Peter B Karadakov

List of Publications by Year
in descending order

105	2,616	201674	223800
papers	citations	27 h-index	46 g-index

107	107	107	2114
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ground- and Excited-State Aromaticity and Antiaromaticity in Benzene and Cyclobutadiene. Journal of Physical Chemistry A, 2008, 112, 7303-7309.	2.5	205
2	Aromaticity and Antiaromaticity in the Low-Lying Electronic States of Cyclooctatetraene. Journal of Physical Chemistry A, 2008, 112, 12707-12713.	2.5	144
3	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343-366.	0.8	143
4	Chemical Bonding and Aromaticity in Furan, Pyrrole, and Thiophene: A Magnetic Shielding Study. Journal of Organic Chemistry, 2013, 78, 8037-8043.	3.2	105
5	ONIOM as an efficient tool for calculating NMR chemical shielding constants in large molecules. Chemical Physics Letters, 2000, 317, 589-596.	2.6	101
6	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
7	Experimental and Theoretical Study of Halogen-Bonded Complexes of DMAP with Di- and Triiodofluorobenzenes. A Complex with a Very Short NÂ·Â·Â·I Halogen Bond. Crystal Growth and Design, 2010, 10, 3710-3720.	3.0	82
8	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
9	Magnetic Shielding, Aromaticity, Antiaromaticity, and Bonding in the Low-Lying Electronic States of Benzene and Cyclobutadiene. Journal of Organic Chemistry, 2016, 81, 11346-11352.	3.2	67
10	Magnetic Shielding in and around Benzene and Cyclobutadiene: A Source of Information about Aromaticity, Antiaromaticity, and Chemical Bonding. Journal of Physical Chemistry A, 2013, 117, 518-523.	2.5	50
11	Shielding in and around Oxazole, Imidazole, and Thiazole: How Does the Second Heteroatom Affect Aromaticity and Bonding?. Journal of Organic Chemistry, 2015, 80, 7150-7157.	3.2	50
12	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
13	Controlling the S₁ Energy Profile by Tuning Excited-State Aromaticity. Journal of the American Chemical Society, 2020, 142, 14985-14992.	13.7	48
14	Halogen-bonded liquid crystals of 4-alkoxystilbazoles with molecular iodine: a very short halogen bond and unusual mesophase stability. Chemical Communications, 2013, 49, 3946.	4.1	47
15	Chemical bonding in oxofluorides of hypercoordinate sulfur. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2247-2254.	1.7	46
16	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
17	Halogenâ€and Hydrogenâ€Bonded Salts and Coâ€crystals Formed from 4â€Haloâ€2,3,5,6â€tetrafluorophenol and Cyclic Secondary and Tertiary Amines: Orthogonal and Nonâ€orthogonal Halogen and Hydrogen Bonding, and Synthetic Analogues of Halogenâ€Bonded Biological Systems. Chemistry - A European Journal, 2014, 20, 6721-6732.	3.3	43
18	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

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19	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
20	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
21	Demonstration of Baird's rule complementarity in the singlet state with implications for excited-state intramolecular proton transfer. Physical Chemistry Chemical Physics, 2019, 21, 11608-11614.	2.8	34
22	Competition and cooperation: hydrogen and halogen bonding in co-crystals involving 4-iodotetrafluorobenzoic acid, 4-iodotetrafluorophenol and 4-bromotetrafluorophenol. CrystEngComm, 2014, 16, 4254-4264.	2.6	32
23	Spin-Coupled Theory for â€˜N Electrons in M Orbitalsâ€™ Active Spaces. Journal of Physical Chemistry A, 2012, 116, 7238-7244.	2.5	31
24	Mesomorphism and Photophysics of Some Metallomesogens Based on Hexasubstituted 2,2â€²:6â€², 2â€²â€²â€²â€¶erpyridines. Chemistry - A European Journal, 2016, 22, 8215-8233.	3.3	31
25	Bonding in YXXY dihalides and dihydrides of dioxygen and disulfur. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3357.	1.7	30
26	Calculations of magnetic shielding for the tin nucleus in a series of tetra-organotin compounds using density functional theory. Physical Chemistry Chemical Physics, 2002, 4, 5925-5932.	2.8	29
27	Exploring Chemical Bonds through Variations in Magnetic Shielding. Journal of Chemical Theory and Computation, 2016, 12, 558-563.	5.3	29
28	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
29	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
30	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
31	Improved convergence of Hartreeâ€“Fock style excited-state wavefunctions using second-order optimisation with an exact Hessian. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	26
32	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
33	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
34	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
35	Spin-coupled descriptions of organic reactivity. International Reviews in Physical Chemistry, 2009, 28, 169-206.	2.3	25
36	Quantum Chemical Investigation of Attractive Non-Covalent Interactions between Halomethanes and Rare Gases. Journal of Physical Chemistry A, 2012, 116, 10621-10628.	2.5	24

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37	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
38	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
39	Calculation of NMR Chemical Shifts in Carbohydrates with ONIOM:â€‰ A Study of the Conformers of Î²-d-Glucopyranose. Journal of Physical Chemistry A, 2003, 107, 292-300.	2.5	22
40	Detailed Visualization of Aromaticity Using Isotropic Magnetic Shielding. Angewandte Chemie - International Edition, 2020, 59, 19275-19281.	13.8	22
41	Mesomorphic 1,2,4-triazine-4-oxides in the synthesis of new heterocyclic liquid crystals. Journal of Materials Chemistry, 2008, 18, 1703.	6.7	21
42	Magnetic Shielding Studies of C₂ and C₂H₂ Support Higher than Triple Bond Multiplicity in C₂. Chemistry - A European Journal, 2017, 23, 12949-12954.	3.3	21
43	Halogen Bonding Interaction between Fluorohalides and Isocyanides. Journal of Physical Chemistry A, 2011, 115, 11079-11086.	2.5	20
44	Chemical bonding in oxohalides of hypercoordinate nitrogen and phosphorus. International Journal of Quantum Chemistry, 1996, 60, 393-400.	2.0	19
45	Modern Valence Bond Description of Gas-Phase Pericyclic Reactions. Theoretical and Computational Chemistry, 2002, 10, 41-53.	0.4	19
46	Magnetic Shielding, Aromaticity, Antiaromaticity and Bonding in the Lowâ€Łying Electronic States of S₂N₂. Chemistry - A European Journal, 2018, 24, 16791-16803.	3.3	19
47	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
48	A spin-coupled study of the Claisen rearrangement of allyl vinyl ether. Theoretical Chemistry Accounts, 2006, 115, 212-220.	1.4	18
49	Modern valence-bond description of the electronic structure of benzocyclobutadiene. International Journal of Quantum Chemistry, 1996, 60, 545-552.	2.0	16
50	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
51	Norcorrole: Aromaticity and Antiaromaticity in Contest. Organic Letters, 2020, 22, 8676-8680.	4.6	15
52	Magnetic Shielding Study of Bonding and Aromaticity in Corannulene and Coronene. Chemistry, 2021, 3, 861-872.	2.2	15
53	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
54	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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55	Do large polycyclic aromatic hydrocarbons and graphene bend? How popular theoretical methods complicate finding the answer to this question. Chemical Physics Letters, 2016, 646, 190-196.	2.6	14
56	Excited-State Aromaticity Reversals in MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2020, 124, 9611-9616.	2.5	13
57	Can Antiâ€Aufbau DFT Calculations Estimate Singlet Excited State Aromaticity? Correspondence on â€œDibenzoarsepins: Planarization of 8Ïâ€Electron System in the Lowest Singlet Excited Stateâ€• Angewandte Chemie - International Edition, 2020, 59, 9228-9230.	13.8	13
58	Electron correlation and basis set effects on the 17O and 1H nuclear magnetic shieldings in water clusters (H2O)n (n=2â€“5). Journal of Molecular Structure, 2002, 602-603, 293-301.	3.6	12
59	Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. International Journal of Quantum Chemistry, 2004, 98, 465-472.	2.0	12
60	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
61	Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011.	1.7	11
62	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
63	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
64	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
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	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
67	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
68	Magnetic shielding paints an accurate and easy-to-visualize portrait of aromaticity. Chemical Communications, 2021, 57, 9504-9513.	4.1	10
69	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
70	Sequential cycloaddition-cycloreversion-cycloaddition-cope rearrangement with an annelated norbornadiene and electrophilic dienes. unusual [Ï€2s + Ï€2a + Ïƒ2a] transformation of a pentacyclo-[11.4.0.17,10.04,13.06,11]octadeca-3,8,14,17-tetraene.1. Tetrahedron, 1993, 49, 4699-4710.	1.9	8
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	A variationally stable compact Hartreeâ€“Fock-style wavefunction for a non-degenerate first excited state. Molecular Physics, 2007, 105, 2363-2373.	1.7	8

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73	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
74	The critical role played by water in controlling Pd catalyst speciation in arylcyanation reactions. Reaction Chemistry and Engineering, 2019, 4, 122-130.	3.7	8
75	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
76	Modern Valence-Bond-Like Representations of SelectedD6hâ€œAromaticâ€•Rings. Journal of Physical Chemistry A, 2006, 110, 7913-7917.	2.5	7
77	Modern valence-bond description of the ground state of Li2 ?. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3751.	1.7	6
78	Modern valence-bond description of (CH3)4Li4. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3363.	1.7	6
79	The spin-coupled picture of clamped benzenes. Molecular Physics, 2006, 104, 677-680.	1.7	6
80	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
81	Does the Electronic Structure of MÃ¶bius Annulenes Follow Heilbronner's Ideas?. ChemPhysChem, 2018, 19, 3186-3190.	2.1	6
82	The spin-coupled description of phenylenedimethylidene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3301-3305.	1.7	5
83	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
84	Bonding in Singlet and Triplet Butalene: Insights from Spin-Coupled Theory. Journal of Physical Chemistry A, 2015, 119, 2169-2175.	2.5	5
85	Modern Valence-Bond Description of Homoaromaticity. Journal of Physical Chemistry A, 2016, 120, 8769-8779.	2.5	5
86	Aromaticity reversals and their effect on bonding in the low-lying electronic states of cyclooctatetraene. Physical Chemistry Chemical Physics, 2021, 23, 24750-24756.	2.8	5
87	Modern valence-bond description of aromatic annulene ions. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4
88	Statistical Thermodynamics Unveils How Ions Influence an Aqueous Dielsâ€Alder Reaction. ChemPhysChem, 2019, 20, 1538-1544.	2.1	4
89	Detailed Visualization of Aromaticity Using Isotropic Magnetic Shielding. Angewandte Chemie, 2020, 132, 19437-19443.	2.0	4
90	Are Multicentre Bond Indices and Related Quantities Reliable Predictors of Excited-State Aromaticity?. Molecules, 2020, 25, 4791.	3.8	4

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91	Mechanism of dye solubilization and de-aggregation by urea. Dyes and Pigments, 2021, 193, 109530.	3.7	4
92	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343.	0.8	4
93	The unusual reaction of tetrachlorothiophene dioxide with an adduct of 5,6-bismethylenenorbornene and hexachloronorbornadiene. Journal of the Chemical Society Chemical Communications, 1991, , 1763.	2.0	3
94	The Effect of Electron Correlation on the 19F Chemical Shifts in Fluorobenzenes. ACS Symposium Series, 1999, , 115-125.	0.5	3
95	Bonding in benzodicyclobutadiene isomers: insights from modern valence bond theory. Molecular Physics, 2014, 112, 2840-2852.	1.7	3
96	Electrophilic bromination of substituted stilbenes and stilbazoles: a quantum-chemical investigation. Physical Chemistry Chemical Physics, 2014, 16, 2576.	2.8	3
97	Nature of the chemical bonding in D_{3h} [MH₃M]⁺ cations (M = Be, Mg). International Journal of Quantum Chemistry, 2020, 120, e26183.	2.0	3
98	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
99	3 Theoretical description of reaction mechanisms: reaction pathways and electronic structure rearrangements. Annual Reports on the Progress of Chemistry Section C, 2001, 97, 61-90.	4.4	2
100	Modern valence-bond descriptions of polycyclic fused aromatic compounds involving cyclopropenyl rings. Computational and Theoretical Chemistry, 2017, 1116, 32-39.	2.5	2
101	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
102	Can Antiâ€Aufbau DFT Calculations Estimate Singlet Excited State Aromaticity? Correspondence on â€œDibenzoarsepins: Planarization of 8Ï€â€Electron System in the Lowest Singlet Excited Stateâ€. Angewandte Chemie, 2020, 132, 9312-9314.	2.0	1
103	Investigating IstvÃ¡n Mayer's â€œimprovedâ€definitions of bond orders and free valence for correlated singletâ€state wave functions. International Journal of Quantum Chemistry, 0, , e26612.	2.0	1
104	Nuclear Magnetic Resonance and Computational Study of trans-(Î¼2:Î·2,Î·2-1,3-Butadiene)bis(trichloroplatinate(II)). Organometallics, 2020, 39, 4723-4734.	2.3	0
105	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