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	Applications of spin-coupled valence bond theory. Chemical Reviews, 1991, 91, 929-964.	47.7	290
2	The electronic structure of the benzene molecule. Nature, 1986, 323, 699-701.	27.8	226
3	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343-366.	0.8	143
4	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
5	Theoretical study of lowâ€lying 1Î£+ and 1Î states of CO. I. Potential energy curves and dipole moments. Journal of Chemical Physics, 1987, 87, 424-432.	3.0	107
6	Theoretical study of lowâ€lying1Î£+and1Î states of CO. II. Transition dipole moments, oscillator strengths, and radiative lifetimes. Journal of Chemical Physics, 1989, 90, 4895-4902.	3.0	102
7	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
8	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
9	Fully variational optimization of modern VB wave functions using the CASVB strategy. International Journal of Quantum Chemistry, 1997, 65, 439-451.	2.0	78
10	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
11	High-Resolution Sizing of Monolayer-Protected Gold Clusters by Differential Centrifugal Sedimentation. ACS Nano, 2013, 7, 8881-8890.	14.6	71
12	Ab initio computation of molecular similarity. The Journal of Physical Chemistry, 1985, 89, 2195-2197.	2.9	67
13	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
14	Silynes (RCâ‰¡SiRâ€²) and Disilynes (RSiâ‰¡SiRâ€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
15	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
16	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
17	The electronic structure of heteroaromatic molecules. Part 3. A comparison of benzene, borazine, and boroxine. Journal of the Chemical Society Perkin Transactions II, 1989, , 719.	0.9	62
18	Expansion of the spin-coupled wavefunction in Slater determinants. Theoretica Chimica Acta, 1993, 85, 261-270.	0.8	61

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19	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
20	Molecular dissimilarity: a momentum-space criterion. Journal of the American Chemical Society, 1992, 114, 4773-4776.	13.7	56
21	Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes. Physical Chemistry Chemical Physics, 2009, 11, 3424.	2.8	54
22	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
23	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
24	Sensitive Analysis of Protein Adsorption to Colloidal Gold by Differential Centrifugal Sedimentation. Analytical Chemistry, 2017, 89, 6807-6814.	6.5	48
25	A novel approach to molecular similarity. Journal of Computer-Aided Molecular Design, 1989, 3, 253-259.	2.9	47
26	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
27	Chemical bonding in oxofluorides of hypercoordinate sulfur. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2247-2254.	1.7	46
28	Nonorthogonal weights of modern VB wavefunctions. Implementation and applications within CASVB. Journal of Mathematical Chemistry, 1998, 23, 105-126.	1.5	46
29	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
30	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
31	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
32	The ab initio spin-coupled description of methane: Hybridization without preconceptions. Computational and Theoretical Chemistry, 1988, 169, 421-436.	1.5	43
33	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
34	The gradient expansions of the kinetic energy and the mean momentum for light diatomic molecules. Journal of Chemical Physics, 1985, 83, 4562-4564.	3.0	42
35	Generalized population analysis of three-center two-electron bonding. International Journal of Quantum Chemistry, 2004, 97, 1002-1011.	2.0	40
36	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

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37	Valence bond calculations of the degree of covalency in a Cî—¸X bond: Application to CH4 and CH3Li. Computational and Theoretical Chemistry, 1988, 169, 437-446.	1.5	39
38	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
39	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
40	Charge partitioning by zeroâ€flux surfaces: The acidities and basicities of simple aliphatic alcohols and amines. Journal of Chemical Physics, 1983, 79, 4967-4972.	3.0	38
41	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
42	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
43	The spin-coupled valence bond description of benzenoid aromatic molecules. Topics in Current Chemistry, 1990, , 41-55.	4.0	38
44	Noble gas molecular ions. Molecular Physics, 1981, 44, 161-172.	1.7	37
45	Distributed multipole analysis from charge partitioning by zero-flux surfaces: The structure of HF complexes. Chemical Physics Letters, 1985, 120, 167-172.	2.6	37
46	The electronic structure of 1,3-dipoles: hypervalent atoms. Journal of the Chemical Society Perkin Transactions II, 1989, , 1187.	0.9	37
47	Theoretical investigation of the Xâ€‰2Î£+ and Câ€‰2Î£+ states of BeH. Journal of Chemical Physics, 1984, 80, 1961-1963.	3.0	36
48	Ab initio investigation of low-lying 2Î£+ and 2Î states of NO2+. Chemical Physics Letters, 1986, 132, 377-382.	2.6	36
49	Molecular similarity of anti-HIV phospholipids. Journal of the American Chemical Society, 1993, 115, 12615-12616.	13.7	36
50	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
51	Ab initio spin-coupled description of the reactions CH2(1A1) + H2 .fwdarw. CH4 and CH4 .fwdarw. CH3(2A1') + H. Journal of the American Chemical Society, 1990, 112, 5054-5060.	13.7	34
52	A momentum-space approach to molecular similarity. Journal of Chemical Information and Computer Sciences, 1992, 32, 587-590.	2.8	34
53	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
54	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

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55	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
56	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
57	Spin-Coupled Theory for â€˜N Electrons in M Orbitalsâ€™ Active Spaces. Journal of Physical Chemistry A, 2012, 116, 7238-7244.	2.5	31
58	Momentum space properties and local density approximations in small molecules: A critical appraisal. Journal of Chemical Physics, 1986, 84, 5594-5605.	3.0	30
59	The electronic structure of heteroaromatic molecules. Part 2. Five-membered rings. Journal of the Chemical Society Perkin Transactions II, 1989, , 263.	0.9	30
60	Bonding in YXXY dihalides and dihydrides of dioxygen and disulfur. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3357.	1.7	30
61	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
62	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
63	On the role of different spin bases within spin-coupled theory. Molecular Physics, 1993, 79, 197-216.	1.7	29
64	A one-electron approximation to domain-averaged Fermi hole analysis. Physical Chemistry Chemical Physics, 2008, 10, 1319.	2.8	29
65	The electronic structure of CH2 and the cycloaddition reaction of methylene with ethene. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1651.	1.1	28
66	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
67	The electronic structure of 1,3-dipoles: spin-coupled descriptions of nitrone and diazomethane. Chemical Physics Letters, 1987, 138, 296-302.	2.6	27
68	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
69	Local density approximations to moments of momentum of diatomic molecules with Hartreeâ€“Fockâ€“Roothaan quality electron distributions. Journal of Chemical Physics, 1985, 83, 239-240.	3.0	26
70	Ionic solids at high pressures and elevated temperatures: MgO (periclase). Journal of Chemical Physics, 1991, 95, 6792-6799.	3.0	26
71	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
72	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

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73	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
74	Theoretical study of the (3sÏ*f*)1Î Rydberg state of CO. Chemical Physics Letters, 1988, 152, 393-396.	2.6	25
75	Momentum-space electron densities and quantum molecular similarity. Topics in Current Chemistry, 1995, , 85-111.	4.0	25
76	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
77	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
78	Spin-coupled descriptions of organic reactivity. International Reviews in Physical Chemistry, 2009, 28, 169-206.	2.3	25
79	Why is the bond multiplicity in C2 so elusive?. Computational and Theoretical Chemistry, 2015, 1053, 189-194.	2.5	25
80	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
81	The dipole moment of LiH(X1Î£+): Spin-coupled valence-bond study. Chemical Physics Letters, 1985, 118, 580-584.	2.6	23
82	Bond formation in momentum space. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 449.	1.1	23
83	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
84	Optimization of virtual orbitals in the framework of a multiconfiguration spin-coupled wave function. Theoretical Chemistry Accounts, 1998, 99, 8-17.	1.4	23
85	The modern valence bond description of naphthalene. Journal of the Chemical Society Chemical Communications, 1989, , 675.	2.0	22
86	The electronic structure of heteroaromatic molecules. Part 1. Six-membered rings. Journal of the Chemical Society Perkin Transactions II, 1989, , 255.	0.9	22
87	Modern valence bond descriptions of molecular excited states: An application of CASVB. International Journal of Quantum Chemistry, 1998, 70, 637-650.	2.0	22
88	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
89	The electronic structure of nitrilimine: absence of the carbenic form. Chemical Communications, 2006, , 1030.	4.1	22
90	Spinâ€“orbit coupling and Î› doubling in NaAr. Journal of Chemical Physics, 1981, 75, 4157-4159.	3.0	21

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91	Ab initio calculation of molecular spinâ€orbit coupling constants using a universal evenâ€tempered basis set of exponential functions. Journal of Chemical Physics, 1982, 76, 6088-6090.	3.0	21
92	Universal systematic sequence of evenâ€tempered exponentialâ€type functions in electronic structure studies. Journal of Chemical Physics, 1982, 77, 5053-5057.	3.0	21
93	Potential CFC replacements: Tropospheric lifetimes of C3 hydrofluorocarbons and hydrofluoroethers. Atmospheric Environment Part A General Topics, 1993, 27, 117-119.	1.3	21
94	Applications of momentum-space similarity. Journal of Computer-Aided Molecular Design, 1995, 9, 331-340.	2.9	20
95	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
96	Structureâ€”property relationships and momentum space quantities: Hammett Ïƒâ€constants. Molecular Physics, 2003, 101, 3159-3162.	1.7	20
97	Accidental predissociation in lithium dimer: A theoretical investigation. Chemical Physics Letters, 1982, 86, 472-476.	2.6	19
98	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. I. Theory and first applications. Chemical Physics, 1994, 186, 233-250.	1.9	19
99	Chemical bonding in oxohalides of hypercoordinate nitrogen and phosphorus. International Journal of Quantum Chemistry, 1996, 60, 393-400.	2.0	19
100	Modern Valence Bond Description of Gas-Phase Pericyclic Reactions. Theoretical and Computational Chemistry, 2002, 10, 41-53.	0.4	19
101	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
102	Reactions of hydrofluorocarbons and hydrochlorofluorocarbons with the hydroxyl radical. Atmospheric Environment Part A General Topics, 1990, 24, 2417-2419.	1.3	18
103	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
104	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
105	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
106	A spin-coupled study of the Claisen rearrangement of allyl vinyl ether. Theoretical Chemistry Accounts, 2006, 115, 212-220.	1.4	18
107	Ab initio calculation of higher order corrections to Î› doubling and spin splitting in diatomic molecules. Journal of Chemical Physics, 1981, 74, 3961-3964.	3.0	17
108	Universal evenâ€tempered basis sets for negative molecular ions. Journal of Chemical Physics, 1983, 78, 2456-2458.	3.0	17

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109	A molecular catastrophe. Nature, 1990, 346, 796-797.	27.8	17
110	Quantum molecular similarity via momentumâ€space indices. Journal of Mathematical Chemistry, 1998, 23, 51-60.	1.5	17
111	Universal systematic sequences of evenâ€tempered basis functions in electronic structure studies of negative ions. Journal of Chemical Physics, 1982, 77, 4551-4554.	3.0	16
112	The Practical Calculation of Interionic Potentials in Solids using Electron Gas Theory. Molecular Simulation, 1990, 4, 269-283.	2.0	16
113	Modern valence-bond description of the electronic structure of benzocyclobutadiene. International Journal of Quantum Chemistry, 1996, 60, 545-552.	2.0	16
114	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
115	AB initio predictions for silicon analogs of astrophysically interesting molecules - SiC2H2, SiH2CN, SiH2C2, and CH2CSi. Astrophysical Journal, 1990, 354, 229.	4.5	16
116	Spinâ€“orbit coupling and spin splitting in HeNe+. Journal of Chemical Physics, 1982, 76, 6443-6444.	3.0	15
117	Studies of molecular states using spin-coupled valence-bond theory. Faraday Symposia of the Chemical Society, 1984, 19, 149.	0.5	15
118	Potential energy surfaces for the reaction of B+ (1S,3P) with H2 using spin-coupled VB theory. Chemical Physics Letters, 1986, 127, 600-608.	2.6	15
119	The spin-coupled description of lithium clusters. Computational and Theoretical Chemistry, 1992, 259, 383-410.	1.5	15
120	Spin coupled valence bond theory of van der Waals systems: application to LiH â€¦ He. Molecular Physics, 1994, 83, 89-100.	1.7	15
121	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
122	Theoretical studies of fluorocarbons part III. Primary, secondary, tertiary and quaternary centres. Journal of Fluorine Chemistry, 1990, 49, 421-432.	1.7	14
123	The modern VB descriptions of CH2, CH2 +, SiH2, and SiH2 +. Journal of the Chemical Society Perkin Transactions II, 1990, , 369.	0.9	14
124	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
125	Ab Initio Modern Valence Bond Theory. Topics in Current Chemistry, 1999, , 105-120.	4.0	14
126	Modern Valence Bond Description of the Electronic Mechanisms of SN2 Identity Reactions. Journal of Physical Chemistry A, 2004, 108, 914-920.	2.5	14

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127	The use of momentum-space descriptors for predicting octanolâ€“water partition coefficients. Computational and Theoretical Chemistry, 2005, 727, 57-61.	1.5	14
128	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
129	Electronic structure of monomeric methyl-lithium. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 151.	1.1	13
130	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
131	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. II. Further applications. Chemical Physics, 1994, 186, 251-273.	1.9	13
132	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
133	Excited-State Aromaticity Reversals in MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2020, 124, 9611-9616.	2.5	13
134	Theoretical study of the HCCS radical. Chemical Physics Letters, 1981, 81, 479-480.	2.6	12
135	Theoretical studies of fluorocarbons. Part I. Small perfluoroalkane molecules. Journal of Fluorine Chemistry, 1990, 46, 317-337.	1.7	12
136	Theoretical Investigation of Thiophene Oligomers:â€‰ A Spin-Coupled Study. Journal of Physical Chemistry A, 1997, 101, 4437-4443.	2.5	12
137	Classification of reaction pathways via momentumâ€“space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213.	2.6	12
138	Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. International Journal of Quantum Chemistry, 2004, 98, 465-472.	2.0	12
139	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
140	Direct summation over vibrational levels: Î› doubling in HF+. Journal of Chemical Physics, 1981, 75, 4502-4506.	3.0	11
141	Theoretical study of AlH+: Spin splitting, core polarization, and interstellar chemistry. Journal of Chemical Physics, 1983, 78, 1371-1376.	3.0	11
142	Spin-coupled valence bond study of low-lying states of LiHe+. Molecular Physics, 1985, 56, 611-620.	1.7	11
143	Theoretical studies of fluorocarbons. Part II. Fluorine and chlorine substituted alkanes. Journal of Fluorine Chemistry, 1990, 47, 489-507.	1.7	11
144	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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145	Molecular Similarity and Momentum Space. , 1995, , 31-55.		11
146	Study of the spectrum and decay of the doubly charged water ion using spinâ€coupled valence bond theory. Journal of Chemical Physics, 1987, 87, 1666-1676.	3.0	10
147	Polar Solids at High Pressure: NaF. Molecular Simulation, 1992, 9, 161-169.	2.0	10
148	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
149	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
150	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
151	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
152	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
153	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
154	Spinâ€“orbit coupling constants for the 2E states of CH3O and CH3F+. Journal of Chemical Physics, 1982, 76, 2765-2766.	3.0	9
155	On the bonding in 2,4-dimethylenecyclobutane-1,3-diyl. Journal of the Chemical Society Chemical Communications, 1989, , 1489.	2.0	9
156	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
157	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
158	Surface tension, density and composition in the methane-pentane system at high pressure. Fluid Phase Equilibria, 2018, 456, 193-202.	2.5	9
159	Spin-coupled valence bond study of the lithium hydride anion. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1713.	1.1	8
160	Hybrids and bond formation: Excursions in momentum space. Computational and Theoretical Chemistry, 1991, 229, 189-196.	1.5	8
161	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
162	Spin-coupled description of the chemical bonding to hypercoordinate chlorine. Theoretical Chemistry Accounts, 2001, 105, 323-327.	1.4	8

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163	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
164	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
165	Local density approximations and momentum-space properties in light molecules and ionic solids. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1675.	1.1	7
166	Momentum space studies of large polyenes. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1519.	1.1	7
167	On the bonding to transition metal atoms in low oxidation states. Journal of the Chemical Society Chemical Communications, 1989, , 1604.	2.0	7
168	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
169	A New Approach to Valence Bond Calculations: CASVB. Molecular Engineering, 1997, 7, 67-85.	0.2	7
170	Modern Valence-Bond-Like Representations of SelectedD6hâ€œAromaticâ€•Rings. Journal of Physical Chemistry A, 2006, 110, 7913-7917.	2.5	7
171	Theoretical study of SiO2-. Molecular Physics, 1981, 44, 799-802.	1.7	6
172	Spin-coupled VB study of the di-cations of methane, ammonia and water. Molecular Physics, 1988, 65, 251-259.	1.7	6
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