

Jack Simons

List of Publications by Year in descending order

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47006

47
h-index

54911

84
g-index

191
all docs

191
docs citations

191
times ranked

3585
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Anions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6401-6511.	2.5	364
2	Ab initio electronic structure of anions. <i>Chemical Reviews</i> , 1987, 87, 535-555.	47.7	336
3	How Do Low-Energy (0.1~2 eV) Electrons Cause DNA-Strand Breaks?. <i>Accounts of Chemical Research</i> , 2006, 39, 772-779.	15.6	331
4	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. <i>Journal of Chemical Physics</i> , 1999, 110, 4763-4771.	3.0	269
5	Theory of electron affinities of small molecules. <i>Journal of Chemical Physics</i> , 1973, 58, 4899-4907.	3.0	267
6	Mechanism for Damage to DNA by Low-Energy Electrons. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7991-7994.	2.6	262
7	The Only Stable State of O ₂ Is the X ² Σ g ⁻ Ground State and It (Still!) Has an Adiabatic Electron Detachment Energy of 0.45 eV. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8521-8529.	2.5	240
8	Small Multiply Charged Anions as Building Blocks in Chemistry. <i>Accounts of Chemical Research</i> , 1996, 29, 497-502.	15.6	170
9	Contribution of electron correlation to the stability of dipole-bound anionic states. <i>Physical Review A</i> , 1996, 54, 1906-1909.	2.5	167
10	The coupled-cluster method with a multiconfiguration reference state. <i>International Journal of Quantum Chemistry</i> , 1981, 19, 207-216.	2.0	163
11	Ab initio analytical molecular gradients and Hessians. <i>Journal of Chemical Physics</i> , 1983, 79, 334-357.	3.0	159
12	A unitary multiconfigurational coupled-cluster method: Theory and applications. <i>Journal of Chemical Physics</i> , 1988, 88, 993-1002.	3.0	156
13	Resonance state lifetimes from stabilization graphs. <i>Journal of Chemical Physics</i> , 1981, 75, 2465-2467.	3.0	152
14	Comparison of the convergence characteristics of some iterative wave function optimization methods. <i>Journal of Chemical Physics</i> , 1982, 76, 543-557.	3.0	152
15	Tetracoordinated Planar Carbon in Pentaatomic Molecules. <i>Journal of the American Chemical Society</i> , 1998, 120, 7967-7972.	13.7	150
16	How to choose a one-electron basis set to reliably describe a dipole-bound anion. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 1024-1038.	2.0	141
17	Propensity rules for vibration-induced electron detachment of anions. <i>Journal of the American Chemical Society</i> , 1981, 103, 3971-3976.	13.7	135
18	Adiabatic electron affinities of small superhalogens: LiF ₂ , LiCl ₂ , NaF ₂ , and NaCl ₂ . <i>Journal of Chemical Physics</i> , 1997, 107, 3867-3875.	3.0	122

#	ARTICLE	IF	CITATIONS
19	Theoretical Study of Negative Molecular Ions. Annual Review of Physical Chemistry, 2011, 62, 107-128.	10.8	106
20	Applications of multiconfigurational coupled-cluster theory. Journal of Chemical Physics, 1982, 76, 4548-4559.	3.0	105
21	Walking on potential energy surfaces. Journal of Chemical Physics, 1990, 92, 340-346.	3.0	105
22	Model Calculations Relevant to Disulfide Bond Cleavage via Electron Capture Influenced by Positively Charged Groups. Journal of Physical Chemistry B, 2003, 107, 13505-13511.	2.6	104
23	Damage to Model DNA Fragments by 0.25-1.0 eV Electrons Attached to a Thymine π^* Orbital. Journal of Physical Chemistry B, 2004, 108, 5800-5805.	2.6	101
24	Electron Attachment Step in Electron Capture Dissociation (ECD) and Electron Transfer Dissociation (ETD). Journal of Physical Chemistry A, 2005, 109, 5801-5813.	2.5	92
25	Theoretical Study of Damage to DNA by 0.2-1.5 eV Electrons Attached to Cytosine. Journal of Physical Chemistry A, 2004, 108, 2999-3005.	2.5	89
26	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
27	Mechanisms for S-S and N-C \pm bond cleavage in peptide ECD and ETD mass spectrometry. Chemical Physics Letters, 2010, 484, 81-95.	2.6	84
28	Direct Calculation of First- and Second-Order Density Matrices. The Higher RPA Method. Journal of Chemical Physics, 1971, 55, 1218-1230.	3.0	78
29	A complete treatment of the electron propagator through third order. Journal of Chemical Physics, 1975, 63, 5302-5304.	3.0	76
30	Complex coordinate rotation of the electron propagator. Journal of Chemical Physics, 1980, 73, 2858-2866.	3.0	75
31	Double-Rydberg anions: Ground-state electronic and geometric stabilities. Journal of Chemical Physics, 1990, 93, 3874-3880.	3.0	74
32	Møller-Plesset perturbation theory for van der Waals complexes bound by electron correlation effects: Ground states of the Ar and Mg dimers. Journal of Chemical Physics, 1987, 87, 3569-3579.	3.0	70
33	Theoretical studies of molecular ions. Ionization potentials of CN $^+$ and BO $^+$. Journal of Chemical Physics, 1976, 64, 3610-3614.	3.0	66
34	Repulsive Coulomb Barriers in Compact Stable and Metastable Multiply Charged Anions. Journal of the American Chemical Society, 2000, 122, 11893-11899.	13.7	63
35	Effects of Base π -Stacking on Damage to DNA by Low-Energy Electrons. Journal of Physical Chemistry A, 2004, 108, 11381-11387.	2.5	63
36	General-Order Many-Body Green's Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61

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37	Vertical and adiabatical ionization potentials of MH^{k+1} anions. Ab initio study of the structure and stability of hypervalent MH_{k+1} molecules. Journal of Chemical Physics, 1993, 99, 4628-4637.	3.0	60
38	Energy-Shift Theory of Low-Lying Excited Electronic States of Molecules. Journal of Chemical Physics, 1972, 57, 3787-3792.	3.0	57
39	Electronic energies, geometries, and vibrational frequencies of the ground and low-lying excited states of the boron trimer. Journal of Chemical Physics, 1991, 94, 2961-2967.	3.0	55
40	A direct ab initio dynamics study of the water-assisted tautomerization of formamide. International Journal of Quantum Chemistry, 1997, 63, 861-874.	2.0	54
41	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. Journal of Physical Chemistry B, 1998, 102, 4205-4208.	2.6	53
42	Stabilization calculation of the energy and lifetime of metastable SO_4^{2-} . Journal of Chemical Physics, 2002, 116, 2848-2851.	3.0	51
43	Is TeF_8^{4-} the MX_2^{n-} dianion with the largest electron detachment energy (5 eV). Journal of Chemical Physics, 1992, 97, 2826-2827.	3.0	50
44	Theoretical search for large Rydberg molecules: NH_3CH_3 , $NH_2(CH_3)_2$, $NH(CH_3)_3$, and $N(CH_3)_4$. Journal of Chemical Physics, 1992, 97, 6621-6627.	3.0	50
45	Negative electron affinities from conventional electronic structure methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	50
46	Direct atomic-orbital-based time-dependent Hartree-Fock calculations of frequency-dependent polarizabilities. Journal of Chemical Physics, 1992, 96, 2978-2987.	3.0	48
47	A combined experimental and theoretical study of the neutral, cationic, and anionic Si_3N cluster molecule. Journal of Chemical Physics, 1994, 101, 2871-2879.	3.0	48
48	Temperature Dependence of the Biotin-Avidin Bond-Rupture Force Studied by Atomic Force Microscopy. Journal of Physical Chemistry B, 2002, 106, 9847-9852.	2.6	48
49	Theoretical studies of molecular ions. Vertical ionization potentials of hydrogen fluoride. Journal of Chemical Physics, 1974, 61, 2670-2674.	3.0	47
50	Application of cholesky-like matrix decomposition methods to the evaluation of atomic orbital integrals and integral derivatives. International Journal of Quantum Chemistry, 1989, 36, 673-688.	2.0	47
51	The electron propagator and superoperator resolvent. Journal of Chemical Physics, 1976, 64, 4541-4543.	3.0	46
52	Modified rotationally adiabatic model for rotational autoionization of dipole-bound molecular anions. Journal of Chemical Physics, 1989, 91, 6858-6865.	3.0	42
53	Ab initio studies of the structures and energies of the $H^+(H_2O)$ and $H^+(H_2O)_2$ complexes. Journal of Chemical Physics, 1987, 87, 2965-2975.	3.0	41
54	Theoretical study of C_2 and $Ca^{+2} : X^{\infty}1\sigma^2 + g$, $a^{\infty}3\sigma^2$, $X^{\infty}2\sigma^2 + g$, and $B^{\infty}2\sigma^2 + u$ potentials. Journal of Chemical Physics, 1987, 86, 6972-6981.	3.0	41

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55	A calculation of the electron detachment energy of NO ₂ ⁻ . Journal of Chemical Physics, 1977, 66, 2427-2430.	3.0	40
56	Theoretical study of the dipole-bound anion (HPPH ₃) ⁻ . Journal of Chemical Physics, 1999, 110, 274-280.	3.0	40
57	Resonance state energies and lifetimes via analytic continuation of stabilization graphs. Journal of Chemical Physics, 1986, 84, 4462-4469.	3.0	39
58	Excess electrons in condensed media: Theory of optical absorption spectrum in molecular solutions. Journal of Chemical Physics, 1978, 68, 415-432.	3.0	38
59	Potential energy curves of M(np ² P)â€¦RG(2 ¹) excited states and M+â€¦RG ground states (M=Li, Na; RG=He, Ne). Journal of Chemical Physics, 1994, 100, 8212-8218.	3.0	38
60	An experimental and theoretical determination of the electron affinity of the ethynyl radical, HC ₂ ⁻ Journal of Chemical Physics, 1979, 71, 2057.	3.0	37
61	Strategies for walking on potential energy surfaces using local quadratic approximations. International Journal of Quantum Chemistry, 1990, 38, 263-276.	2.0	35
62	A calculation of the electron affinity of the lithium molecule. Journal of Chemical Physics, 1976, 64, 4548-4550.	3.0	33
63	Perturbative solution of equations of motion for excitation and ionization processes. Journal of Chemical Physics, 1976, 64, 1413-1418.	3.0	32
64	Complex coordinate rotation calculation of branching ratios. International Journal of Quantum Chemistry, 1982, 21, 727-739.	2.0	32
65	Ab initio electronic structure of HCN ⁻ and HNC ⁻ dipole-bound anions and a description of electron loss upon tautomerization. Journal of Chemical Physics, 2001, 114, 7443-7449.	3.0	32
66	Dipole-Bound Anion of the HNNH ₃ Isomer of Hydrazine. An Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 625-631.	2.5	31
67	Theoretical studies of molecular ions: Be ⁺ 2. Journal of Chemical Physics, 1976, 65, 1601-1602.	3.0	30
68	A potentially size-consistent multiconfiguration based coupled electron pair approximation. Journal of Chemical Physics, 1989, 90, 3671-3679.	3.0	30
69	Ab initio study of the internal rotation barrier of formamide and the formamide-H ₂ O complex. International Journal of Quantum Chemistry, 1993, 45, 123-132.	2.0	30
70	A dipole-bound dianion. Journal of Chemical Physics, 2000, 112, 6563-6570.	3.0	30
71	Analysis of the equation-of-motion theory of electron affinities and ionization potentials. Chemical Physics, 1976, 14, 145-158.	1.9	28
72	Comment on the electronic structure of small beryllium and magnesium clusters and their anions. Journal of Chemical Physics, 1980, 72, 2889-2890.	3.0	28

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73	Anionic states of LiFl. <i>Journal of Chemical Physics</i> , 1994, 100, 1308-1311.	3.0	28
74	Why Are (MgO) _n Clusters and Crystalline MgO So Reactive?. <i>The Journal of Physical Chemistry</i> , 1996, 100, 8023-8030.	2.9	28
75	Low-energy (0.1 eV) electron attachment S ₂ S bond cleavage assisted by Coulomb stabilization. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 838-846.	2.0	28
76	Monte Carlo simulation of small hydrate clusters of NO ⁻ . <i>Journal of Chemical Physics</i> , 1980, 73, 1814-1826.	3.0	27
77	Geometrical derivatives of dipole moments and polarizabilities. <i>International Journal of Quantum Chemistry</i> , 1984, 25, 1135-1150.	2.0	27
78	Dissociative Recombination of H ₃ O ⁺ . <i>Journal of Physical Chemistry A</i> , 1999, 103, 6552-6563.	2.5	27
79	Analytical Model for Rates of Electron Attachment and Intramolecular Electron Transfer in Electron Transfer Dissociation Mass Spectrometry. <i>Journal of the American Chemical Society</i> , 2010, 132, 7074-7085.	13.7	27
80	An excess electron bound to urea. I. Canonical and zwitterionic tautomers. <i>Journal of Chemical Physics</i> , 2001, 115, 8373-8380.	3.0	26
81	Peculiar Structures of Small Magnesium Carbide Clusters: MgC ₂ , (MgC ₂) ₂ , and (MgC ₂) ₄ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 2215-2217.	2.5	25
82	Rydberg bonding in ammonium dimer ((NH ₄) ₂). <i>The Journal of Physical Chemistry</i> , 1992, 96, 8840-8843.	2.9	23
83	Ab initio study of geometrically metastable multiprotonated species: MH _k ⁿ⁺ . <i>Journal of Chemical Physics</i> , 1992, 97, 4272-4281.	3.0	23
84	Two-photon ionization spectroscopy and all-electron ab initio study of LiCa. <i>Journal of Chemical Physics</i> , 1998, 109, 6655-6665.	3.0	23
85	Analysis of the $\hat{\sigma}^{\text{TM}}\hat{\sigma}^{\text{TM}}$ charge resonance $\hat{\sigma}^{\text{TM}}\hat{\sigma}^{\text{TM}}$ transition in anthracene dimer anion. <i>Journal of Chemical Physics</i> , 1980, 72, 425-428.	3.0	22
86	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. <i>Journal of Chemical Physics</i> , 1993, 98, 7012-7019.	3.0	22
87	Theoretical study of electron capture dissociation of [Mg(H ₂ O) _n] ²⁺ clusters. <i>International Journal of Mass Spectrometry</i> , 2008, 277, 166-174.	1.5	22
88	Refinements to the Utah-Washington Mechanism of Electron Capture Dissociation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7892-7901.	2.6	22
89	Excess electrons in condensed media. A model for migration in dilute molecular solutions. <i>Journal of Chemical Physics</i> , 1977, 67, 389-398.	3.0	20
90	Electronic structure of small metal clusters. II. Anions of Li ₂ , LiNa, and Na ₂ . <i>Journal of Chemical Physics</i> , 1978, 69, 1788-1789.	3.0	20

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91	Resolvent operator approach to many-body perturbation theory. II. Open shells. Journal of Chemical Physics, 1982, 76, 1979-1994.	3.0	20
92	An excess electron bound to urea. III. The urea dimer as an electron trap. Journal of Chemical Physics, 2002, 116, 6118-6125.	3.0	20
93	Translational and rotational symmetries in integral derivatives. Journal of Chemical Physics, 1985, 82, 4566-4576.	3.0	19
94	Propensity rules for vibration-rotation-induced electron detachment of diatomic anions: application to amidogen(1-) ion. Journal of Physical Chemistry, 1988, 92, 3086-3091.	2.9	19
95	Polarization Green's function with multiconfiguration self-consistent-field reference states. International Journal of Quantum Chemistry, 1979, 16, 1209-1237.	2.0	18
96	Ab initio potential energy surfaces for Cd(1P)+H2=CdH(X ^{2Σ+})+H, HCdH(X ^{1Σ+g}), Cd(3P)+H2, and Cd(1S)+H+H. Journal of Chemical Physics, 1992, 96, 6555-6564.	3.0	18
97	Is 9-acridinamine anion a dispersion-bound anion?. Journal of Chemical Physics, 2001, 115, 11193-11199.	3.0	18
98	A calculation of the photodetachment energy of NH2 ⁻ . Journal of Chemical Physics, 1976, 65, 5393-5397.	3.0	17
99	Calculation of hyperfine coupling constants of the ground state X ^{3Σ⁻} of NH and B2. Journal of Chemical Physics, 1993, 99, 5995-6003.	3.0	17
100	Line shapes of charge-transfer spectra. Journal of Chemical Physics, 1979, 70, 4974-4981.	3.0	16
101	Associative electron detachment: O ⁻ +H ⁺ OH+e ⁻ . Journal of Chemical Physics, 1985, 83, 3888-3893.	3.0	16
102	Mixed valence/dipole-bound dianions. Journal of Chemical Physics, 1999, 111, 9469-9474.	3.0	16
103	On the Possibility of Mixed Rydberg-Valence Bonds. Journal of Physical Chemistry A, 1999, 103, 3575-3580.	2.5	16
104	On the lowest sigma and pi anion states of Be2 and Be3. Journal of Chemical Physics, 1982, 77, 5250-5252.	3.0	15
105	A multiconfiguration self-consistent-field group function method for problems with repeating potentials. Journal of Chemical Physics, 1983, 79, 6104-6111.	3.0	15
106	Roles Played by Metastable States in Chemistry. ACS Symposium Series, 1984, , 3-16.	0.5	15
107	On the possibility of binding of two electrons to dipole potentials. International Journal of Quantum Chemistry, 2000, 76, 197-204.	2.0	15
108	First-Order geometrical response equations for state-averaged multiconfigurational self-consistent field (SA-MCSCF) wave functions. International Journal of Quantum Chemistry, 1991, 40, 361-378.	2.0	14

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109	Singlet \leftrightarrow triplet energy transfer via $1\hat{1}/3\hat{1}+1$ curve crossings in group 2 and 12 metal \hat{c} atom/rare \hat{c} gas systems. Journal of Chemical Physics, 1993, 99, 3815-3822.	3.0	14
110	Interaction of an aluminum atom with an alkaline earth atom: Spectroscopic and ab initio investigations of AlCa. Journal of Chemical Physics, 1994, 101, 5441-5453.	3.0	14
111	Inversion in the relative stabilities of HBO and BOH upon ionization. Journal of Chemical Physics, 1999, 110, 3765-3768.	3.0	14
112	Ejecting Electrons from Molecular Anions via Shine, Shake/Rattle, and Roll. Journal of Physical Chemistry A, 2020, 124, 8778-8797.	2.5	14
113	Fate of Dipole-Bound Anion States when Hydrated. Journal of Physical Chemistry A, 2020, 124, 2064-2076.	2.5	14
114	An analysis of the natural orbital theory of ionization potentials. Journal of Chemical Physics, 1977, 66, 1067-1069.	3.0	13
115	New anionic states of the lithium trimer. Journal of Chemical Physics, 1994, 101, 4867-4877.	3.0	13
116	Laser Photolysis of Matrix-Isolated Methyl Nitrate: \hat{c} % Experimental and Theoretical Characterization of the Infrared Spectrum of Imine Peroxide (HNOO). Journal of the American Chemical Society, 1998, 120, 12327-12333.	13.7	13
117	Direct analytical calculation of first \hat{c} order density matrix elements through third order. Journal of Chemical Physics, 1973, 59, 2436-2440.	3.0	12
118	Spectroscopy of binary solutions. The benzene \hat{c} iodine charge \hat{c} transfer spectrum. Journal of Chemical Physics, 1978, 69, 1406-1417.	3.0	12
119	Dissociation of vibronic states of \hat{c} 1A \hat{c} 2 DCN: Quantum treatment. Journal of Chemical Physics, 1984, 80, 176-185.	3.0	12
120	Dipole-bound anions supported by charge-transfer interaction: Anionic states of HnF3?nN ? BH3 and H3N ? BHnF3?n (n = 0, 1, 2, 3). International Journal of Quantum Chemistry, 2003, 92, 367-375.	2.0	12
121	Equations of motion methods for computing electron affinities and ionization potentials. , 2005, , 443-464.		12
122	Dynamics of molecules in contact with an external medium at equilibrium. International Journal of Quantum Chemistry, 1978, 13, 553-562.	2.0	11
123	Coordinate rotation studies of H?, He?, Be?, Mg? resonances: Basis set and configuration list dependence. International Journal of Quantum Chemistry, 1983, 23, 1723-1738.	2.0	11
124	Translation \hat{c} rotation invariance for N \hat{c} particle systems: Internal coordinates and search for stationary points in reduced spaces. Journal of Chemical Physics, 1985, 83, 3500-3506.	3.0	11
125	Interactions of the B3 cluster with H atoms and H2 molecules. Journal of Chemical Physics, 1992, 96, 8251-8257.	3.0	11
126	Collisional energy transfer in bimolecular ion \hat{c} molecule dynamics M++(H2; D2; or HD) \hat{c} (MH++H); Tj ETQq0 0 0 ggBT /Overlock 10 Tf	3.0	11

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127	Potential energy surfaces and reactive dynamics of Zn(3P) with H ₂ . Journal of Chemical Physics, 1996, 105, 10919-10924.	3.0	11
128	Time-Domain and Tunneling Pictures of Nonadiabatic Induced Electron Ejection in Molecular Anions. Journal of Physical Chemistry A, 1999, 103, 9408-9416.	2.5	11
129	First- and Second-Order Density Matrices of Symmetry-Projected Single-Determinant Wavefunctions. Journal of Chemical Physics, 1969, 51, 296-301.	3.0	10
130	Graphical description of the symmetries of potential energy surfaces. Journal of Chemical Physics, 1993, 98, 8801-8809.	3.0	10
131	Interpretation of the hyperfine coupling constants of the boron trimer in rare-gas matrices. Journal of Chemical Physics, 1993, 98, 3060-3065.	3.0	10
132	Semiquantum Expressions for Electronically Nonadiabatic Electron Ejection Rates. Journal of Physical Chemistry A, 1998, 102, 6035-6042.	2.5	10
133	Characterization of the Rydberg Bonding in (NH ₄) ₂ ⁻ . Journal of Physical Chemistry A, 2000, 104, 10855-10858.	2.5	10
134	A Note on Differences Between Operator-Level and Function-Level Equations of Motion. International Journal of Quantum Chemistry, 1977, 12, 227-229.	2.0	9
135	Lifetimes of electronically metastable double-Rydberg anions: FH ⁻² . Journal of Chemical Physics, 1990, 93, 2546-2553.	3.0	9
136	Polyhedral Ionic Molecules. Journal of the American Chemical Society, 1997, 119, 4618-4621.	13.7	9
137	Analysis of Stabilization and Extrapolation Methods for Determining Energies and Lifetimes of Metastable Electronic States. Journal of Physical Chemistry A, 2021, 125, 7735-7749.	2.5	9
138	Resolvent operator approach to many-body perturbation theory. I. Closed shells. Journal of Chemical Physics, 1982, 76, 1972-1978.	3.0	8
139	Resolvent operator approach to many-body perturbation theory. III. Applications. Journal of Chemical Physics, 1982, 76, 1995-2002.	3.0	8
140	Reactive dynamics for Zn(3P)+H ₂ /D ₂ /HD†ZnH/ZnD+H/D: Rotational populations in ZnH/ZnD products. Journal of Chemical Physics, 1999, 110, 229-240.	3.0	8
141	Are HBO ⁻ and BOH ⁻ electronically stable?. Molecular Physics, 2003, 101, 1259-1265.	1.7	8
142	Electron detachment energies in high-symmetry alkali halide solvated-electron anions. Journal of Chemical Physics, 2003, 119, 902-908.	3.0	8
143	One-Electron Electron-Molecule Potentials Consistent with ab Initio Møller-Plesset Theory². Journal of Physical Chemistry A, 2010, 114, 8631-8643.	2.5	8
144	Semiclassical vibrational wave functions for electronically excited DCN: A highly quantum mechanical system. Journal of Chemical Physics, 1985, 82, 4199-4220.	3.0	7

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145	Finding transition states when second-order Jahn-Teller instability occurs. International Journal of Quantum Chemistry, 1993, 48, 211-218.	2.0	7
146	Al ₃ H stable and transition state structures. Journal of Chemical Physics, 1994, 101, 10746-10752.	3.0	7
147	Ab Initio Study of the Mechanism of Photolytic Deazation of 2,3-Diazabicyclo[2.2.2]oct-2-ene and 2,3-Diazabicyclo[2.2.1]hept-2-ene. Journal of Physical Chemistry A, 1997, 101, 2379-2383.	2.5	7
148	Sponge Model for the Kinetics of Surface Thermal Decomposition of Microcrystalline Solids: Application to HMX. Journal of Physical Chemistry B, 1999, 103, 8650-8656.	2.6	7
149	An excess electron bound to urea oligomers. II. Chains and ribbons. Journal of Chemical Physics, 2001, 115, 10731-10737.	3.0	7
150	One-particle green's function with multiconfiguration reference states. International Journal of Quantum Chemistry, 1978, 14, 389-404.	2.0	7
151	Nature of the autodetaching sub $2P_{1/2}$ threshold states of the alkali anions. International Journal of Quantum Chemistry, 1978, 14, 333-336.	2.0	6
152	Electronic spectroscopy in condensed media: Spectra of styrene and cyclooctatetraene anions. Journal of Chemical Physics, 1978, 69, 5538-5544.	3.0	6
153	Electronic spectroscopy in condensed media: The lowest $n \rightarrow \pi^*$ transition of the solvated nitrite anion. Journal of Chemical Physics, 1979, 71, 60-67.	3.0	6
154	Application of spectral quantization to metastable states of $Ca^{1A}DCN$. Journal of Chemical Physics, 1986, 85, 5826-5837.	3.0	6
155	Ab Initio Predictions of New Carbon Hypermagnesium Species: Mg_2C and Mg_3C . Journal of Physical Chemistry A, 1997, 101, 902-906.	2.5	6
156	An Unstable Anion Stabilized in a Molecular Trap. Journal of Physical Chemistry A, 2000, 104, 712-717.	2.5	6
157	An analytical model for vibrational non-Born-Oppenheimer induced electron ejection in molecular anions. Journal of Chemical Physics, 2002, 117, 9124-9132.	3.0	6
158	Multiconfigurational wavefunction optimization using the unitary group method. International Journal of Quantum Chemistry, 1980, 18, 211-228.	2.0	6
159	Do not forget the Rydberg orbitals. Journal of Chemical Physics, 2022, 156, 100901.	3.0	6
160	The Siegert methods in resonance scattering: Relation to L ₂ methods. International Journal of Quantum Chemistry, 1981, 20, 779-780.	2.0	5
161	The B ₃ Li molecule's electronic and geometrical structure. Journal of Chemical Physics, 1992, 97, 8357-8360.	3.0	5
162	Valence-Rydberg Bonding in Bimolecular $Ca \rightarrow NH_2 \rightarrow Ca$ Complexes. Journal of the American Chemical Society, 2000, 122, 369-377.	13.7	5

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163	A survey of some theoretical studies of negative ions. International Journal of Quantum Chemistry, 1977, 11, 971-978.	2.0	4
164	Should one use complex basis functions in coordinate rotation calculations on molecules?. Journal of Chemical Physics, 1980, 73, 992-993.	3.0	4
165	Coordinate rotated TDHF excitation energies Li? 1S ?1P. International Journal of Quantum Chemistry, 1982, 22, 275-288.	2.0	4
166	Reply to "Comment on: "Translation" rotation invariance for N-particle systems: Internal coordinates and search for stationary points in reduced spaces". Journal of Chemical Physics, 1986, 84, 3581-3581.	3.0	4
167	A two-dimensional model for collisional energy transfer in bimolecular ion-molecule dynamics: M++(H2; D2; or HD)?(MH++H; MD++D; MH++D; or MD++H). Theoretica Chimica Acta, 1995, 90, 357-381.	0.8	4
168	13C carbonyl chemical shielding tensors: Comparing SCF, MBPT (2), and DFT predictions to experiment. International Journal of Quantum Chemistry, 1997, 63, 875-894.	2.0	4
169	The complex coordinate rotation method and exterior scaling: A simple example. International Journal of Quantum Chemistry, 1980, 18, 113-121.	2.0	4
170	Selected boron, aluminum, and gallium trihalide and trihydride anions. Chemical Physics, 2017, 482, 387-392.	1.9	4
171	Unusual and Conventional Dative Bond Formation by s^{2} Lone Pair Donation from Alkaline Earth Metal Atoms to BH_{3} , AlH_{3} , and GaH_{3} . Journal of Physical Chemistry A, 2020, 124, 5369-5377.	2.5	4
172	How to choose a one-electron basis set to reliably describe a dipole-bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	4
173	Diffusion of excess electrons in one- and two-component molecular solutions. A theoretical model. Journal of Chemical Physics, 1978, 68, 1695-1700.	3.0	3
174	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. International Journal of Quantum Chemistry, 1992, 41, 793-810.	2.0	3
175	Second-order Jahn-Teller instability and the activation energy for $Al(1S) + H_{2} \rightarrow AlH(2^{+}) + H$. International Journal of Quantum Chemistry, 1993, 48, 309-317.	2.0	3
176	Role of angular electron pair correlation in stabilizing C_{2}^{60} . International Journal of Quantum Chemistry, 2006, 106, 507-513.	2.0	3
177	$F + H_{2} \rightarrow FH + H$ potential energy surface: Construction of the reference configuration state function space and MR-ACPF-2 results. International Journal of Quantum Chemistry, 2006, 106, 1516-1527.	2.0	3
178	Finding Valence Antibonding Levels while Avoiding Rydberg, Pseudo-continuum, and Dipole-Bound Orbitals. Journal of the American Chemical Society, 0, , .	13.7	3
179	Combining doubly charged cations and anions to form new species. Journal of Chemical Physics, 1994, 100, 5778-5784.	3.0	2
180	Effects of local Coulomb potentials on acid and base protonation-deprotonation rates and equilibria. International Journal of Quantum Chemistry, 2009, 109, 3120-3130.	2.0	2

#	ARTICLE	IF	CITATIONS
181	Direct calculation of density matrices: Natural orbitals and occupation numbers of model conjugated molecules. <i>International Journal of Quantum Chemistry</i> , 2009, 8, 323-333.	2.0	2
182	Caralumane Superacids of Lewis and Brønsted Character. <i>Journal of Physical Chemistry A</i> , 2021, 125, 999-1011.	2.5	2
183	A rigorous upper bound energy for the unitary coupled electron pair approximation method. <i>Journal of Chemical Physics</i> , 1991, 94, 5252-5252.	3.0	1
184	Application of the coordinate rotation method to metastable atom-diatom scattering resonances. <i>International Journal of Quantum Chemistry</i> , 2009, 18, 467-475.	2.0	1
185	Electron propagator studies of molecular anions. <i>International Journal of Quantum Chemistry</i> , 2009, 22, 575-581.	2.0	1
186	Thymine dimer repair by electron transfer from photo-excited 2,3,5-tri-O-acetyl-8-oxo-7,8-dihydroguanosine or 2,3,5-tri-O-acetyl-riboseyluric acid – a theoretical study. <i>Molecular Physics</i> , 2013, 111, 1580-1588.	2.0	0
187	How Do Low-energy (0.1–2 eV) Electrons Cause DNA Strand Breaks?. <i>AIP Conference Proceedings</i> , 2007, , .	0.4	0
188	The electronic structure of singlet cyclopentadienylidene. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 349-353.	2.0	0
189	Concluding remarks for advances in ion spectroscopy <i>Faraday Discussion</i> . <i>Faraday Discussions</i> , 2019, 217, 623-643.	3.2	0
190	Tribute to Alexander I. Boldyrev. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9261-9263.	2.5	0