Jack Simons

List of Publications by Year
in descending order

190 papers	8,038 citations	47006 47 h-index	54911 84 g-index
191 all docs	191 docs citations	191 times ranked	3585 citing authors

#	Article	IF	Citations
1	Do not forget the Rydberg orbitals. Journal of Chemical Physics, 2022, 156, 100901.	3.0	6
2	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
3	Caralumane Superacids of Lewis and BrÃ¸nsted Character. Journal of Physical Chemistry A, 2021, 125, 999-1011.	2.5	2
4	Tribute to Alexander I. Boldyrev. Journal of Physical Chemistry A, 2021, 125, 9261-9263.	2.5	0
5	Ejecting Electrons from Molecular Anions via Shine, Shake/Rattle, and Roll. Journal of Physical Chemistry A, 2020, 124, 8778-8797.	2.5	14
6	Unusual and Conventional Dative Bond Formation by s² Lone Pair Donation from Alkaline Earth Metal Atoms to BH₃, AlH₃, and GaH₃. Journal of Physical Chemistry A, 2020, 124, 5369-5377.	2.5	4
7	Fate of Dipole-Bound Anion States when Hydrated. Journal of Physical Chemistry A, 2020, 124, 2064-2076.	2.5	14
8	Concluding remarks for advances in ion spectroscopy Faraday Discussion. Faraday Discussions, 2019, 217, 623-643.	3.2	0
9	Selected boron, aluminum, and gallium trihalide and trihydride anions. Chemical Physics, 2017, 482, 387-392.	1.9	4
10	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61
11	Negative electron affinities from conventional electronic structure methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	50
12	Refinements to the Utahâ€“Washington Mechanism of Electron Capture Dissociation. Journal of Physical Chemistry B, 2014, 118, 7892-7901.	2.6	22
13	Thymine dimer repair by electron transfer from photo-excited 2â€²,3â€²,5â€²-tri-O-acetyl-8-oxo-7,8-dihydroguanosine or 2â€²,3â€²,5â€²-tri-O-acetyl-ribosyluric acid â€“ a theoretical study. Molecular Physics, 2013, 111, 1580-1588.	1.7	1
14	Theoretical Study of Negative Molecular Ions. Annual Review of Physical Chemistry, 2011, 62, 107-128.	10.8	106
15	Mechanisms for Sâ€“S and Nâ€“CÎ± bond cleavage in peptide ECD and ETD mass spectrometry. Chemical Physics Letters, 2010, 484, 81-95.	2.6	84
16	One-Electron Electronâ^'Molecule Potentials Consistent with ab Initio MÃ¸llerâ^'Plesset Theory^{â€}. Journal of Physical Chemistry A, 2010, 114, 8631-8643.	2.5	8
17	Analytical Model for Rates of Electron Attachment and Intramolecular Electron Transfer in Electron Transfer Dissociation Mass Spectrometry. Journal of the American Chemical Society, 2010, 132, 7074-7085.	13.7	27
18	Application of the coordinate rotation method to metastable atom-diatom scattering resonances. International Journal of Quantum Chemistry, 2009, 18, 467-475.	2.0	1

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19	Electron propagator studies of molecular anions. International Journal of Quantum Chemistry, 2009, 22, 575-581.	2.0	1
20	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
21	Direct calculation of density matrices: Natural orbitals and occupation numbers of model conjugated molecules. International Journal of Quantum Chemistry, 2009, 8, 323-333.	2.0	2
22	Theoretical study of electron capture dissociation of [Mg(H2O)n]2+ clusters. International Journal of Mass Spectrometry, 2008, 277, 166-174.	1.5	22
23	Molecular Anions. Journal of Physical Chemistry A, 2008, 112, 6401-6511.	2.5	364
24	How Do Low-energy (0.1â€“2 eV) Electrons Cause DNA Strand Breaks?. AIP Conference Proceedings, 2007, , .	0.4	0
25	How Do Low-Energy (0.1â^'2 eV) Electrons Cause DNA-Strand Breaks?. Accounts of Chemical Research, 2006, 39, 772-779.	15.6	331
26	Role of angular electron pair correlation in stabilizing C2â^'60. International Journal of Quantum Chemistry, 2006, 106, 507-513.	2.0	3
27	F + H2 â†' 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
28	Low-energy (0.1 eV) electron attachment S?S bond cleavage assisted by Coulomb stabilization. International Journal of Quantum Chemistry, 2005, 102, 838-846.	2.0	28
29	Equations of motion methods for computing electron affinities and ionization potentials. , 2005, , 443-464.		12
30	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
31	Effects of Base Ï€-Stacking on Damage to DNA by Low-Energy Electrons. Journal of Physical Chemistry A, 2004, 108, 11381-11387.	2.5	63
32	Damage to Model DNA Fragments by 0.25â^'1.0 eV Electrons Attached to a Thymine Ï€* Orbital. Journal of Physical Chemistry B, 2004, 108, 5800-5805.	2.6	101
33	Theoretical Study of Damage to DNA by 0.2â^'1.5 eV Electrons Attached to Cytosineâ€. Journal of Physical Chemistry A, 2004, 108, 2999-3005.	2.5	89
34	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
35	The Only Stable State of O2-Is the X2ÎgGround State and It (Still!) Has an Adiabatic Electron Detachment Energy of 0.45 eV. Journal of Physical Chemistry A, 2003, 107, 8521-8529.	2.5	240
36	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

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37	Are HBOâˆ’and BOHâˆ’electronically stable?. Molecular Physics, 2003, 101, 1259-1265.	1.7	8
38	Electron detachment energies in high-symmetry alkali halide solvated-electron anions. Journal of Chemical Physics, 2003, 119, 902-908.	3.0	8
39	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
40	An analytical model for vibrational non-Bornâ€“Oppenheimer induced electron ejection in molecular anions. Journal of Chemical Physics, 2002, 117, 9124-9132.	3.0	6
41	Stabilization calculation of the energy and lifetime of metastable SO42âˆ’. Journal of Chemical Physics, 2002, 116, 2848-2851.	3.0	51
42	Mechanism for Damage to DNA by Low-Energy Electronsâ€. Journal of Physical Chemistry B, 2002, 106, 7991-7994.	2.6	262
43	Temperature Dependence of the Biotinâˆ’Avidin Bond-Rupture Force Studied by Atomic Force Microscopy. Journal of Physical Chemistry B, 2002, 106, 9847-9852.	2.6	48
44	An excess electron bound to urea. I. Canonical and zwitterionic tautomers. Journal of Chemical Physics, 2001, 115, 8373-8380.	3.0	26
45	Ab initio electronic structure of HCNâˆ’ and HNCâˆ’ dipole-bound anions and a description of electron loss upon tautomerization. Journal of Chemical Physics, 2001, 114, 7443-7449.	3.0	32
46	Is 9-acridinamine anion a dispersion-bound anion?. Journal of Chemical Physics, 2001, 115, 11193-11199.	3.0	18
47	An excess electron bound to urea oligomers. II. Chains and ribbons. Journal of Chemical Physics, 2001, 115, 10731-10737.	3.0	7
48	On the possibility of binding of two electrons to dipole potentials. International Journal of Quantum Chemistry, 2000, 76, 197-204.	2.0	15
49	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	141
50	A dipole-bound dianion. Journal of Chemical Physics, 2000, 112, 6563-6570.	3.0	30
51	Characterization of the Rydberg Bonding in (NH4)2-. Journal of Physical Chemistry A, 2000, 104, 10855-10858.	2.5	10
52	An Unstable Anion Stabilized in a Molecular Trap. Journal of Physical Chemistry A, 2000, 104, 712-717.	2.5	6
53	Repulsive Coulomb Barriers in Compact Stable and Metastable Multiply Charged Anions. Journal of the American Chemical Society, 2000, 122, 11893-11899.	13.7	63
54	Valenceâˆ’Rydberg Bonding in Bimolecular Râˆ’Ca+â€¢NH2âˆ’Râ€˜ Complexes. Journal of the American Chemical Society, 2000, 122, 369-377.	13.7	5

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55	How to choose a oneâ€electron basis set to reliably describe a dipoleâ€bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	4
56	Reactive dynamics for Zn(3P)+H2/D2/HDâ†'ZnH/ZnD+H/D: Rotational populations in ZnH/ZnD products. Journal of Chemical Physics, 1999, 110, 229-240.	3.0	8
57	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. Journal of Chemical Physics, 1999, 110, 4763-4771.	3.0	269
58	Mixed valence/dipole-bound dianions. Journal of Chemical Physics, 1999, 111, 9469-9474.	3.0	16
59	Theoretical study of the dipole-bound anion (HPPH3)â^'. Journal of Chemical Physics, 1999, 110, 274-280.	3.0	40
60	Inversion in the relative stabilities of HBO and BOH upon ionization. Journal of Chemical Physics, 1999, 110, 3765-3768.	3.0	14
61	On the Possibility of Mixed Rydberg-Valence Bonds. Journal of Physical Chemistry A, 1999, 103, 3575-3580.	2.5	16
62	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
63	Dipole-Bound Anion of the HNNH3Isomer of Hydrazine. An Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 625-631.	2.5	31
64	Sponge Model for the Kinetics of Surface Thermal Decomposition of Microcrystalline Solids:â€‰ Application to HMX. Journal of Physical Chemistry B, 1999, 103, 8650-8656.	2.6	7
65	Dissociative Recombination of H3O+. Journal of Physical Chemistry A, 1999, 103, 6552-6563.	2.5	27
66	Tetracoordinated Planar Carbon in Pentaatomic Molecules. Journal of the American Chemical Society, 1998, 120, 7967-7972.	13.7	150
67	Laser Photolysis of Matrix-Isolated Methyl Nitrate:â€‰ 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
68	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. Journal of Physical Chemistry B, 1998, 102, 4205-4208.	2.6	53
69	Semiquantum Expressions for Electronically Nonadiabatic Electron Ejection Rates. Journal of Physical Chemistry A, 1998, 102, 6035-6042.	2.5	10
70	Two-photon ionization spectroscopy and all-electron ab initio study of LiCa. Journal of Chemical Physics, 1998, 109, 6655-6665.	3.0	23
71	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. Journal of Chemical Physics, 1997, 107, 3867-3875.	3.0	122
72	Polyhedral Ionic Molecules. Journal of the American Chemical Society, 1997, 119, 4618-4621.	13.7	9

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73	Ab Initio Predictions of New Carbon Hypermagnesium Species:â€‰ Mg2C and Mg3C. Journal of Physical Chemistry A, 1997, 101, 902-906.	2.5	6
74	Peculiar Structures of Small Magnesium Carbide Clusters:Â MgC2, (MgC2)2, and (MgC2)4. Journal of Physical Chemistry A, 1997, 101, 2215-2217.	2.5	25
75	Ab Initio Study of the Mechanism of Photolytic Deazatization 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
76	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
77	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
78	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
79	Small Multiply Charged Anions as Building Blocks in Chemistry. Accounts of Chemical Research, 1996, 29, 497-502.	15.6	170
80	Why Are (MgO)nClusters and Crystalline MgO So Reactive?. The Journal of Physical Chemistry, 1996, 100, 8023-8030.	2.9	28
81	Contribution of electron correlation to the stability of dipole-bound anionic states. Physical Review A, 1996, 54, 1906-1909.	2.5	167
82	Potential energy surfaces and reactive dynamics of Zn(3P) with H2. Journal of Chemical Physics, 1996, 105, 10919-10924.	3.0	11
83	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
84	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
85	Combining doubly charged cations and anions to form new species. Journal of Chemical Physics, 1994, 100, 5778-5784.	3.0	2
86	New anionic states of the lithium trimer. Journal of Chemical Physics, 1994, 101, 4867-4877.	3.0	13
87	Anionic states of LiFLi. Journal of Chemical Physics, 1994, 100, 1308-1311.	3.0	28
88	Potential energy curves of M(npâ€‰2P)â‹…RG(2Î) 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
89	Al3H stable and transition state structures. Journal of Chemical Physics, 1994, 101, 10746-10752.	3.0	7
90	A combined experimental and theoretical study of the neutral, cationic, and anionic Si3N cluster molecule. Journal of Chemical Physics, 1994, 101, 2871-2879.	3.0	48

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91	Ab initio study of the internal rotation barrier of formamide and the formamide-H2O complex. International Journal of Quantum Chemistry, 1993, 45, 123-132.	2.0	30
92	Finding transition states when second-order Jahn-Teller instability occurs. International Journal of Quantum Chemistry, 1993, 48, 211-218.	2.0	7
93	Second-order Jahn-Teller instability and the activation energy for Al+(1S) + H2 ? AlH+(2?+) + H. International Journal of Quantum Chemistry, 1993, 48, 309-317.	2.0	3
94	Singletâ€toâ€triplet energy transfer via 1Î1/3Î£+1 curve crossings in group 2 and 12 metalâ€“atom/rareâ€gas systems. Journal of Chemical Physics, 1993, 99, 3815-3822.	3.0	14
95	Collisional energy transfer in bimolecular ionâ€“molecule dynamics M++(H2; D2; or HD)â†'(MH++H;) Tj ETQq1 1 0.784314 rgBT /Ove	3.0	11
96	Vertical and adiabatical ionization potentials of MHâ^'K+1 anions. Ab initio study of the structure and stability of hypervalent MHk+1 molecules. Journal of Chemical Physics, 1993, 99, 4628-4637.	3.0	60
97	Calculation of hyperfine coupling constants of the ground state Xâ€‰3Î£â^' of NH and B2. Journal of Chemical Physics, 1993, 99, 5995-6003.	3.0	17
98	Graphical description of the symmetries of potential energy surfaces. Journal of Chemical Physics, 1993, 98, 8801-8809.	3.0	10
99	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. Journal of Chemical Physics, 1993, 98, 7012-7019.	3.0	22
100	Interpretation of the hyperfine coupling constants of the boron trimer in rareâ€gas matrices. Journal of Chemical Physics, 1993, 98, 3060-3065.	3.0	10
101	Rydberg bonding in ammonium dimer ((NH4)2). The Journal of Physical Chemistry, 1992, 96, 8840-8843.	2.9	23
102	Ab initio potentialâ€energy surfaces for Cd(1P)+H2=CdH(Xâ€‰2Î£+)+H, HCdH(Xâ€‰1Î£+g), Cd(3P)+H2, and Cd(1S)+H+H. Journal of Chemical Physics, 1992, 96, 6555-6564.	3.0	18
103	The B3Li moleculeâ€™s electronic and geometrical structure. Journal of Chemical Physics, 1992, 97, 8357-8360.	3.0	5
104	Direct atomicâ€orbitalâ€based timeâ€dependent Hartreeâ€“Fock calculations of frequencyâ€dependent polarizabilities. Journal of Chemical Physics, 1992, 96, 2978-2987.	3.0	48
105	Interactions of the B3 cluster with H atoms and H2 molecules. Journal of Chemical Physics, 1992, 96, 8251-8257.	3.0	11
106	Ab initio study of geometrically metastable multiprotonated species: MHk+n. Journal of Chemical Physics, 1992, 97, 4272-4281.	3.0	23
107	Is TeF2â^'8the MX2â^'ndianion with the largest electron detachment energy (5 eV). Journal of Chemical Physics, 1992, 97, 2826-2827.	3.0	50
108	Theoretical search for large Rydberg molecules: NH3CH3, NH2(CH3)2, NH(CH3)3, and N(CH3)4. Journal of Chemical Physics, 1992, 97, 6621-6627.	3.0	50

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109	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
110	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
111	Electronic energies, geometries, and vibrational frequencies of the ground and lowâ€lying excited states of the boron trimer. Journal of Chemical Physics, 1991, 94, 2961-2967.	3.0	55
112	A rigorous upper bound energy for the unitary coupled electron pair approximation method. Journal of Chemical Physics, 1991, 94, 5252-5252.	3.0	1
113	Strategies for walking on potential energy surfaces using local quadratic approximations. International Journal of Quantum Chemistry, 1990, 38, 263-276.	2.0	35
114	Doubleâ€Rydberg anions: Groundâ€state electronic and geometric stabilities. Journal of Chemical Physics, 1990, 93, 3874-3880.	3.0	74
115	Lifetimes of electronically metastable doubleâ€Rydberg anions: FHâ^'2. Journal of Chemical Physics, 1990, 93, 2546-2553.	3.0	9
116	Walking on potential energy surfaces. Journal of Chemical Physics, 1990, 92, 340-346.	3.0	105
117	A potentially sizeâ€consistent multiconfiguration based coupled electron pair approximation. Journal of Chemical Physics, 1989, 90, 3671-3679.	3.0	30
118	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
119	Modified rotationally adiabatic model for rotational autoionization of dipoleâ€bound molecular anions. Journal of Chemical Physics, 1989, 91, 6858-6865.	3.0	42
120	A unitary multiconfigurational coupledâ€cluster method: Theory and applications. Journal of Chemical Physics, 1988, 88, 993-1002.	3.0	156
121	Propensity rules for vibration-rotation-induced electron detachment of diatomic anions: application to amidogen(1-) ion .fwdarw. imidogen + electron. The Journal of Physical Chemistry, 1988, 92, 3086-3091.	2.9	19
122	Ab initio studies of the structures and energies of the Hâ^'(H2O) and Hâ^'(H2O)2 complexes. Journal of Chemical Physics, 1987, 87, 2965-2975.	3.0	41
123	Mo/llerâ€“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
124	Theoretical study of C2 and Câ^'2 : Xâ€‰1Î£+g , aâ€‰3Îu , Xâ€‰2Î£+g , and Bâ€‰2Î£+u potentials. Journal of Chemical Physics, 1987, 86, 6972-6981.	3.0	41
125	Ab initio electronic structure of anions. Chemical Reviews, 1987, 87, 535-555.	47.7	336
126	Reply to â€˜â€˜Comment on: â€˜Translationâ€“rotation invariance for Nâ€particle systems: Internal coordinates and search for stationary points in reduced spacesâ€™â€‰â€™. Journal of Chemical Physics, 1986, 84, 3581-3581.	3.0	4

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127	Resonance state energies and lifetimes via analytic continuation of stabilization graphs. Journal of Chemical Physics, 1986, 84, 4462-4469.	3.0	39
128	Application of spectral quantization to metastable states of Câ€‰1Aâ€™DCN. Journal of Chemical Physics, 1986, 85, 5826-5837.	3.0	6
129	Translationâ€rotation invariance for Nâ€particle systems: Internal coordinates and search for stationary points in reduced spaces. Journal of Chemical Physics, 1985, 83, 3500-3506.	3.0	11
130	Semiclassical vibrational wave functions for electronically excited DCN: A highly quantum mechanical system. Journal of Chemical Physics, 1985, 82, 4199-4220.	3.0	7
131	Associative electron detachment: Oâ^'+Hâ†'OH+eâ^'. Journal of Chemical Physics, 1985, 83, 3888-3893.	3.0	16
132	Translational and rotational symmetries in integral derivatives. Journal of Chemical Physics, 1985, 82, 4566-4576.	3.0	19
133	Roles Played by Metastable States in Chemistry. ACS Symposium Series, 1984, , 3-16.	0.5	15
134	Dissociation of vibronic states ofCâ€“1Aâ€² DCN: Quantum treatment. Journal of Chemical Physics, 1984, 80, 176-185.	3.0	12
135	Geometrical derivatives of dipole moments and polarizabilities. International Journal of Quantum Chemistry, 1984, 25, 1135-1150.	2.0	27
136	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
137	Ab initio analytical molecular gradients and Hessians. Journal of Chemical Physics, 1983, 79, 334-357.	3.0	159
138	A multiconfiguration selfâ€consistentâ€field group function method for problems with repeating potentials. Journal of Chemical Physics, 1983, 79, 6104-6111.	3.0	15
139	Resolvent operator approach to manyâ€body perturbation theory. I. Closed shells. Journal of Chemical Physics, 1982, 76, 1972-1978.	3.0	8
140	On the lowest sigma and pi anion states of Be2 and Be3. Journal of Chemical Physics, 1982, 77, 5250-5252.	3.0	15
141	Resolvent operator approach to manyâ€body perturbation theory. II. Open shells. Journal of Chemical Physics, 1982, 76, 1979-1994.	3.0	20
142	Resolvent operator approach to manyâ€body perturbation theory. III. Applications. Journal of Chemical Physics, 1982, 76, 1995-2002.	3.0	8
143	Applications of multiconfigurational coupledâ€cluster theory. Journal of Chemical Physics, 1982, 76, 4548-4559.	3.0	105
144	Comparison of the convergence characteristics of some iterative wave function optimization methods. Journal of Chemical Physics, 1982, 76, 543-557.	3.0	152

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145	Complex coordinate rotation calculation of branching ratios. International Journal of Quantum Chemistry, 1982, 21, 727-739.	2.0	32
146	Coordinate rotatedTDHF excitation energies Li? 1S ?1P. International Journal of Quantum Chemistry, 1982, 22, 275-288.	2.0	4
147	Propensity rules for vibration-induced electron detachment of anions. Journal of the American Chemical Society, 1981, 103, 3971-3976.	13.7	135
148	The coupled-cluster method with a multiconfiguration reference state. International Journal of Quantum Chemistry, 1981, 19, 207-216.	2.0	163
149	The Siegert methods in resonance scattering: Relation toL2 methods. International Journal of Quantum Chemistry, 1981, 20, 779-780.	2.0	5
150	Resonance state lifetimes from stabilization graphs. Journal of Chemical Physics, 1981, 75, 2465-2467.	3.0	152
151	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
152	Monte Carlo simulation of small hydrate clusters of NOâ‾2. Journal of Chemical Physics, 1980, 73, 1814-1826.	3.0	27
153	Analysis of the â€™â€™charge resonanceâ€™â€™ transition in anthracene dimer anion. Journal of Chemical Physics, 1980, 72, 425-428.	3.0	22
154	Should one use complex basis functions in coordinate rotation calculations on molecules?. Journal of Chemical Physics, 1980, 73, 992-993.	3.0	4
155	Complex coordinate rotation of the electron propagator. Journal of Chemical Physics, 1980, 73, 2858-2866.	3.0	75
156	The complex coordinate rotation method and exterior scaling: A simple example. International Journal of Quantum Chemistry, 1980, 18, 113-121.	2.0	4
157	Multiconfigurational wavefunction optimization using the unitary group method. International Journal of Quantum Chemistry, 1980, 18, 211-228.	2.0	6
158	The electronic structure of singlet cyclopentadienylidene. International Journal of Quantum Chemistry, 1980, 18, 349-353.	2.0	0
159	Line shapes of chargeâ€transfer spectra. Journal of Chemical Physics, 1979, 70, 4974-4981.	3.0	16
160	Electronic spectroscopy in condensed media: The lowestnâ€Ï€* transition of the solvated nitrite anion. Journal of Chemical Physics, 1979, 71, 60-67.	3.0	6
161	Polarization Green's function with multiconfiguration self-consistent-field reference states. International Journal of Quantum Chemistry, 1979, 16, 1209-1237.	2.0	18
162	An experimental and theoretical determination of the electron affinity of the ethynyl radical, HC2â‹…. Journal of Chemical Physics, 1979, 71, 2057.	3.0	37

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163	Dynamics of molecules in contact with an external medium at equilibrium. International Journal of Quantum Chemistry, 1978, 13, 553-562.	2.0	11
164	Nature of the autodetaching sub2PÂ½threshold states of the alkali anions. International Journal of Quantum Chemistry, 1978, 14, 333-336.	2.0	6
165	Excess electrons in condensed media: Theory of optical absorption spectrum in molecular solutions. Journal of Chemical Physics, 1978, 68, 415-432.	3.0	38
166	Electronic spectrocopy in condensed media: Spectra of styrene and cycloâ€octatetraene anions. Journal of Chemical Physics, 1978, 69, 5538-5544.	3.0	6
167	Diffusion of excess electrons in oneâ€and twoâ€component molecular solutions. A theoretical model. Journal of Chemical Physics, 1978, 68, 1695-1700.	3.0	3
168	Spectroscopy of binary solutions. The benzeneâ€“iodine chargeâ€transfer spectrum. Journal of Chemical Physics, 1978, 69, 1406-1417.	3.0	12
169	Electronic structure of small metal clusters. II. Anions of Li2, LiNa, and Na2. Journal of Chemical Physics, 1978, 69, 1788-1789.	3.0	20
170	One-particle green's function with multiconfiguration reference states. International Journal of Quantum Chemistry, 1978, 14, 389-404.	2.0	7
171	A calculation of the electron detachment energy of NO2â^'. Journal of Chemical Physics, 1977, 66, 2427-2430.	3.0	40
172	An analysis of the natural orbital theory of ionization potentials. Journal of Chemical Physics, 1977, 66, 1067-1069.	3.0	13
173	Excess electrons in condensed media. A model for migration in dilute molecular solutions. Journal of Chemical Physics, 1977, 67, 389-398.	3.0	20
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