters, 1983, 50, 675-678.	7.8	77
131	Photoelectron spectra of and ab initio calculations on chlorobenzenes. 1. Chlorobenzene and dichlorobenzenes. The Journal of Physical Chemistry, 1981, 85, 1486-1489.	2.9	46
132	Photoelectron spectra of and ab initio calculations on chlorobenzenes. 2. Trichlorobenzenes, tetrachlorobenzenes, and pentachlorobenzene. The Journal of Physical Chemistry, 1981, 85, 1490-1495.	2.9	17
133	Photoelectron spectra of and ab initio calculations on chlorobenzenes. 3. Hexachlorobenzene. The Journal of Physical Chemistry, 1981, 85, 1495-1497.	2.9	7
134	Application of photoelectron spectroscopy to biologically active molecules and their constituent parts. 6. Opiate narcotics. Journal of the American Chemical Society, 1979, 101, 7477-7482.	13.7	20
135	Photoelectron Spectroscopy of Heterocycles. Fluorene Analogues. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1978, 33, 1006-1012.	1.5	46
136	Photoelectron spectroscopy of the heterocycles imidazole and methylimidazoles. International Journal of Quantum Chemistry, 1978, 14, 367-371.	2.0	9
137	Photoelectron Spectroscopy of Substituted N-Benzylideneanilines. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1977, 32, 1291-1295.	0.7	9
138	Photoelectron Spectroscopy of Heterocycles. Indene Analogs. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1976, 31, 1051-1056.	1.5	37
139	Graph theory and molecular orbitals. XII. Acyclic polyenes. Journal of Chemical Physics, 1975, 62, 3399.	3.0	588
140	A collaborative informatics infrastructure for multi-scale science. , 0, , .		16
141	Active Thermochemical Tables: the thermophysical and thermochemical properties of methyl, CH3, and methylene, CH2, corrected for nonrigid rotor and anharmonic oscillator effects. Molecular Physics, 0, , e1969046.	1.7	12