Branko Ruscic

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	31.2	980
2	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. Journal of Chemical Physics, 2006, 125, 144108.	3.0	646
3	Graph theory and molecular orbitals. XII. Acyclic polyenes. Journal of Chemical Physics, 1975, 62, 3399.	3.0	588
4	Introduction to Active Thermochemical Tables: Several "Key―Enthalpies of Formation Revisitedâ€. Journal of Physical Chemistry A, 2004, 108, 9979-9997.	2.5	582
5	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
6	High-accuracy extrapolated <i>ab initio</i> thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	3.0	367
7	Active Thermochemical Tables: thermochemistry for the 21st century. Journal of Physics: Conference Series, 2005, 16, 561-570.	0.4	360

$_{8}$ Standard electrode potentials involving radicals in aqueous solution: inorganic radicals (IUPAC) Tj ETQq0 0 0 rgBT /Overlock $_{10}^{10}$ Tf 50 46

9	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
10	Photoionization mass spectrometric studies of SiHn (n=1–4). Journal of Chemical Physics, 1987, 86, 1235-1248.	3.0	263
11	Active Thermochemical Tables: Accurate Enthalpy of Formation of Hydroperoxyl Radical, HO2â€. Journal of Physical Chemistry A, 2006, 110, 6592-6601.	2.5	255
12	Vacuum ultraviolet photoionization mass spectrometric study of C60. Journal of Chemical Physics, 1992, 96, 911-918.	3.0	195
13	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
14	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
15	Uncertainty quantification in thermochemistry, benchmarking electronic structure computations, and Active Thermochemical Tables. International Journal of Quantum Chemistry, 2014, 114, 1097-1101.	2.0	177
16	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
17	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
18	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

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19	lonization 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
20	The ethyl radical: Photoionization and theoretical studies. Journal of Chemical Physics, 1989, 91, 114-121.	3.0	108
21	Photoionization studies of (BH3)n(n=1,2). Journal of Chemical Physics, 1988, 88, 5580-5593.	3.0	106
22	Active Thermochemical Tables: Water and Water Dimer. Journal of Physical Chemistry A, 2013, 117, 11940-11953.	2.5	99
23	Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	95
24	Photoionization studies of GeHn (n=2–4). Journal of Chemical Physics, 1990, 92, 1865-1875.	3.0	94
25	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
26	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. Chemical Physics, 2009, 356, 14-24.	1.9	92
27	Heats of Formation of C ₆ H ₅ [•] , C ₆ H ₅ ⁺ , and C ₆ H ₅ NO by Threshold Photoelectron Photoion Coincidence and Active Thermochemical Tables Analysis. Journal of Physical Chemistry A. 2010. 114. 13134-13145.	2.5	87
28	The ionization potentials of CH4 and CD4. Journal of Chemical Physics, 1987, 86, 674-676.	3.0	86
29	Thermal Decomposition of NH ₂ OH 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
30	A photoionization study of the COOH species. Journal of Chemical Physics, 1989, 91, 6780-6785.	3.0	84
31	Photoionization mass spectrometry of CH2S and HCS. Journal of Chemical Physics, 1993, 98, 2568-2579.	3.0	84
32	On the heats of formation of trifluoromethyl radical CF3and its cation CF3+. Journal of Chemical Physics, 1997, 106, 210-221.	3.0	81
33	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
34	Photochemical formation and transport of ozone in Athens, Greece. Atmospheric Environment, 1988, 22, 1855-1861.	1.0	79
35	Photoionization of Atomic Chlorine. Physical Review Letters, 1983, 50, 675-678.	7.8	77
36	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

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37	Photoionization mass spectrometric studies of the isomeric transient species CD2OH and CD3O. Journal of Chemical Physics, 1991, 95, 4033-4039.	3.0	76
38	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
39	Photoionization mass spectrometric studies of the transient species Si2Hn (n=2–5). Journal of Chemical Physics, 1991, 95, 2416-2432.	3.0	72
40	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. Theoretical Chemistry Accounts, 2014, 133, .	1.4	72
41	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
42	Toward Hartreeâ^'Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. Journal of Physical Chemistry A, 2002, 106, 10396-10407.	2.5	68
43	Experimental determination of ΔH0f(HOBr) and ionization potentials (HOBr): Implications for corresponding properties of HOI. Journal of Chemical Physics, 1994, 101, 7795-7803.	3.0	66
44	A photoionization study of the vinyl radical. Journal of Chemical Physics, 1988, 88, 7396-7404.	3.0	61
45	Photoionization mass spectrometric studies of the isomeric transient species CH2SH and CH3S. Journal of Chemical Physics, 1992, 97, 1818-1823.	3.0	61
46	Heat of formation of hydroxymethyl and methanol D0(H-CH2OH). The Journal of Physical Chemistry, 1993, 97, 11451-11455.	2.9	61
47	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Born–Oppenheimer corrections for a â€̃simple' organic molecule. Computational and Theoretical Chemistry, 2007, 811, 345-353.	1.5	60
48	Photoionization mass spectrometric study of N2H2and N2H3: N–H, N=N bond energies and proton affinity of N2. Journal of Chemical Physics, 1991, 95, 4378-4384.	3.0	59
49	The H–NCO bond energy and ΔH0f (NCO) from photoionization mass spectrometric studies of HNCO and NCO. Journal of Chemical Physics, 1994, 100, 4498-4508.	3.0	59
50	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.5	59
51	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
52	High-accuracy extrapolated <i>ab initio</i> thermochemistry. IV. A modified recipe for computational efficiency. Journal of Chemical Physics, 2019, 150, 224102.	3.0	58
53	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
54	Superstructural ordering in low-temperature phase of superionic Cu2Se. Solid State Ionics, 1987, 23, 37-47.	2.7	53

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55	Photoionisation of atomic bromine. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 1503-1514.	1.6	51
56	Photoelectron spectra of the lanthanide trihalides and their interpretation. Journal of Chemical Physics, 1983, 78, 5443-5467.	3.0	50
57	Pulsed field-ionization photoelectron-photoion coincidence study of the process N2+hν→N++N+eâ^': Bond dissociation energies of N2 and N2+. Journal of Chemical Physics, 2005, 123, 074330.	3.0	50
58	Reflected Shock Tube Studies of High-Temperature Rate Constants for OH + NO2→ HO2+ NO and OH + HO2→ H2O + O2â€. Journal of Physical Chemistry A, 2006, 110, 6602-6607.	2.5	50
59	Photoelectron Spectroscopy of Heterocycles. Fluorene Analogues. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1978, 33, 1006-1012.	1.5	46
60	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
61	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
62	Highâ€ŧemperature rate constants for H/D + C ₂ H ₆ and C ₃ H ₈ . International Journal of Chemical Kinetics, 2012, 44, 194-205.	1.6	45
63	On the heat of formation of carbonyl fluoride, CF2O. Journal of Chemical Physics, 1996, 105, 9781-9795.	3.0	42
64	A master equation simulation for the •OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105.	3.0	42
65	Photoionâ€pair formation and photoelectronâ€induced dissociative attachment in C2H2:D0(HCC–H). Journal of Chemical Physics, 1990, 93, 5586-5593.	3.0	41
66	High-temperature chemistry of HCl and Cl2. Combustion and Flame, 2015, 162, 2693-2704.	5.2	41
67	Photoelectron Spectroscopy of Heterocycles. Indene Analogs. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1976, 31, 1051-1056.	1.5	37
68	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	1.9	37
69	Photoionisation of atomic sulphur. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, 2825-2840.	1.6	36
70	Direct identification of propargyl radical in combustion flames by vacuum ultraviolet photoionization mass spectrometry. Journal of Chemical Physics, 2006, 124, 074302.	3.0	36
71	IS HO ⁺ ₂ A DETECTABLE INTERSTELLAR MOLECULE?. Astrophysical Journal, 2009, 697, 601-609.	4.5	35
72	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

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73	The H–NCS bond energy, ΔH○f (HNCS), ΔH○f (NCS), and IP(NCS) from photoionization mass spectromet studies of HNCS, NCS, and (NCS)2. Journal of Chemical Physics, 1994, 101, 7975-7989.	ric _{3.0}	33
74	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806.	2.5	33
75	Photoionization of As2and As4: Implications for group V clusters. Journal of Chemical Physics, 1992, 96, 6696-6709.	3.0	32
76	On the HCN – HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934.	2.5	32
77	Inhibition of hydrogen oxidation by HBr and Br2. Combustion and Flame, 2012, 159, 528-540.	5.2	31
78	Prompt NO formation in flames: The influence of NCN thermochemistry. Proceedings of the Combustion Institute, 2013, 34, 657-666.	3.9	31
79	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
80	Enthalpy of Formation of N ₂ H ₄ (Hydrazine) Revisited. Journal of Physical Chemistry A, 2017, 121, 6187-6198.	2.5	31
81	Thermochemistry. Computer Aided Chemical Engineering, 2019, 45, 3-114.	0.5	31
82	Mechanisms of photodissociative ionization of HCOOH: The heat of formation of COOH+. Journal of Chemical Physics, 1989, 91, 6772-6779.	3.0	28
83	Photoionization mass spectrometric study of Si2H6. Journal of Chemical Physics, 1991, 95, 2407-2415.	3.0	28
84	A photoionization study of trifluoromethanol, CF3OH, trifluoromethyl hypofluorite, CF3OF, and trifluoromethyl hypochlorite, CF3OCI. Journal of Chemical Physics, 1997, 106, 9111-9121.	3.0	28
85	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
86	Photoionization mass spectrometric study of CH3OF. Journal of Chemical Physics, 1991, 95, 7957-7961.	3.0	26
87	Direct observation of the ionization threshold of triplet methylene by photoionization mass spectrometry. Journal of Chemical Physics, 1998, 108, 6748-6755.	3.0	26
88	Hartree–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
89	Near-threshold shape resonance in the photoionization of 2-butyne. Journal of Chemical Physics, 2012, 136, 154303.	3.0	23
90	Photoionisation of atomic fluorine. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, L79-L83.	1.6	22

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91	Photoelectron spectra, electronic structure and long-range electronic interaction in some steroids. Pure and Applied Chemistry, 1989, 61, 2139-2150.	1.9	22
92	A vacuum ultraviolet laser pulsed field ionization-photoion study of methane (CH ₄): determination of the appearance energy of methylium from methane with unprecedented precision and the resulting impact on the bond dissociation energies of CH ₄ and CH ₄ ⁺ . Physical Chemistry Chemical Physics, 2017, 19, 9592-9605.	2.8	21
93	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
94	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
95	An Experimental and Theoretical Study of the Thermal Decomposition of C ₄ H ₆ Isomers. Journal of Physical Chemistry A, 2017, 121, 3827-3850.	2.5	20
96	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538.	4.6	20
97	Photoion-pair formation in Cl2. Chemical Physics, 1988, 123, 317-328.	1.9	19
98	A Collaborative Informatics Infrastructure for Multi-Scale Science. Cluster Computing, 2005, 8, 243-253.	5.0	18
99	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
100	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
101	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
102	Electric field effects in the photoionization of N2near threshold. Journal of Chemical Physics, 1990, 93, 1741-1746.	3.0	17
103	A collaborative informatics infrastructure for multi-scale science. , 0, , .		16
104	Photoionisation of atomic selenium. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, 2841-2845.	1.6	15
105	Three laws for D0 (BiF). Chemical Physics, 1992, 166, 215-227.	1.9	15
106	Theoretical calculations on the reaction of ethylene with oxygen. Chemical Physics, 2005, 311, 335-341.	1.9	15
107	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
108	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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109	Active Thermochemical Tables: The Partition Function of Hydroxymethyl (CH2OH) Revisited. Journal of Physical Chemistry A, 2019, 123, 4212-4231.	2.5	13
110	Photoionization of HBr and DBr near threshold. Journal of Chemical Physics, 1990, 93, 1747-1754.	3.0	12
111	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
112	Substitution Effects on Electronic Structure of Thiophene. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1985, 40, 1214-1218.	0.7	11
113	Fourier transform photoelectron spectroscopy: The correlation function and the harmonic oscillator approximation. Journal of Chemical Physics, 1986, 85, 3776-3784.	3.0	11
114	Photoionization mass spectrometric studies of Sb2 and Bi2. Journal of Chemical Physics, 1993, 99, 8445-8450.	3.0	11
115	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
116	On the generalized approach to the structure count. Theoretica Chimica Acta, 1986, 69, 107-117.	0.8	10
117	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
118	Photoionization of Group V trimers and tetramers. Journal of Electron Spectroscopy and Related Phenomena, 1993, 66, 39-54.	1.7	10
119	Theoretical investigation of the transition states leading to HCI elimination in 2-chloropropene. Molecular Physics, 2002, 100, 865-874.	1.7	10
120	Toward accurate high temperature anharmonic partition functions. Proceedings of the Combustion Institute, 2019, 37, 315-322.	3.9	10
121	Photoelectron Spectroscopy of Substituted N-Benzylideneanilines. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1977, 32, 1291-1295.	0.7	9
122	Autoionization in atomic chlorine: Comparison of theories and experiment. Physical Review A, 1989, 40, 6716-6718.	2.5	9
123	Threshold photoelectron spectrum of HOBr. Journal of Chemical Physics, 1994, 101, 9215-9218.	3.0	9
124	Portal-based Knowledge Environment for Collaborative Science. Concurrency Computation Practice and Experience, 2007, 19, 1703-1716.	2.2	9
125	Photoelectron spectroscopy of the heterocycles imidazole and methylimidazoles. International Journal of Quantum Chemistry, 1978, 14, 367-371.	2.0	9
126	Enthalpy of Formation of C ₂ H ₂ O ₄ (Oxalic Acid) from High-Level Calculations and the Active Thermochemical Tables Approach. Journal of Physical Chemistry A, 2019, 123, 3481-3496.	2.5	9

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127	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
128	Photoelectron spectra of and ab initio calculations on chlorobenzenes. 3. Hexachlorobenzene. The Journal of Physical Chemistry, 1981, 85, 1495-1497.	2.9	7
129	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
130	Photoelectron spectra of Ga20, In20 and Tl20. Journal of Electron Spectroscopy and Related Phenomena, 1986, 41, 357-384.	1.7	7
131	Reactions of NO ₃ 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
132	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
133	A Grid Service-Based Active Thermochemical Table Framework. Lecture Notes in Computer Science, 2002, , 25-38.	1.3	6
134	Determination of consecutive bond energies by photoionization of SbHn (n=1–3). Journal of Chemical Physics, 1993, 99, 5840-5848.	3.0	4
135	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
136	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
137	Photoionization of atomic bismuth. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 1743-1759.	1.5	2
138	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
139	Some recent developments in the chemistry of hypofluorites. Journal of Fluorine Chemistry, 1991, 54, 1.	1.7	1
140	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part 1 ChemInform, 2005, 36, no.	0.0	1
141	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. Highlights in Theoretical Chemistry, 2015, , 31-46.	0.0	1