Frank Weinhold

List of Publications by Year
in descending order

229 papers	57,241 citations	12303 69 h-index	1216 227 g-index
277 all docs	277 docs citations	277 times ranked	23843 citing authors

#	Article	IF	Citations
1	Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. Chemical Reviews, 1988, 88, 899-926.	23.0	15,946
2	Natural population analysis. Journal of Chemical Physics, 1985, 83, 735-746.	1.2	8,757
3	Natural hybrid orbitals. Journal of the American Chemical Society, 1980, 102, 7211-7218.	6.6	4,505
4	Natural bond orbital analysis of nearâ€Hartreeâ€“Fock water dimer. Journal of Chemical Physics, 1983, 78, 4066-4073.	1.2	2,775
5	Natural localized molecular orbitals. Journal of Chemical Physics, 1985, 83, 1736-1740.	1.2	2,019
6	Analysis of the geometry of the hydroxymethyl radical by the â€œdifferent hybrids for different spinsâ€• natural bond orbital procedure. Computational and Theoretical Chemistry, 1988, 169, 41-62.	1.5	1,905
7	NBO 6.0: Natural bond orbital analysis program. Journal of Computational Chemistry, 2013, 34, 1429-1437.	1.5	1,269
8	Natural bond orbital methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 1-42.	6.2	1,153
9	NATURAL BOND ORBITALS AND EXTENSIONS OF LOCALIZED BONDING CONCEPTS. Chemistry Education Research and Practice, 2001, 2, 91-104.	1.4	732
10	Electronic Basis of Improper Hydrogen Bonding:Â A Subtle Balance of Hyperconjugation and Rehybridization. Journal of the American Chemical Society, 2003, 125, 5973-5987.	6.6	700
11	Natural resonance theory: I. General formalism. Journal of Computational Chemistry, 1998, 19, 593-609.	1.5	621
12	What is NBO analysis and how is it useful?. International Reviews in Physical Chemistry, 2016, 35, 399-440.	0.9	585
13	Metric geometry of equilibrium thermodynamics. Journal of Chemical Physics, 1975, 63, 2479-2483.	1.2	560
14	Natural bond orbital analysis: A critical overview of relationships to alternative bonding perspectives. Journal of Computational Chemistry, 2012, 33, 2363-2379.	1.5	515
15	Natural resonance theory: II. Natural bond order and valency. Journal of Computational Chemistry, 1998, 19, 610-627.	1.5	480
16	Natural bond orbital analysis of molecular interactions: Theoretical studies of binary complexes of HF, H2O, NH3, N2, O2, F2, CO, and CO2 with HF, H2O, and NH3. Journal of Chemical Physics, 1986, 84, 5687-5705.	1.2	474
17	Natural resonance theory: III. Chemical applications. Journal of Computational Chemistry, 1998, 19, 628-646.	1.5	460
18	The Natural Bond Orbital Lewis Structure Concept for Molecules, Radicals, and Radical Ions. , 1988, , 227-236.		392

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19	Resonance properties of complex-rotated hamiltonians. Molecular Physics, 1978, 36, 1613-1630.	0.8	369
20	Collagen Stability:Â Insights from NMR Spectroscopic and Hybrid Density Functional Computational Investigations of the Effect of Electronegative Substituents on Prolyl Ring Conformations. Journal of the American Chemical Society, 2002, 124, 2497-2505.	6.6	318
21	Quantum-mechanical studies on the origin of barriers to internal rotation about single bonds. Journal of the American Chemical Society, 1979, 101, 1700-1709.	6.6	312
22	Natural chemical shielding analysis of nuclear magnetic resonance shielding tensors from gauge-including atomic orbital calculations. Journal of Chemical Physics, 1997, 107, 1173-1184.	1.2	258
23	Natural bond orbital analysis of steric interactions. Journal of Chemical Physics, 1997, 107, 5406-5421.	1.2	257
24	NBO 7.0: New vistas in localized and delocalized chemical bonding theory. Journal of Computational Chemistry, 2019, 40, 2234-2241.	1.5	249
25	A new twist on molecular shape. Nature, 2001, 411, 539-541.	13.7	234
26	Structure and spectroscopy of (HCN)n clusters: Cooperative and electronic delocalization effects in Câ€“Hâ‹…â‹…â‹…N hydrogen bonding. Journal of Chemical Physics, 1995, 103, 333-347.	1.2	220
27	Nature of H-bonding in clusters, liquids, and enzymes: an ab initio, natural bond orbital perspective. Computational and Theoretical Chemistry, 1997, 398-399, 181-197.	1.5	219
28	What is a hydrogen bond? Mutually consistent theoretical and experimental criteria for characterizing H-bonding interactions. Molecular Physics, 2012, 110, 565-579.	0.8	195
29	Metric geometry of equilibrium thermodynamics. II. Scaling, homogeneity, and generalized Gibbsâ€“Duhem relations. Journal of Chemical Physics, 1975, 63, 2484-2487.	1.2	179
30	Natural Bond Orbital Analysis of Internal Rotation Barriers and Related Phenomena. Israel Journal of Chemistry, 1991, 31, 277-285.	1.0	179
31	Natural steric analysis of internal rotation barriers. International Journal of Quantum Chemistry, 1999, 72, 269-280.	1.0	179
32	Natural steric analysis:Ab initiovan der Waals radii of atoms and ions. Journal of Chemical Physics, 1997, 107, 5422-5432.	1.2	173
33	Antiâ€Electrostatic Hydrogen Bonds. Angewandte Chemie - International Edition, 2014, 53, 11214-11217.	7.2	171
34	On the role of d orbitals in sulfur hexafluoride. Journal of the American Chemical Society, 1986, 108, 3586-3593.	6.6	168
35	Rebuttal to the Bickelhauptâ€“Baerends Case for Steric Repulsion Causing the Staggered Conformation of Ethane. Angewandte Chemie - International Edition, 2003, 42, 4188-4194.	7.2	160
36	Quantum cluster equilibrium theory of liquids: General theory and computer implementation. Journal of Chemical Physics, 1998, 109, 367-372.	1.2	153

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37	Dynamic polarizabilities of twoâ€electron atoms, with rigorous upper and lower bounds. Journal of Chemical Physics, 1976, 65, 4913-4926.	1.2	136
38	The Nature of the Siliconâ€“Oxygen Bond. Organometallics, 2011, 30, 5815-5824.	1.1	135
39	Moment-theory investigations of photoabsorption and dispersion profiles in atoms and ions. Physical Review A, 1976, 14, 1042-1056.	1.0	133
40	Experimental and theoretical determination of the temperature dependence of deuteron and oxygen quadrupole coupling constants of liquid water. Journal of Chemical Physics, 1995, 103, 6941-6950.	1.2	132
41	Spectroscopic Evidence for Clusters of Likeâ€Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. ChemPhysChem, 2016, 17, 458-462.	1.0	115
42	Origin of Methyl Internal Rotation Barriers. Accounts of Chemical Research, 1999, 32, 983-993.	7.6	113
43	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
44	Understanding barriers to internal rotation in substituted toluenes and their cations. Journal of Chemical Physics, 1995, 102, 6787-6805.	1.2	110
45	Quantum Cluster Equilibrium Theory of Liquids:Â Temperature Dependence of Hydrogen Bonding in LiquidN-Methylacetamide Studied by IR Spectra. Journal of Physical Chemistry B, 1998, 102, 9312-9318.	1.2	110
46	Quantum cluster equilibrium theory of liquids: Illustrative application to water. Journal of Chemical Physics, 1998, 109, 373-384.	1.2	107
47	Metric geometry of equilibrium thermodynamics. V. Aspects of heterogeneous equilibrium. Journal of Chemical Physics, 1976, 65, 559-564.	1.2	105
48	NaturalJ-Coupling Analysis:Â Interpretation of ScalarJ-Couplings in Terms of Natural Bond Orbitals. Journal of the American Chemical Society, 2001, 123, 12026-12036.	6.6	102
49	Investigation of the differences in stability of the OCâ‹…â‹…â‹…HF and COâ‹…â‹…â‹…HF complexes. Journal of Chemical Physics, 1985, 82, 2679-2687.	1.2	101
50	The role of delocalization in benzene. Journal of the American Chemical Society, 1993, 115, 10952-10957.	6.6	100
51	Theoretical study of hydrogen bonding in liquid and gaseous N-methylformamide. Journal of Chemical Physics, 1997, 107, 499-507.	1.2	99
52	Origin of Trans-Bent Geometries in Maximally Bonded Transition Metal and Main Group Molecules. Journal of the American Chemical Society, 2006, 128, 7335-7345.	6.6	99
53	Reduced Density Matrices of Atoms and Molecules. II. On the Nâ€Representability Problem. Journal of Chemical Physics, 1967, 47, 2298-2311.	1.2	97
54	What is a hydrogen bond? Resonance covalency in the supramolecular domain. Chemistry Education Research and Practice, 2014, 15, 276-285.	1.4	97

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55	Hyperconjugative Interactions in Permethylated Siloxanes and Ethers: The Nature of the SiO Bond. Journal of the American Chemical Society, 2013, 135, 5762-5767.	6.6	94
56	Reduced Density Matrices of Atoms and Molecules. I. The 2 Matrix of Doubleâ€Occupancy, Configurationâ€Interaction Wavefunctions for Singlet States. Journal of Chemical Physics, 1967, 46, 2752-2758.	1.2	93
57	NMR Investigations ofClostridium pasteurianumRubredoxin. Origin of Hyperfine1H,2H,13C, and15N NMR Chemical Shifts in Ironâ^'Sulfur Proteins As Determined by Comparison of Experimental Data with Hybrid Density Functional Calculationsâ€. Journal of the American Chemical Society, 1998, 120, 4806-4814.	6.6	93
58	Efficient optimization of natural resonance theory weightings and bond orders by gramâ€based convex programming. Journal of Computational Chemistry, 2019, 40, 2028-2035.	1.5	91
59	Natural bond critical point analysis: Quantitative relationships between natural bond orbitalâ€based and QTAIMâ€based topological descriptors of chemical bonding. Journal of Computational Chemistry, 2012, 33, 2440-2449.	1.5	89
60	Metric geometry of equilibrium thermodynamics. III. Elementary formal structure of a vectorâ€algebraic representation of equilibrium thermodynamics. Journal of Chemical Physics, 1975, 63, 2488-2495.	1.2	87
61	Observation of an Eclipsed Csp3-CH3 Bond in a Tricyclic Orthoamide; Experimental and Theoretical Evidence for Cï£¿Hâƒ›O Hydrogen Bonds. Angewandte Chemie International Edition in English, 1987, 26, 1175-1177.	4.4	87
62	Metric geometry of equilibrium thermodynamics. IV. Vectorâ€algebraic evaluation of thermodynamic derivatives. Journal of Chemical Physics, 1975, 63, 2496-2501.	1.2	86
63	Experimental and theoretical studies of hydrogen bonding in neat, liquid formamide. Journal of Chemical Physics, 1995, 102, 5118-5125.	1.2	85
64	CHEMISTRY: High Bond Orders in Metal-Metal Bonding. Science, 2007, 316, 61-63.	6.0	81
65	Upper and Lower Bounds to Quantum-Mechanical Properties. Advances in Quantum Chemistry, 1972, , 299-331.	0.4	80
66	Quantum cluster equilibrium theory of liquids: Freezing of QCE/3-21G water to tetrakaidecahedral â€œBucky-iceâ€. Journal of Chemical Physics, 1999, 110, 508-515.	1.2	75
67	Quantum cluster equilibrium theory of liquids: molecular clusters and thermodynamics of liquid ethanol. Molecular Physics, 1999, 97, 465-477.	0.8	75
68	Some remarks on nonorthogonal orbitals in quantum chemistry. Computational and Theoretical Chemistry, 1988, 165, 189-202.	1.5	70
69	Blue-Shifted and Red-Shifted Hydrogen Bonds in Hypervalent Rare-Gas FRgâ^'HÂ·Â·Â·Y Sandwiches. Journal of Physical Chemistry A, 2004, 108, 4720-4730.	1.1	70
70	Criteria of Accuracy of Approximate Wavefunctions. Journal of Mathematical Physics, 1970, 11, 2127-2138.	0.5	69
71	Imaginaryâ€frequency polarizability and van der Waals force constants of twoâ€electron atoms, with rigorous bounds. Journal of Chemical Physics, 1977, 66, 191-198.	1.2	67
72	Dipole oscillator strengths, with rigorous limits of error, for He andLi+. Physical Review A, 1974, 9, 118-128.	1.0	66

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73	Transferability of natural bond orbitals. Journal of the American Chemical Society, 1988, 110, 368-372.	6.6	65
74	Protonation of Rhenium Alkyne Complexes Produces Î·3-Allyl Rhenium Complexes via Observable 1-Metallacyclopropene Intermediates. Journal of the American Chemical Society, 1998, 120, 12500-12511.	6.6	65
75	Structure of Liquid N-Methylacetamide:â€‰ Temperature Dependence of NMR Chemical Shifts and Quadrupole Coupling Constants. Journal of Physical Chemistry A, 1997, 101, 8861-8870.	1.1	64
76	Calculation of Upper and Lower Bounds to Oscillator Strengths. Journal of Chemical Physics, 1971, 54, 1874-1881.	1.2	61
77	Complex-coordinate studies of helium autoionizing resonances. International Journal of Quantum Chemistry, 1978, 14, 727-736.	1.0	61
78	Bayâ€•type HÂ·Â·Â·H â€œbondingâ€•in cisâ€2â€butene and related species: QTAIM versus NBO description. Journal of Computational Chemistry, 2014, 35, 1499-1508.	1.5	59
79	A theoretical model of bonding in hyperlithiated carbon compounds. Journal of the American Chemical Society, 1985, 107, 1919-1921.	6.6	58
80	Common Textbook and Teaching Misrepresentations of Lewis Structures. Journal of Chemical Education, 1995, 72, 583.	1.1	57
81	Conceptual model of "through-bonds" interactions. Journal of the American Chemical Society, 1976, 98, 4392-4393.	6.6	56
82	Photoelectron spectroscopy of free radicals with cmâ¯1 resolution: The benzyl cation. Journal of Chemical Physics, 1991, 95, 8665-8668.	1.2	56
83	Structures of the aluminum oxides studied by ab initio methods with natural bond orbital analysis. Journal of Chemical Physics, 1992, 97, 3420-3430.	1.2	55
84	High Harmonic Generation Spectra of Neutral Helium by the Complex-Scaled (t,tâ€²) Method: Role of Dynamical Electron Correlation. Physical Review Letters, 1997, 78, 2100-2103.	2.9	54
85	Solvent and concentration dependence of the hydroxyl chemical shift of methanol. Molecular Physics, 1998, 93, 145-151.	0.8	54
86	Resonance Character of Hydrogenâ€bonding Interactions in Water and Other Hâ€bonded Species. Advances in Protein Chemistry, 2005, 72, 121-155.	4.4	53
87	Joint treatment of ab initio and experimental data in molecular force field calculations with Tikhonovâ€™s method of regularization. Journal of Chemical Physics, 1994, 100, 1414-1424.	1.2	52
88	Rabbit-ears hybrids, VSEPR sterics, and other orbital anachronisms. Chemistry Education Research and Practice, 2014, 15, 417-434.	1.4	52
89	Temperature dependence of hydrogen bonding in neat, liquid formamide. Journal of Chemical Physics, 1995, 103, 3636-3642.	1.2	49
90	Radical hydrogen bonding: Origin of stability of radical-molecule complexes. Journal of Chemical Physics, 2007, 127, 164102.	1.2	49

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91	3c/4e ÏƒÌ‚-Type Long-Bonding: A Novel Transitional Motif toward the Metallic Delocalization Limit. Inorganic Chemistry, 2013, 52, 5154-5166.	1.9	48
92	Valence and extra-valence orbitals in main group and transition metal bonding. Journal of Computational Chemistry, 2007, 28, 198-203.	1.5	46
93	Bonding Analysis of TM(cAAC)₂ (TM = Cu, Ag, and Au) and the Importance of Reference State. Organometallics, 2015, 34, 3442-3449.	1.1	46
94	Resonance Theory Reboot. Journal of the American Chemical Society, 2019, 141, 4156-4166.	6.6	45
95	Bond-antibond analysis of internal rotation barriers in glyoxal and related molecules: WhereINDO fails. International Journal of Quantum Chemistry, 1981, 19, 781-791.	1.0	43
96	Calculations of one-, two- and three-bond nuclear spin-spin couplings in a model peptide and correlations with experimental data. Journal of Biomolecular NMR, 1994, 4, 519-542.	1.6	43
97	Structure of Magnesium Cluster Grignard Reagents. Inorganic Chemistry, 1995, 34, 2980-2983.	1.9	43
98	Quantum cluster equilibrium theory of liquids: temperature dependent chemical shifts, quadrupole coupling constants and vibrational frequencies in liquid ethanol. Molecular Physics, 1999, 97, 479-486.	0.8	43
99	Trans-Hydrogen-Bondh2JNNandh1JNHCouplings in the DNA Aâˆ’T Base Pair:Â Natural Bond Orbital Analysis. Journal of the American Chemical Society, 2002, 124, 1190-1191.	6.6	43
100	Some remarks on the Câ€“H bond dipole moment. Journal of Chemical Physics, 1986, 84, 2428-2430.	1.2	42
101	Chemical Bonding as a Superposition Phenomenon. Journal of Chemical Education, 1999, 76, 1141.	1.1	42
102	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie - International Edition, 2015, 54, 2600-2602.	7.2	42
103	Theoretical Studies of Protium/Deuterium Fractionation Factors and Cooperative Hydrogen Bonding in Peptides. Journal of the American Chemical Society, 1995, 117, 9619-9624.	6.6	41
104	Quadrupole coupling constants in linear (HCN)nclusters: Theoretical and experimental evidence for cooperativity effects in Câ€“Hâ‹…â‹…â‹…N hydrogen bonding. Journal of Chemical Physics, 1995, 103, 348-352.	1.2	40
105	Predicting the Ionic Product of Water. Scientific Reports, 2017, 7, 10244.	1.6	40
106	Antisymmetrization effects in bondâ€orbital models of internal rotation barriers. Journal of Chemical Physics, 1980, 72, 2866-2868.	1.2	39
107	Comment on â€œObservation of alkaline earth complexes M(CO) ₈ (M = Ca, Sr, or Ba) that mimic transition metalsâ€• Science, 2019, 365, .	6.0	39
108	Theoretical Prediction of Robust Second-Row Oxyanion Clusters in the Metastable Domain of Antielectrostatic Hydrogen Bonding. Inorganic Chemistry, 2018, 57, 2035-2044.	1.9	38

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109	Comment on â€œNatural Bond Orbitals and the Nature of the Hydrogen Bondâ€• Journal of Physical Chemistry A, 2018, 122, 724-732.	1.1	38
110	Boron oxides:Ab initiostudies with natural bond orbital analysis. Journal of Chemical Physics, 1993, 98, 1329-1335.	1.2	37
111	Electron-correlation effects in the positions and widths of two-electron autoionizing resonances. Physical Review A, 1979, 20, 27-31.	1.0	35
112	Syn and anti bent hydrazine radical cations. Effect of .sigma.,.pi. mixing on spectral properties. Journal of the American Chemical Society, 1985, 107, 143-149.	6.6	34
113	Photodissociation of (CO)+2: Theoretical studies of ground 2Bu and excited 2Bg potential energy surfaces. Journal of Chemical Physics, 1987, 87, 392-410.	1.2	34
114	Quantum cluster equilibrium theory of liquids part I: Molecular clusters and thermodynamics of liquid ammonia. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 197-204.	0.9	33
115	Torsion-vibration interactions in hydrogen peroxide. 1. Calculation of the trans barrier for hydroxyls overtone excitations up to v = 8. The Journal of Physical Chemistry, 1988, 92, 4295-4306.	2.9	32
116	Effective Oâ€17 quadrupole moments for the calibrated computation of quadrupole coupling parameters at different levels of theory. Journal of Chemical Physics, 1996, 105, 8223-8230.	1.2	32
117	Theoretical studies of O2?:(H2O)n clusters. Journal of Computational Chemistry, 1986, 7, 294-305.	1.5	31
118	Threshold photoionization spectra of benzyl radical: Cation vibrational states and ab initio calculations. Journal of Chemical Physics, 1996, 104, 8886-8895.	1.2	31
119	Hyperfine-Shifted ¹³C Resonance Assignments in an Ironâ€“Sulfur Protein with Quantum Chemical Verification: Aliphatic Câ€“HÂ·Â·Â·S 3-Centerâ€“4-Electron Interactions. Journal of the American Chemical Society, 2011, 133, 1310-1316.	6.6	31
120	Inadequacies of the Point-Dipole Approximation for Describing Electronâ€“Nuclear Interactions in Paramagnetic Proteins:â€‰ Hybrid Density Functional Calculations and the Analysis of NMR Relaxation of High-Spin Iron(III) Rubredoxin. Journal of Physical Chemistry B, 1998, 102, 8300-8305.	1.2	30
121	Torsion-vibration interactions in overtone excited states of hydrogen peroxide. The Journal of Physical Chemistry, 1986, 90, 6405-6408.	2.9	29
122	Eine C_{sp}³â€gebundene Methylgruppe in ekliptischer Konformation; experimenteller und theoretischer Nachweis von Cï¿H â€¦ Oâ€WasserstoffbrÃ¼cken. Angewandte Chemie, 1987, 99, 1216-1218.	1.6	29
123	Estimates of ? and ? torsion angles in proteins from one-, two- and three-bond nuclear spin-spin couplings: Application to staphylococcal nuclease. Journal of Biomolecular NMR, 1994, 4, 543-551.	1.6	29
124	Quantum cluster equilibrium theory of liquids part II: Temperature dependent chemical shifts, quadrupole coupling constants and vibrational frequencies in liquid ammonia. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 205-212.	0.9	29
125	Critical test of quantum cluster equilibrium theory: Formic acid at B3LYP/6-31+G* hybrid density functional level. Journal of Chemical Physics, 1998, 109, 5945-5947.	1.2	29
126	Diamagnetism of helium. Journal of Chemical Physics, 2000, 113, 8667-8670.	1.2	28

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127	Improved Lower Bounds to the Overlap Integral of an Approximate Wavefunction with the True Wavefunction. Journal of Chemical Physics, 1967, 46, 2448-2449.	1.2	27
128	Variational Upper and Lower Bounds to Dipole Transition Moments. Physical Review Letters, 1970, 25, 907-909.	2.9	27
129	Dynamic polarizabilities of metastable 2â€‰1,3S excited states of He and Li+, with rigorous upper and lower bounds. Journal of Chemical Physics, 1977, 66, 185-190.	1.2	27
130	Criteria of accuracy of resonance eigenvalues. International Journal of Quantum Chemistry, 1980, 17, 1201-1211.	1.0	26
131	Quantum cluster equilibrium theory of liquids: light and heavy QCE/3-21G model water. Physical Chemistry Chemical Physics, 2000, 2, 1613-1619.	1.3	26
132	Molecular Composition of Liquid Sulfur. Angewandte Chemie - International Edition, 2002, 41, 3199-3202.	7.2	26
133	Insight into the Mechanism of the Michael Reaction. ChemPhysChem, 2016, 17, 2022-2034.	1.0	26
134	Lower bounds to expectation values. Journal of Physics A, 1968, 1, 305-313.	1.6	25
135	Relative accuracy of length and velocity forms in oscillator-strength calculations. Physical Review A, 1974, 10, 1457-1463.	1.0	25
136	The principle of maximum overlap. Journal of the American Chemical Society, 1976, 98, 3745-3749.	6.6	25
137	Natural bond orbitals in multiconfigurational expansions: Local treatment of electron correlation in molecules. Journal of Chemical Physics, 1992, 97, 1095-1108.	1.2	25
138	Polyion Covalency: Exotic Species from the Unexplored World of Electrostatically Shielded Molecular Ion Chemistry. Angewandte Chemie - International Edition, 2017, 56, 14577-14581.	7.2	25
139	New Formulas for Lower Bounds to Expectation Values. Physical Review, 1969, 183, 142-147.	2.7	24
140	Geometric representation of equilibrium thermodynamics. Accounts of Chemical Research, 1976, 9, 236-240.	7.6	24
141	Torsion-vibration interactions in hydrogen peroxide. 2. Natural bond orbital analysis. The Journal of Physical Chemistry, 1988, 92, 4306-4313.	2.9	24
142	Calculation of nuclear spin-spin coupling constants with ab initio molecular orbital wave functions. The Journal of Physical Chemistry, 1993, 97, 11657-11665.	2.9	24
143	Quantum Chemical Calculations on Structural Models of the Catalytic Site of Chymotrypsin:Â Comparison of Calculated Results with Experimental Data from NMR Spectroscopy. Journal of the American Chemical Society, 2002, 124, 14373-14381.	6.6	24
144	News from the Periodic Table: An Introduction to "Periodicity Symbols, Tables, and Models for Higher-Order Valency and Donorâ€“Acceptor Kinships". Journal of Chemical Education, 2007, 84, 1145.	1.1	24

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145	Mass polarization and Breit-Pauli corrections for the polarizability of helium-4. The Journal of Physical Chemistry, 1982, 86, 1111-1116.	2.9	23
146	Comments on â€œIs It Time To Retire the Hybrid Atomic Orbital?â€• Journal of Chemical Education, 2012, 89, 570-572.	1.1	23
147	Resonance Character of Copper/Silver/Gold Bonding in Small Moleculeâ‹…â‹…â‹…Mï£¿X (X=F, Cl, Br,) Tj ETQq1 1 0.784314 rgBT /Ove	1.0	23
148	Quantum Cluster Equilibrium Theory of Liquids: Isotopically substituted QCE/3-21G Model Water. Zeitschrift Fur Physikalische Chemie, 2002, 216, .	1.4	21
149	The Path to Natural Bond Orbitals. Israel Journal of Chemistry, 2022, 62, .	1.0	21
150	On the dipole moment of three identical spherical atoms. Molecular Physics, 1978, 35, 1205-1210.	0.8	20
151	Resonance Bonding Patterns of Peroxide Chemistry:Â Cyclic Three-Center Hyperbonding in â€œPhosphadioxiraneâ€•Intermediates. Journal of the American Chemical Society, 2006, 128, 11850-11859.	6.6	20
152	18â€•electron rule and the 3c/4e hyperbonding saturation limit. Journal of Computational Chemistry, 2016, 37, 237-241.	1.5	20
153	Variational calculation of continuum corrections to overlap. Journal of Chemical Physics, 1973, 59, 355-362.	1.2	19
154	3c/4e î„‘-type long-bonding competes with Ï‰-bonding in noble-gas hydrides HNgY (Ng = He, Ne, Ar, Kr, Xe, Rn;) Tj ETQq0 0 0 rgBT /Ove	1.3	19
155	Natural resonance theory: II. Natural bond order and valency. Journal of Computational Chemistry, 1998, 19, 610-627.	1.5	19
156	What Is the Nature of Supramolecular Bonding? Comprehensive NBO/NRT Picture of Halogen and Pnicogen Bonding in RPH2Â·Â·Â·IF/FI Complexes (R = CH3, OH, CF3, CN, NO2). Molecules, 2019, 24, 2090.	1.7	18
157	Variational Extensions of Lower Bounds to Expectation Values. Physical Review A, 1970, 1, 122-124.	1.0	17
158	Calculations of one-, two- and three-bond nuclear spin-spin couplings in a model peptide and correlations with experimental data. Journal of Biomolecular NMR, 1995, 5, 332.	1.6	17
159	Accurate Structure and Dynamics of the Metal-Site of Paramagnetic Metalloproteins from NMR Parameters Using Natural Bond Orbitals. Journal of the American Chemical Society, 2012, 134, 4670-4682.	6.6	17
160	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie, 2015, 127, 2636-2638.	1.6	17
161	9-(9-Borabicyclo[3.3.1]nonyl)-9-azabicyclo[3.3.1]nonane radical cation: a failure of Bredt's rule kinetic stabilization. Journal of Organic Chemistry, 1980, 45, 2116-2119.	1.7	16
162	Coupling of internal rotations in propanelike molecules. International Journal of Quantum Chemistry, 1982, 21, 487-509.	1.0	16

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163	Addendum: Antiâ€Electrostatic Hydrogen Bonds. Angewandte Chemie - International Edition, 2014, 53, 12992-12992.	7.2	16
164	Ab Initio Calculations of Protium/Deuterium Fractionation Factors in O2H5+ Clusters. The Journal of Physical Chemistry, 1995, 99, 8013-8016.	2.9	15
165	Ab initioand regularized force fields of haloethanes: CH3CH2Cl, CH3CHCl2, CH3CF2Cl, and CH3CFCl2. Journal of Chemical Physics, 1998, 109, 7286-7299.	1.2	15
166	Nuclear motion and Breitâ€“Pauli corrections to the diamagnetism of atomic helium. Journal of Chemical Physics, 2002, 117, 3243-3247.	1.2	15
167	Kinetics and Mechanism of Water Cluster Equilibria. Journal of Physical Chemistry B, 2014, 118, 7792-7798.	1.2	15
168	Upper and lower bounds to quantum-mechanical sum rules. Journal of Physics A, 1968, 1, 655-660.	1.6	14
169	Upper and lower bounds to the van der Waals interactions between atoms. Journal of Physics B: Atomic and Molecular Physics, 1969, 2, 517-520.	1.6	14
170	Lower Bounds to Expectation Values: Two-Electron Atoms. Canadian Journal of Chemistry, 1973, 51, 260-264.	0.6	14
171	Experimental and theoretical study of the relaxation of vibrationally excited HF by NO and CO. Journal of Chemical Physics, 1989, 91, 1688-1696.	1.2	14
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