David L Cooper

List of Publications by Year
in descending order

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233	5,636	87888	133252
papers	citations	38	59
		h-index	g-index

241	241	241	2557
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spin-Coupled Generalized Valence Bond Theory: New Perspectives on the Electronic Structure of Molecules and Chemical Bonds. Journal of Physical Chemistry A, 2021, 125, 2021-2050.	2.5	26
2	Role of Dynamical Electron Correlation in the Differences in Bonding between CaAlH3 and MgAlH3. Journal of Physical Chemistry A, 2021, 125, 3912-3919.	2.5	0
3	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
4	Comparison of DAFH and FALDI-like approaches. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
5	Excited-State Aromaticity Reversals in MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2020, 124, 9611-9616.	2.5	13
6	Are Multicentre Bond Indices and Related Quantities Reliable Predictors of Excited-State Aromaticity?. Molecules, 2020, 25, 4791.	3.8	4
7	Resolving a puzzling anomaly in the spinâ€coupled generalized valence bond description of benzene. Journal of Computational Chemistry, 2020, 41, 1421-1426.	3.3	6
8	Nature of the chemical bonding in D_{3h} [MH₃M]⁺ cations (M = Be, Mg). International Journal of Quantum Chemistry, 2020, 120, e26183.	2.0	3
9	Is the S₂N₂ ring a singlet diradical? Critical analysis of alternative valence bond descriptions. International Journal of Quantum Chemistry, 2019, 119, e25845.	2.0	8
10	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
11	Electronic Structure and Bonding Situation in M₂O₂ (M = Be, Mg, Ca) Rhombic Clusters. Journal of Physical Chemistry A, 2018, 122, 2816-2822.	2.5	34
12	Surface tension, density and composition in the methane-pentane system at high pressure. Fluid Phase Equilibria, 2018, 456, 193-202.	2.5	9
13	Magnetic Shielding, Aromaticity, Antiaromaticity and Bonding in the Lowâ€lying Electronic States of S₂N₂. Chemistry - A European Journal, 2018, 24, 16791-16803.	3.3	19
14	Does the Electronic Structure of MÃ¶bius Annulenes Follow Heilbronner's Ideas?. ChemPhysChem, 2018, 19, 3186-3190.	2.1	6
15	Study of the antimalarial activity of 4-aminoquinoline compounds against chloroquine-sensitive and chloroquine-resistant parasite strains. Journal of Molecular Modeling, 2018, 24, 237.	1.8	24
16	Theoretical investigations of the chemical bonding in MMâ€²2O2 clusters (M, Mâ€²â€‰=â€‰Be, Mg, Ca). Journal of Molecular Modeling, 2018, 24, 226.	1.8	2
17	Reassessing spin-coupled (full generalized valence bond) descriptions of ozone using three-center bond indices. Computational and Theoretical Chemistry, 2017, 1116, 40-49.	2.5	5
18	Modern valence-bond descriptions of polycyclic fused aromatic compounds involving cyclopropenyl rings. Computational and Theoretical Chemistry, 2017, 1116, 32-39.	2.5	2

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19	Sensitive Analysis of Protein Adsorption to Colloidal Gold by Differential Centrifugal Sedimentation. Analytical Chemistry, 2017, 89, 6807-6814.	6.5	48
20	Insights from domain-averaged Fermi hole (DAFH) analysis and multicenter bond indices into the nature of Be(0) bonding. Structural Chemistry, 2017, 28, 1033-1043.	2.0	13
21	Combining rival Ï€â€space descriptions of <scp>O</scp>₃ and of <scp>SO</scp>₂. International Journal of Quantum Chemistry, 2016, 116, 718-730.	2.0	8
22	Modern Valence-Bond Description of Homoaromaticity. Journal of Physical Chemistry A, 2016, 120, 8769-8779.	2.5	5
23	New insights from domain-averaged Fermi holes and bond order analysis into the bonding conundrum in C₂. Molecular Physics, 2016, 114, 1270-1284.	1.7	32
24	Three-dimensional networks containing rectangular Sr4and Ba4units: Synthesis, structure, bonding, and potential application for Ne gas separation. International Journal of Quantum Chemistry, 2015, 115, 1501-1510.	2.0	6
25	Combining symmetry-separated and bent-bond spin-coupled models of cylindrically symmetric multiple bonding. Molecular Physics, 2015, 113, 1690-1694.	1.7	3
26	Bonding in Singlet and Triplet Butalene: Insights from Spin-Coupled Theory. Journal of Physical Chemistry A, 2015, 119, 2169-2175.	2.5	5
27	Are orbital-resolved shared-electron distribution indices and Cioslowski covalent bond orders useful for molecules?. Molecular Physics, 2015, 113, 1682-1689.	1.7	5
28	Why is the bond multiplicity in C2 so elusive?. Computational and Theoretical Chemistry, 2015, 1053, 189-194.	2.5	25
29	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
30	Bonding in benzodicyclobutadiene isomers: insights from modern valence bond theory. Molecular Physics, 2014, 112, 2840-2852.	1.7	3
31	Modern valence-bond description of aromatic annulene ions. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4
32	Bond formation in diatomic transition metal hydrides: Insights from the analysis of domainâ€averaged fermi holes. International Journal of Quantum Chemistry, 2013, 113, 102-111.	2.0	4
33	High-Resolution Sizing of Monolayer-Protected Gold Clusters by Differential Centrifugal Sedimentation. ACS Nano, 2013, 7, 8881-8890.	14.6	71
34	Spin-Coupled Theory for â€˜N Electrons in M Orbitalsâ€™ Active Spaces. Journal of Physical Chemistry A, 2012, 116, 7238-7244.	2.5	31
35	Variational second order density matrix study of $mathrm{F_3^-}$F3â^': Importance of subspace constraints for size-consistency. Journal of Chemical Physics, 2011, 134, 054115.	3.0	14
36	Chemical verification of variational second-order density matrix based potential energy surfaces for the N2 isoelectronic series. Journal of Chemical Physics, 2010, 132, 114112.	3.0	30

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37	Influence of Atoms-in-Molecules Methods on Shared-Electron Distribution Indices and Domain-Averaged Fermi Holes^{â€}. Journal of Physical Chemistry A, 2010, 114, 8754-8763.	2.5	38
38	Modern valence bond description of the electronic mechanism of a [1,3] sigmatropic rearrangement linking bicyclo[3.2.0]heptâ€2â€ene and bicyclo[2.2.1]heptâ€2â€ene (norbornene). International Journal of Quantum Chemistry, 2009, 109, 1807-1811.	2.0	5
39	Comparison between the performances of the spinâ€projected Hartreeâ€“Fock, generalized valenceâ€bond, and spinâ€coupled approaches. International Journal of Quantum Chemistry, 2009, 109, 2447-2455.	2.0	6
40	Anatomy of bond formation: Insights from the analysis of domainâ€averaged Fermi holes in momentum space. International Journal of Quantum Chemistry, 2009, 109, 2383-2392.	2.0	4
41	QSAR using momentum-space and trivial feature count descriptors â€“ An application to Tetrahymena pyriformis toxicity. Computational and Theoretical Chemistry, 2009, 901, 56-59.	1.5	3
42	Spin-coupled descriptions of organic reactivity. International Reviews in Physical Chemistry, 2009, 28, 169-206.	2.3	25
43	Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes. Physical Chemistry Chemical Physics, 2009, 11, 3424.	2.8	54
44	Analytic Models of Domainâ€Averaged Fermi Holes: A New Tool for the Study of the Nature of Chemical Bonds. Chemistry - A European Journal, 2008, 14, 3338-3345.	3.3	43
45	Spin-Coupled Description of Aromaticity in the Retro Dielsâ^'Alder Reaction of Norbornene. Journal of Physical Chemistry A, 2008, 112, 12823-12828.	2.5	9
46	A one-electron approximation to domain-averaged Fermi hole analysis. Physical Chemistry Chemical Physics, 2008, 10, 1319.	2.8	29
47	Anatomy of bond formation. Bond length dependence of the extent of electron sharing in chemical bonds from the analysis of domain-averaged Fermi holes. Faraday Discussions, 2007, 135, 31-42.	3.2	65
48	The unusual electronic mechanism of the [1,5] hydrogen shift in (Z)-1,3-pentadiene predicted by modern valence bond theory. Faraday Discussions, 2007, 135, 285-297.	3.2	10
49	Anatomy of Bond Formation. Domain-Averaged Fermi Holes as a Tool for the Study of the Nature of the Chemical Bonding in Li₂, Li₄, and F₂. Journal of Physical Chemistry A, 2007, 111, 11294-11301.	2.5	40
50	Investigating the utility of momentum-space descriptors for predicting bloodâ€“brain barrier penetration. Journal of Molecular Graphics and Modelling, 2007, 26, 607-612.	2.4	15
51	The electronic structure of nitrilimine: absence of the carbenic form. Chemical Communications, 2006, , 1030.	4.1	22
52	Modern Valence-Bond-Like Representations of SelectedD6hâ€œAromaticâ€•Rings. Journal of Physical Chemistry A, 2006, 110, 7913-7917.	2.5	7
53	The spin-coupled picture of clamped benzenes. Molecular Physics, 2006, 104, 677-680.	1.7	6
54	A spin-coupled study of the Claisen rearrangement of allyl vinyl ether. Theoretical Chemistry Accounts, 2006, 115, 212-220.	1.4	18

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55	The use of momentum-space descriptors for predicting octanolâ€“water partition coefficients. Computational and Theoretical Chemistry, 2005, 727, 57-61.	1.5	14
56	Anatomy of bond formation. Bond length dependence of the extent of electron sharing in chemical bonds. Computational and Theoretical Chemistry, 2005, 727, 133-138.	1.5	47
57	The quantitative use of momentum-space descriptors. Chemical Physics Letters, 2005, 416, 376-380.	2.6	6
58	Spin-Coupled Study of the Electronic Mechanism of the Hetero-Dielsâ^'Alder Reaction of Acrolein and Ethene. Journal of Physical Chemistry A, 2005, 109, 231-235.	2.5	10
59	Multicenter bonding and the structure of electron-rich molecules. Model of three-center four-electron bonding reconsidered. Theoretical Chemistry Accounts, 2004, 112, 419-430.	1.4	52
60	Generalized population analysis of three-center two-electron bonding. International Journal of Quantum Chemistry, 2004, 97, 1002-1011.	2.0	40
61	Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. International Journal of Quantum Chemistry, 2004, 98, 465-472.	2.0	12
62	Modern Valence Bond Description of the Electronic Mechanisms of SN2 Identity Reactions. Journal of Physical Chemistry A, 2004, 108, 914-920.	2.5	14
63	Aromatic vs Diradical Character in the Transition States of the Cope Rearrangements of 1,5-Hexadiene and Its Cyano Derivatives. Journal of Physical Chemistry A, 2004, 108, 194-202.	2.5	25
64	Classification of reaction pathways via momentumâ€“space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213.	2.6	12
65	Modern Valence-Bond Description of Chemical Reaction Mechanisms:â€‰ The 1,3-Dipolar Addition of Methyl Azide to Ethene. Journal of Physical Chemistry A, 2003, 107, 2548-2559.	2.5	10
66	Electron Reorganization in Chemical Reactions. Structural Changes from the Analysis of Bond Order Profiles. Journal of Physical Chemistry A, 2003, 107, 2100-2105.	2.5	20
67	Structureâ€”property relationships and momentum space quantities: Hammett Ïƒâ€”constants. Molecular Physics, 2003, 101, 3159-3162.	1.7	20
68	Modern Valence Bond Description of Gas-Phase Pericyclic Reactions. Theoretical and Computational Chemistry, 2002, 10, 41-53.	0.4	19
69	Semi-empirical valence bond models of conjugated alkenes with donor and acceptor substituents. Physical Chemistry Chemical Physics, 2001, 3, 2419-2423.	2.8	3
70	Modern Valence-Bond Description of Chemical Reaction Mechanisms:Â The 1,3-Dipolar Addition of Diazomethane to Ethene. Journal of Organic Chemistry, 2001, 66, 4285-4292.	3.2	25
71	Reply to Comment â€œElectronic Reorganization in 1,3-Dipolar Cycloaddition of Fulminic Acid to Acetyleneâ€• Journal of Physical Chemistry A, 2001, 105, 10946-10946.	2.5	8
72	Spin-coupled description of the chemical bonding to hypercoordinate chlorine. Theoretical Chemistry Accounts, 2001, 105, 323-327.	1.4	8

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73	Silynes (RCa‰¡SiRa€²) and Disilynes (RSia‰¡SiRa€²): Why Are Less Bonds Worth Energetically More? The research is supported by an Israel Science Foundation (ISF) and a Niedersachsen grant (to S.S.), by a U.S.â€“Israel Binational Science Foundation (BSF) grant (to Y.A.) and by the Minerva Foundation. S.S. and F.O. thank the European Union for a Marie Curie Fellowship (Contract number: MCFI-1999-00145). S.S. and D.D. thank P. C. Hiberty for the helpful advice.. Angewandte Chemie - International Edition, 2001, 40, 4023.	13.8	65
74	Confronting modern valence bond theory with momentum-space quantum similarity and with pair density analysis. Mathematical and Computational Chemistry, 2001, , 169-185.	0.3	1
75	Spin-Coupled Model of the Bonding in First-Row Transition Metal Methylene Monocations. Journal of Physical Chemistry A, 2000, 104, 7091-7098.	2.5	10
76	Ab Initio Modern Valence Bond Theory. Topics in Current Chemistry, 1999, , 105-120.	4.0	14
77	Hypercoordinate bonding to main group elements: the spin-coupled point of view. Theoretical and Computational Chemistry, 1999, , 537-553.	0.4	2
78	Bent-bond versus separated-bond models: A spin-coupled survey for a few organic and inorganic systems. International Journal of Quantum Chemistry, 1999, 74, 223-229.	2.0	22
79	The spin-coupled description of aromatic, antiaromatic and nonaromatic systems. Theoretical and Computational Chemistry, 1999, , 503-518.	0.4	6
80	Bentâ€bond versus separatedâ€bond models: A spinâ€coupled survey for a few organic and inorganic systems. International Journal of Quantum Chemistry, 1999, 74, 223-229.	2.0	2
81	Nonorthogonal weights of modern VB wavefunctions. Implementation and applications within CASVB. Journal of Mathematical Chemistry, 1998, 23, 105-126.	1.5	46
82	Quantum molecular similarity via momentumâ€space indices. Journal of Mathematical Chemistry, 1998, 23, 51-60.	1.5	17
83	The spin-coupled description of phenylenedimethylidene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3301-3305.	1.7	5
84	Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H2. Chemical Physics, 1998, 233, 9-27.	1.9	44
85	A quantum molecular similarity approach to anti-HIV activity. Computational and Theoretical Chemistry, 1998, 423, 113-123.	1.5	5
86	Modern valence bond descriptions of molecular excited states: An application of CASVB. International Journal of Quantum Chemistry, 1998, 70, 637-650.	2.0	22
87	Optimization of virtual orbitals in the framework of a multiconfiguration spin-coupled wave function. Theoretical Chemistry Accounts, 1998, 99, 8-17.	1.4	23
88	Spin-coupled calculations based on projected spin eigenfunctions. Theoretical Chemistry Accounts, 1998, 99, 64-67.	1.4	4
89	Modern valence-bond description of chemical reaction mechanisms: the 1,3-dipolar addition of fulminic acid to ethyne. Theoretical Chemistry Accounts, 1998, 100, 222-229.	1.4	39
90	Spin-coupled description of fluorocyclophosphazenes (NPF2)3, (NPF2)4, (NPF2)5. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1541-1545.	1.7	2

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91	Modern Valence-Bond Description of Chemical Reaction Mechanisms:Â Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 1998, 120, 3975-3981.	13.7	45
92	Potential energy curves and â^,/â^,R couplings for electron capture in low-energy collisions of silicon ions with helium and atomic hydrogen. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3295-3299.	1.7	6
93	Modern VB representations of CASSCF wave functions and the fully-variational optimization of modern VB wave functions using the CASVB strategy. Advances in Quantum Chemistry, 1998, , 51-67.	0.8	67
94	The biorthogonal method for optimizing modern valence bond wavefunctions. Molecular Physics, 1998, 93, 663-674.	1.7	4
95	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
96	Chemical bonding in oxofluorides of hypercoordinate sulfur. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2247-2254.	1.7	46
97	Study of the electronic states of the allyl radical using spin-coupled valence bond theory. Journal of Chemical Physics, 1997, 106, 3663-3672.	3.0	26
98	Spin-Coupled Valence Bond Study of the Reaction between Benzene and a Methyl Cation. Journal of Physical Chemistry A, 1997, 101, 2886-2892.	2.5	16
99	Theoretical Investigation of Thiophene Oligomers:â€‰ A Spin-Coupled Study. Journal of Physical Chemistry A, 1997, 101, 4437-4443.	2.5	12
100	A New Approach to Valence Bond Calculations: CASVB. Molecular Engineering, 1997, 7, 67-85.	0.2	7
101	Normalization of projected spin eigenfunctions. Journal of Mathematical Chemistry, 1997, 22, 249-254.	1.5	2
102	Symmetry adaptation and the utilization of point group symmetry in valence bond calculations, including CASVB. Theoretica Chimica Acta, 1997, 95, 131-150.	0.8	38
103	The electronic structure of borabenzene: Combination of an aromatic ?-sextet and a reactive ?-framework. International Journal of Quantum Chemistry, 1997, 63, 441-449.	2.0	26
104	Fully variational optimization of modern VB wave functions using the CASVB strategy. International Journal of Quantum Chemistry, 1997, 65, 439-451.	2.0	78
105	Fully variational optimization of modern VB wave functions using the CASVB strategy. International Journal of Quantum Chemistry, 1997, 65, 439-451.	2.0	1
106	Symmetry adaptation and the utilization of point group symmetry in valence bond calculations, including CASVB. Theoretica Chimica Acta, 1997, 95, 131.	0.8	6
107	A New Approach to Valence Bond Calculations: CASVB. Topics in Molecular Organization and Engineering, 1997, , 67-85.	0.1	3
108	Exact transformations of CI spaces, VB representations of CASSCF wavefunctions and the optimization of VB wavefunctions. Theoretica Chimica Acta, 1996, 94, 233-245.	0.8	57

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109	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343-366.	0.8	143
110	Pair populations and effective valencies from ab initio SCF and spin-coupled wave functions. International Journal of Quantum Chemistry, 1996, 57, 501-518.	2.0	36
111	Chemical bonding in oxohalides of hypercoordinate nitrogen and phosphorus. International Journal of Quantum Chemistry, 1996, 60, 393-400.	2.0	19
112	Modern valence-bond description of the electronic structure of benzocyclobutadiene. International Journal of Quantum Chemistry, 1996, 60, 545-552.	2.0	16
113	Momentum-space electron densities?localized orbitals in hydrocarbons, boranes, and transition metal complexes. International Journal of Quantum Chemistry, 1996, 60, 579-592.	2.0	4
114	A modern valence bond approach for interatomic potentials. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 175-189.	0.6	2
115	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343.	0.8	4
116	Exact transformations of CI spaces, VB representations of CASSCF wavefunctions and the optimization of VB wavefunctions. Theoretica Chimica Acta, 1996, 94, 233.	0.8	30
117	Momentum-space similarity. Advances in Molecular Similarity, 1996, , 61-87.	0.5	6
118	Applications of momentum-space similarity. Journal of Computer-Aided Molecular Design, 1995, 9, 331-340.	2.9	20
119	The unusual coordination of carbon atoms in bicyclic l,6-methano[10]annulene: a modern valence bond study. Computational and Theoretical Chemistry, 1995, 338, 257-265.	1.5	9
120	Modern valence-bond description of bonding in strained three-membered rings: cyclopropane, aziridine, ethene oxide, phosphirane and thiirane. Computational and Theoretical Chemistry, 1995, 341, 13-24.	1.5	10
121	Momentum-space electron densities and quantum molecular similarity. Topics in Current Chemistry, 1995, , 85-111.	4.0	25
122	The Electronic Structure of Cyclooctatetraene and the Modern Valence-Bond Understanding of Antiaromaticity. The Journal of Physical Chemistry, 1995, 99, 10186-10195.	2.9	39
123	SPINS: A collection of algorithms for symbolic generation and transformation of many-electron spin eigenfunctions. Theoretica Chimica Acta, 1995, 90, 51-73.	0.8	49
124	Modern valence-bond description of the ground state of Li2 ?. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3751.	1.7	6
125	Bonding in YXXY dihalides and dihydrides of dioxygen and disulfur. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3357.	1.7	30
126	Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011.	1.7	11

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127	Catalytic chemistry of furan and thiophene. Ab initio calculations, using the spin-coupled valence bond method, of the interaction of furan and thiophene with a positively charged centre. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 749.	1.7	7
128	Modern valence-bond description of (CH3)4Li4. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3363.	1.7	6
129	Molecular Similarity and Momentum Space. , 1995, , 31-55.		11
130	Spin coupled valence bond theory of van der Waals systems: application to LiH â€¦ He. Molecular Physics, 1994, 83, 89-100.	1.7	15
131	The calculation of molecular response properties using perturbed spinâ€coupled wave functions. I. Basic theory. Journal of Chemical Physics, 1994, 100, 4408-4416.	3.0	6
132	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. II. Further applications. Chemical Physics, 1994, 186, 251-273.	1.9	13
133	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. I. Theory and first applications. Chemical Physics, 1994, 186, 233-250.	1.9	19
134	A topological classification. Nature, 1994, 371, 651-652.	27.8	6
135	Spin-coupled description of organic reaction pathways: the cycloaddition reaction of two ethene molecules. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1643.	1.7	10
136	Study of the electronic states of the benzene molecule using spinâ€coupled valence bond theory. Journal of Chemical Physics, 1994, 101, 3866-3887.	3.0	63
137	The calculation of molecular response properties using perturbed spinâ€coupled wave functions. II. Polarizability and magnetic susceptibility of H2 and LiH as functions of internuclear distance. Journal of Chemical Physics, 1994, 100, 4417-4431.	3.0	18
138	Spin-Coupled Study of the Electronic Structure of Polyenyl Radicals C3H5-C9H11. Journal of the American Chemical Society, 1994, 116, 2075-2084.	13.7	18
139	Chemical Bonding to Hypercoordinate Second-Row Atoms: d Orbital Participation versus Democracy. Journal of the American Chemical Society, 1994, 116, 4414-4426.	13.7	98
140	The Nature of the Carbon-Carbon Bonds in Cyclopropane and Cyclobutane: A Comparison Based on Spin-Coupled Theory. Journal of the American Chemical Society, 1994, 116, 7714-7721.	13.7	23
141	The Coulson-Fischer +r12wavefunction for H2. Molecular Physics, 1994, 81, 921-935.	1.7	6
142	Expansion of the spin-coupled wavefunction in Slater determinants. Theoretica Chimica Acta, 1993, 85, 261-270.	0.8	61
143	On the role of different spin bases within spin-coupled theory. Molecular Physics, 1993, 79, 197-216.	1.7	29
144	Ionic halides and oxides at high pressure: calculated Hugoniots, isotherms and thermal pressures. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4369.	1.7	18

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145	Molecular similarity of anti-HIV phospholipids. Journal of the American Chemical Society, 1993, 115, 12615-12616.	13.7	36
146	The Lowest Singlet and Triplet States of oâ€Benzyne: Spinâ€Coupled Interpretation of the Electronic Structure at CAS SCF Equilibrium Geometries. Israel Journal of Chemistry, 1993, 33, 253-264.	2.3	27
147	Bent versus .sigma.-.pi. bonds in ethene and ethyne: the spin-coupled point of view. Journal of the American Chemical Society, 1993, 115, 6863-6869.	13.7	34
148	Potential CFC replacements: Tropospheric lifetimes of C3 hydrofluorocarbons and hydrofluoroethers. Atmospheric Environment Part A General Topics, 1993, 27, 117-119.	1.3	21
149	Spin-coupled description of cyclobutadiene and 2,4-dimethylenecyclobutane-1,3-diyl: antipairs. The Journal of Physical Chemistry, 1992, 96, 7943-7952.	2.9	44
150	Population of long-lived vibrational levels of CO:I1Î£â^'andD1Î". Physical Review Letters, 1992, 68, 3865-3868.	7.8	5
151	Coreâ€valence separation in the spinâ€coupled wave function: A fully variational treatment based on a secondâ€order constrained optimization procedure. Journal of Chemical Physics, 1992, 97, 7637-7655.	3.0	76
152	Chemical bonding to lithium clusters: interaction of Li5 with H atoms. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 2309.	1.7	5
153	Tropospheric lifetimes of potential CFC replacements: Rate coefficients for reaction with the hydroxyl radical. Atmospheric Environment Part A General Topics, 1992, 26, 1331-1334.	1.3	32
154	Molecular dissimilarity: a momentum-space criterion. Journal of the American Chemical Society, 1992, 114, 4773-4776.	13.7	56
155	Polar Solids at High Pressure: NaF. Molecular Simulation, 1992, 9, 161-169.	2.0	10
156	A momentum-space approach to molecular similarity. Journal of Chemical Information and Computer Sciences, 1992, 32, 587-590.	2.8	34
157	The spin-coupled description of lithium clusters. Computational and Theoretical Chemistry, 1992, 259, 383-410.	1.5	15
158	Applications of spin-coupled valence bond theory. Chemical Reviews, 1991, 91, 929-964.	47.7	290
159	On the bonding in B2H6 and the lone pairs in H2O: The use of localized molecular orbitals in spin-coupled calculations. Computational and Theoretical Chemistry, 1991, 229, 155-162.	1.5	13
160	Hybrids and bond formation: Excursions in momentum space. Computational and Theoretical Chemistry, 1991, 229, 189-196.	1.5	8
161	The Ab initio spin-coupled description of the process HCNâ†'CH+N. Computational and Theoretical Chemistry, 1991, 229, 279-289.	1.5	6
162	Theoretical studies of fluorocarbons, hydrofluorocarbons and hydrochlorofluorocarbons. Journal of Fluorine Chemistry, 1991, 54, 229.	1.7	1

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163	Ionic solids at high pressures and elevated temperatures: MgO (periclase). Journal of Chemical Physics, 1991, 95, 6792-6799.	3.0	26
164	Electronic structure of diborane and octahydrotriborate(1-): boron-hydrogen-boron bridges and closed boron-boron-boron bonds. The Journal of Physical Chemistry, 1991, 95, 10617-10623.	2.9	28
165	A molecular catastrophe. Nature, 1990, 346, 796-797.	27.8	17
166	Theoretical studies of fluorocarbons. Part I. Small perfluoroalkane molecules. Journal of Fluorine Chemistry, 1990, 46, 317-337.	1.7	12
167	Theoretical studies of fluorocarbons. Part II. Fluorine and chlorine substituted alkanes. Journal of Fluorine Chemistry, 1990, 47, 489-507.	1.7	11
168	Theoretical studies of fluorocarbons part III. Primary, secondary, tertiary and quaternary centres. Journal of Fluorine Chemistry, 1990, 49, 421-432.	1.7	14
169	The Spin-coupled Approach to Electronic Structure. Molecular Simulation, 1990, 4, 293-312.	2.0	4
170	The modern VB descriptions of CH2, CH2 +, SiH2, and SiH2 +. Journal of the Chemical Society Perkin Transactions II, 1990, , 369.	0.9	14
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