David F Feller

List of Publications by Citations

183 papers	16,246 citations	64 h-index	124 g-index
189 ext. papers	17,073 ext. citations	5.3 avg, IF	6.87 L-index

#	Paper	IF	Citations
183	The role of databases in support of computational chemistry calculations. *Journal of Computational Chemistry*, **1996**, 17, 1571-1586	3.5	1909
182	Application of systematic sequences of wave functions to the water dimer. *Journal of Chemical Physics*, **1992**, 96, 6104-6114	3.9	1007
181	Basis set selection for molecular calculations. *Chemical Reviews*, **1986**, 86, 681-696	68.1	680
180	The use of systematic sequences of wave functions for estimating the complete basis set, full configuration interaction limit in water. *Journal of Chemical Physics*, **1993**, 98, 7059-7071	3.9	526
179	Hydrogen Bond Energy of the Water Dimer. *The Journal of Physical Chemistry*, **1996**, 100, 2993-2997		433
178	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	2.8	422
177	An Ab Initio Investigation of the Structure and Alkali Metal Cation Selectivity of 18-Crown-6. *Journal of the American Chemical Society*, **1994**, 116, 10657-10669	16.4	335
176	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	317
175	A survey of factors contributing to accurate theoretical predictions of atomization energies and molecular structures. *Journal of Chemical Physics*, **2008**, 129, 204105	3.9	302
174	Re-examination of atomization energies for the Gaussian-2 set of molecules. *Journal of Chemical Physics*, **1999**, 110, 8384-8396	3.9	251
173	Extended benchmark studies of coupled cluster theory through triple excitations. *Journal of Chemical Physics*, **2001**, 115, 3484-3496	3.9	236
172	An examination of intrinsic errors in electronic structure methods using the Environmental Molecular Sciences Laboratory computational results database and the Gaussian-2 set. *Journal of Chemical Physics*, **1998**, 108, 154-176	3.9	235
171	Cation-Water Interactions: The M+(H2O)n Clusters for Alkali Metals, M = Li, Na, K, Rb, and Cs. *The Journal of Physical Chemistry*, **1995**, 99, 3060-3067		222
170	One-electron properties of several small molecules using near Hartree–Fock limit basis sets. *Journal of Chemical Physics*, **1987**, 86, 3424-3440	3.9	221
169	An extended basis set ab initio study of alkali metal cation–water clusters. *Journal of Chemical Physics*, **1995**, 103, 3526-3542	3.9	214
168	On the effectiveness of CCSD(T) complete basis set extrapolations for atomization energies. *Journal of Chemical Physics*, **2011**, 135, 044102	3.9	210
167	Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. *Journal of Chemical Physics*, **2003**, 118, 3510-3522	3.9	184

166	An approximation to frozen natural orbitals through the use of the Hartree–Fock exchange potential. *Journal of Chemical Physics*, **1981**, 74, 3977-3979	3.9	184
165	Enthalpies of formation of gas-phase N3, N3-, N5+, and N5- from Ab initio molecular orbital theory, stability predictions for N5(+)N3(-) and N5(+)N5(-), and experimental evidence for the instability of N5(+)N3(-). *Journal of the American Chemical Society*, **2004**, 126, 834-43	16.4	182
164	Electron momentum spectroscopy of the valence orbitals of H2O and D2O: Quantitative comparisons using Hartree–Fock limit and correlated wavefunctions. *Chemical Physics*, **1987**, 113, 19-42	2.3	169
163	Sources of error in electronic structure calculations on small chemical systems. *Journal of Chemical Physics*, **2006**, 124, 054107	3.9	168
162	Performance of CCSDT for diatomic dissociation energies. *Journal of Chemical Physics*, **2000**, 113, 485-493	3.9	168
161	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	2.8	161
160	Ab initio configuration interaction calculations of the hyperfine structure in small radicals. *Journal of Chemical Physics*, **1984**, 80, 1006-1017	3.9	158
159	The Nature of K+/Crown Ether Interactions: A Hybrid Quantum Mechanical-Molecular Mechanical Study. *The Journal of Physical Chemistry*, **1994**, 98, 10465-10476		154
158	An extended basis set ab initio study of Li+(H2O)n, n=1–5. *Journal of Chemical Physics*, **1994**, 100, 4981-4997	3.9	151
157	Systematic approach to extended even-tempered orbital bases for atomic and molecular calculations. *Theoretica Chimica Acta*, **1979**, 52, 231-251		151
156	Predicting the Heats of Formation of Model Hydrocarbons up to Benzene. *Journal of Physical Chemistry A*, **2000**, 104, 3048-3056	2.8	140
155	Cation–Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+(1,2-dimethoxyethane)x, x = 1 and 2, and Li+(12-crown-4). *The Journal of Physical Chemistry*, **1996**, 100, 16116-16125		140
154	Dication–Water Interactions: M2+(H2O)n Clusters for Alkaline Earth Metals M = Mg, Ca, Sr, Ba, and Ra. *The Journal of Physical Chemistry*, **1996**, 100, 4790-4797		140
153	Further benchmarks of a composite, convergent, statistically calibrated coupled-cluster-based approach for thermochemical and spectroscopic studies. *Molecular Physics*, **2012**, 110, 2381-2399	1.7	139
152	Cation–Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+[O(CH3)2]x, x = 1–4. *The Journal of Physical Chemistry*, **1996**, 100, 1605-1614		138
151	Strength of the Benzene–Water Hydrogen Bond. *Journal of Physical Chemistry A*, **1999**, 103, 7558-7561	2.8	136
150	Heats of Formation of Simple Perfluorinated Carbon Compounds. *Journal of Physical Chemistry A*, **1999**, 103, 4744-4751	2.8	129
149	Estimating the Strength of the Water/Single-Layer Graphite Interaction. *Journal of Physical Chemistry A*, **2000**, 104, 9971-9975	2.8	119

148	Theoretical Study of the Heats of Formation of Small Silicon-Containing Compounds. *Journal of Physical Chemistry A*, **1999**, 103, 6413-6419	2.8	118
147	Binding Enthalpies for Alkali CationBenzene Complexes Revisited. *Journal of Physical Chemistry A*, **2000**, 104, 11414-11419	2.8	115
146	Heats of formation and ionization energies of NHx, x=0 3. *Journal of Chemical Physics*, **2001**, 115, 2576-2581	3.9	112
145	Experimental evidence for a C2v (2B1) ground-state structure of the methane cation radical: ESR and ab initio CI investigations of methane cation radicals (CH4+ and CD2H2+) in neon matrixes at 4 K. *Journal of the American Chemical Society*, **1984**, 106, 3700-3701	16.4	108
144	A CCSDT study of the effects of higher order correlation on spectroscopic constants. I. First row diatomic hydrides. *Journal of Chemical Physics*, **2000**, 112, 5604-5610	3.9	107
143	Structures and binding enthalpies of M+(H2O)n clusters, M=Cu, Ag, Au. *Journal of Chemical Physics*, **1999**, 110, 1475-1491	3.9	105
142	Ab InitioStudy of M+:18-Crown-6 Microsolvation. *Journal of Physical Chemistry A*, **1997**, 101, 2723-2731	2.8	103
141	Heats of Formation of CF2, FCO, and CF2O. *Journal of Physical Chemistry A*, **1998**, 102, 8209-8216	2.8	100
140	Coupled Cluster Theory Determination of the Heats of Formation of Combustion-Related Compounds: CO, HCO, CO2, HCO2, HOCO, HC(O)OH, and HC(O)OOH. *Journal of Physical Chemistry A*, **2003**, 107, 1604-1617	2.8	94
139	A multireference CI determination of the isotropic hyperfine constants for first row atoms B E. *Journal of Chemical Physics*, **1988**, 88, 7580-7587	3.9	93
138	Ab initio study of hydrogen bonding in the phenol water system. *Journal of Computational Chemistry*, **1993**, 14, 1027-1035	3.5	92
137	An Ab Initio Investigation of the Structure and Alkaline Earth Divalent Cation Selectivity of 18-Crown-6. *Journal of the American Chemical Society*, **1996**, 118, 6052-6059	16.4	91
136	A complete basis set estimate of cation- bond strengths: Na+(ethylene) and Na+(benzene). *Chemical Physics Letters*, **2000**, 322, 543-548	2.5	90
135	Theoretical Study of Cation/Ether Complexes: Alkali Metal Cations with 1,2-Dimethoxyethane and 12-Crown-4. *Journal of Physical Chemistry A*, **1998**, 102, 3813-3819	2.8	87
134	MCSCF/CI investigation of the low-lying potential energy surfaces of the formyloxyl radical, HCO2.cntdot.. *Journal of the American Chemical Society*, **1983**, 105, 1459-1466	16.4	87
133	Difficulties inab initio CI calculations of the hyperfine structure of small radicals. *Theoretica Chimica Acta*, **1985**, 68, 57-67		86
132	Heats of Formation of Simple Boron Compounds. *Journal of Physical Chemistry A*, **1998**, 102, 7053-7059	2.8	84
131	Coupled Cluster Theory and Multireference Configuration Interaction Study of FO, F2O, FO2, and FOOF. *Journal of Physical Chemistry A*, **2003**, 107, 9641-9651	2.8	83

130	Probing the limits of accuracy in electronic structure calculations: is theory capable of results uniformly better than "chemical accuracy"?. *Journal of Chemical Physics*, **2007**, 126, 114105	3.9	82
129	ESR and ab initio theoretical studies of the cation radicals 14N+4 and 15N+4: The trapping of ion–neutral reaction products in neon matrices at 4 K. *Journal of Chemical Physics*, **1987**, 87, 885-897	3.9	82
128	Decomposition Pathways of Peroxynitrous Acid: Gas-Phase and Solution Energetics. *Journal of Physical Chemistry A*, **2002**, 106, 3191-3196	2.8	77
127	A comparison of techniques for predicting higher order correlation effects: Diatomic dissociation energies. *Journal of Chemical Physics*, **1999**, 111, 4373-4382	3.9	75
126	The role of databases in support of computational chemistry calculations **1996**, 17, 1571		75
125	A Practical Guide to Reliable First Principles Computational Thermochemistry Predictions Across the Periodic Table. *Annual Reports in Computational Chemistry*, **2012**, 1-28	1.8	74
124	Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	72
123	Ab initio study of m-benzoquinodimethane. *Journal of the American Chemical Society*, **1983**, 105, 1791-1795	16.4	69
122	Theoretical Conformational Analysis of Thiacrown Macrocycles. *Journal of Physical Chemistry A*, **2000**, 104, 652-660	2.8	68
121	Benchmarks of improved complete basis set extrapolation schemes designed for standard CCSD(T) atomization energies. *Journal of Chemical Physics*, **2013**, 138, 074103	3.9	66
120	The electron affinity of oxygen: A systematic configuration interaction approach. *Journal of Chemical Physics*, **1989**, 90, 1024-1030	3.9	65
119	Ab initio studies of [1.1.1]- and [2.2.2]propellane. *Journal of the American Chemical Society*, **1987**, 109, 4133-4139	16.4	63
118	Accurate Calculations of the Electron Affinity and Ionization Potential of the Methyl Radical. *Journal of Physical Chemistry A*, **1997**, 101, 9405-9409	2.8	60
117	A comparison of unrestricted Hartree–Fock- and restricted open-shell Hartree–Fock-based methods for determining the magnetic hyperfine parameters of NO (X 2Π). *Journal of Chemical Physics*, **1993**, 99, 2829-2840	3.9	60
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115	Improved accuracy benchmarks of small molecules using correlation consistent basis sets. *Theoretical Chemistry Accounts*, **2014**, 133,	1.9	59
114	Electron spin resonance investigations of 11B12C, 11B13C, and 10B12C in neon, argon, and krypton matrices at 4 K: Comparison with theoretical results. *Journal of Chemical Physics*, **1989**, 90, 690-699	3.9	58
113	Theoretical Study of Cation/Ether Complexes: The Alkali Metals and Dimethyl Ether. *Journal of Physical Chemistry A*, **1997**, 101, 6125-6131	2.8	57

112	Laser sputtering generation of B2 for ESR matrix isolation studies: comparison with ab initio CI theoretical calculations. *Journal of the American Chemical Society*, **1987**, 109, 3521-3525	16.4	57
111	The generation and trapping of the high-temperature oxosilyliumyl cation radicals (28SiO+ and 29SiO+) in neon matrixes at 4 K; an ESR and ab initio CI theoretical investigation. *Journal of the American Chemical Society*, **1985**, 107, 2857-2864	16.4	56
110	Concerted dihydrogen exchange between ethane and ethylene. SCF and FORS calculations of the barrier. *Journal of the American Chemical Society*, **1982**, 104, 960-967	16.4	56
109	The structure and binding energy of K+□ther complexes: A comparison of MP2, RI-MP2, and density functional methods. *Journal of Chemical Physics*, **1996**, 105, 1940-1950	3.9	55
108	An ab initio study of the magnetic hyperfine properties of F□(2□u). *Journal of Chemical Physics*, **1990**, 93, 579-589	3.9	54
107	Ab initio multireference CI determinations of the electron affinity of carbon and oxygen. *Journal of Chemical Physics*, **1985**, 82, 4135-4141	3.9	54
106	Molecular properties of water. *Chemical Physics Letters*, **1984**, 104, 54-58	2.5	52
105	Potential surface for the methylenecyclopropane rearrangement. *Journal of the American Chemical Society*, **1982**, 104, 967-972	16.4	52
104	Barrier for the H2CO-H2+CO reaction: A discrepancy between high-level electronic structure calculations and experiment. *Journal of Chemical Physics*, **2000**, 113, 218-226	3.9	51
103	A theoretical study of the acetaldehyde-derived radical. *Journal of the American Chemical Society*, **1982**, 104, 2956-2959	16.4	51
102	Calibration study of the CCSD(T)-F12a/b methods for C2 and small hydrocarbons. *Journal of Chemical Physics*, **2010**, 133, 184102	3.9	50
101	Heats of formation of the H1,2OmSn (m, n = 0-3) molecules from electronic structure calculations. *Journal of Physical Chemistry A*, **2009**, 113, 11343-53	2.8	50
100	Anharmonic zero point vibrational energies: tipping the scales in accurate thermochemistry calculations?. *Journal of Chemical Physics*, **2013**, 138, 044311	3.9	49
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98	Novel Binding Modes in Tetramethoxycalix[4]arene:□Implications for Ligand Design. *Journal of the American Chemical Society*, **2000**, 122, 10083-10089	16.4	48
97	Allylic resonance - when is it unimportant?. *Journal of the American Chemical Society*, **1984**, 106, 2513-2518	16.4	48
96	Molecular orbital studies of hyperfine coupling constants in the H2CN and H(HO)CN radicals. *The Journal of Physical Chemistry*, **1991**, 95, 4702-4708		46
95	ESR and ab initio theoretical studies of the cation radicals 12C2 16O+2, 12,13C2 16O+2, 13C2 16O+2, 12C2 16,17O+2, 12C2 17O+2, and 12,13C2 16,17O+2 isolated in neon matrices at 4 K. The use of matrix isolation for trapping ion□eutral reaction products. *Journal of Chemical Physics*, **1984**, 80, 4593-4604	3.9	46

94	Theoretical study of cation/ether complexes: 15-crown-5 and its alkali metal complexes. *International Journal of Mass Spectrometry*, **2000**, 201, 41-58	1.9	45
93	Neon matrix electron spin resonance and theoretical investigations of 10,11BH2, 12,13CH2, and 12,13CH+2. *Journal of Chemical Physics*, **1989**, 91, 4468-4476	3.9	45
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91	Dependence of the singlet-triplet splitting in heterosubstituted carbenes on the heteroatom electronegativity and conformation. *Chemical Physics Letters*, **1980**, 71, 22-26	2.5	45
90	An expanded calibration study of the explicitly correlated CCSD(T)-F12b method using large basis set standard CCSD(T) atomization energies. *Journal of Chemical Physics*, **2013**, 139, 084110	3.9	43
89	Molecular Dynamics Study of WaterBenzene Interactions at the Liquid/Vapor Interface of Water. *Journal of Physical Chemistry B*, **2000**, 104, 4403-4407	3.4	42
88	The singlet and triplet state rotational potential surfaces for dihydroxycarbene. *Journal of Chemical Physics*, **1979**, 71, 4987	3.9	41
87	Molecular Structure, Vibrational Frequencies, and Energetics of the HCO, HOCO, and HCO2 Anions. *Journal of Physical Chemistry A*, **2003**, 107, 186-190	2.8	40
86	Theoretical and neon matrix electron spin resonance studies of the methanol cation: CH3OH+, CH3OD+, CH2DOH+, and 13CH3OH+. *Journal of Chemical Physics*, **1992**, 97, 5363-5376	3.9	40
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83	The CCSD(T) complete basis set limit for Ne revisited. *Journal of Chemical Physics*, **2008**, 129, 194115	3.9	38
82	Structures and heats of formation of simple alkaline earth metal compounds: fluorides, chlorides, oxides, and hydroxides for Be, Mg, and Ca. *Journal of Physical Chemistry A*, **2010**, 114, 9349-58	2.8	37
81	The gas and solution phase acidities of HNO, HOONO, HONO, and HONO2. *International Journal of Mass Spectrometry*, **2003**, 227, 421-438	1.9	37
80	High level ab initio energies and structures for the rotamers of 1,3-butadiene. *Journal of Physical Chemistry A*, **2009**, 113, 1601-7	2.8	36
79	A Theoretical Case Study of Substituent Effects and Microsolvation on the Binding Specificity of Crown Ethers. *Journal of Physical Chemistry A*, **1997**, 101, 7292-7298	2.8	36
78	Theoretical investigations of the electronic states of porphyrins. III. Low-lying electronic states of porphinatoiron(II). *International Journal of Quantum Chemistry*, **1985**, 28, 773-796	2.1	36
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76	Hydrogen fluoride: a critical comparison of theoretical and experimental results. *Computational and Theoretical Chemistry*, **1997**, 400, 69-92		35
75	Ab initio structures for 90 degrees -twisted s-trans-1,3-butadiene and cyclooctatetraene: the naked sp2-sp2 bond. *Journal of Physical Chemistry A*, **2008**, 112, 2131-3	2.8	35
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73	Ab initio coupled cluster determination of the heats of formation of C2H2F2, C2F2, and C2F4. *Journal of Physical Chemistry A*, **2011**, 115, 1440-51	2.8	34
72	Refined theoretical estimates of the atomization energies and molecular structures of selected small oxygen fluorides. *Journal of Physical Chemistry A*, **2010**, 114, 613-23	2.8	34
71	High level coupled cluster determination of the structure, frequencies, and heat of formation of water. *Journal of Chemical Physics*, **2009**, 131, 154306	3.9	34
70	A theoretical determination of the electron affinity of methylene. *Journal of Chemical Physics*, **1982** , 77, 6134-6143	3.9	34
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68	Improved estimates of the total correlation energy in the ground state of the water molecule. *Journal of Chemical Physics*, **1997**, 106, 7706-7708	3.9	32
67	Structures and heats of formation of simple alkali metal compounds: hydrides, chlorides, fluorides, hydroxides, and oxides for Li, Na, and K. *Journal of Physical Chemistry A*, **2010**, 114, 4272-81	2.8	31
66	Calculation of zero field splitting parameters for trimethylenemethane. *Journal of Chemical Physics*, **1981**, 74, 2256-2259	3.9	30
65	Neon matrix ESR and CI theoretical investigation of 10BF+ and 11BF+: Photoionization of BF from reactive laser sputtering and high temperature sources. *Journal of Chemical Physics*, **1986**, 85, 5437-5445	3.9	29
64	Accurate ab initio study of the energetics of phosphorus nitride: Heat of formation, ionization potential, and electron affinity. *Journal of Chemical Physics*, **2003**, 118, 8290-8295	3.9	28
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61	A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. *Journal of Chemical Physics*, **2014**, 141, 104302	3.9	27
60	Ab initio coupled cluster determination of the equilibrium structures of cis- and trans-1,2-difluoroethylene and 1,1-difluoroethylene. *Journal of Physical Chemistry A*, **2011**, 115, 94-8	2.8	25
59	A Nonparametrized Ab Initio Determination of the Heat of Formation of Hydroxylamine, NH2OH. *Journal of Physical Chemistry A*, **2003**, 107, 10419-10427	2.8	25

58	Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions. *Reviews in Computational Chemistry*, **2007**, 1-43		22
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56	Enthalpy of Formation of NH (Hydrazine) Revisited. *Journal of Physical Chemistry A*, **2017**, 121, 6187-6198	2.8	21
55	The generation of 12C31P and 13C31P by reactive laser vaporization for rare gas matrix electron spin resonance studies: Comparison with ab initio theoretical calculations. *Journal of Chemical Physics*, **1988**, 88, 3441-3450	3.9	21
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53	Vibrational spectroscopy of 1,1-difluorocyclopropane-d0, -d2, and -d4: the equilibrium structure of difluorocyclopropane. *Journal of Physical Chemistry A*, **2007**, 111, 2498-506	2.8	20
52	Ab Initio CI Calculations of the Energy Difference between Trimethylenemethane and Butadiene. *Israel Journal of Chemistry*, **1983**, 23, 105-108	3.4	20
51	Configuration interaction calculations on the X1Sigma+ground state and low-lying A1Pi and1Delta excited states of the PN molecule. I. Potential energy curve of the X1Sigma+state of PN. Miscellaneous spectroscopic observables. *Journal of Physics B: Atomic, Molecular and Optical Physics*	1.3	18
50	Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using HartreeFock limit and configuration interaction wavefunctions for hydrogen fluoride.. *Chemical Physics*, **1993**, 171, 303-317	2.3	18
49	Configuration interaction calculations on the propane radical cation, C3H +8. *Theoretica Chimica Acta*, **1990**, 77, 111-122		18
48	Infrared spectra of CF(2)=CHD and CF(2)=CD(2): scaled quantum-chemical force fields and an equilibrium structure for 1,1-difluoroethylene. *Journal of Physical Chemistry A*, **2010**, 114, 9309-18	2.8	17
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43	Electron spin resonance rare gas matrix studies of 12CO2□13CO2□and C17O2□: Comparison with ab initio calculations. *Journal of Chemical Physics*, **1996**, 105, 5672-5686	3.9	16
42	When is allylic resonance unimportant?. *Journal of the American Chemical Society*, **1983**, 105, 3347-3348	16.4	16
41	Configuration-interaction calculations of miscellaneous properties of the CP and molecules: I. CP ground state. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1996**, 29, 5283-5303	1.3	15

40	Configuration interaction calculations on the P2molecule. I. Potential energy curves of the X1Sigmag+and a3Sigmau+states of P2; spectroscopic properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1994**, 27, 1657-1670	1.3	15
39	Thermodynamic properties of arsenic compounds and the heat of formation of the As atom from high level electronic structure calculations. *Journal of Physical Chemistry A*, **2011**, 115, 14667-76	2.8	14
38	Configuration interaction calculations on the X1Sigma+ground state and low-lying A1Pi and1Delta excited states of the PN molecule. II. Potential energy curves of the A1Pi and1Delta excited states of PN and spectroscopic properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1993**, 26, 1915-1934	1.3	13
37	Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: Comparison with EMS experiments. *Chemical Physics*, **1990**, 147, 45-50	2.3	13
36	Heats of formation of MHxCly (M = Si, P, As, Sb) compounds and main group fluorides from high level electronic structure calculations. *Journal of Physical Chemistry A*, **2012**, 116, 3717-27	2.8	12
35	Configuration interaction calculations on the state of CP and the - transition bands. Miscellaneous properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1998**, 31, 5053-5075	1.3	12
34	Some aspects of the triplet di-.pi.-methane rearrangement: comparison of the ring opening of cyclopropyldicarbinyl and cyclopropylcarbinyl. *Journal of the American Chemical Society*, **1985**, 107, 5054-5059	16.4	12
33	The cyclic isomer of CO2. *Journal of Chemical Physics*, **1980**, 73, 4517-4520	3.9	12
32	Ab initio calculation of the properties and the geometry of the lowest triplet state of pyrazine. *The Journal of Physical Chemistry*, **1982**, 86, 1583-1588		12
31	Statistical Electronic Structure Calibration Study of the CCSD(T*)-F12b Method for Atomization Energies. *Journal of Physical Chemistry A*, **2015**, 119, 7375-87	2.8	11
30	Density Functional Theory and the Basis Set Truncation Problem with Correlation Consistent Basis Sets: Elephant in the Room or Mouse in the Closet?. *Journal of Physical Chemistry A*, **2018**, 122, 2598-2603	2.8	11
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