Frank Weinhold

List of Publications by Year
in descending order

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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	The Path to Natural Bond Orbitals. Israel Journal of Chemistry, 2022, 62, .	1.0	21
2	Anti-Electrostatic Pi-Hole Bonding: How Covalency Conquers Coulombics. Molecules, 2022, 27, 377.	1.7	6
3	Chlorine dioxide: An exception that proves the rules of localized chemical bonding. Journal of Chemical Physics, 2022, 156, 124303.	1.2	4
4	High-Density â€œWindowpaneâ€•Coordination Patterns of Water Clusters and Their NBO/NRT Characterization. Molecules, 2022, 27, 4218.	1.7	1
5	Sulfur Tetrahydride and Allied Superhydride Clusters: Whenâ€‰Resonance Takes Precedence. Chemistry - A European Journal, 2021, 27, 6748-6759.	1.7	0
6	6 Natural bond orbital theory: Discovering chemistry with NBO7. , 2021, , 129-156.		10
7	Comment on â€œSuperposition of Waves or Densities: Which Is the Nature of Chemical Resonance?â€•[J. Comput. Chem. 2021, 42, 412â€“417]. Journal of Computational Chemistry, 2021, 42, 1338-1340.	1.5	2
8	Time-Conjugation in a Unified Quantum Theory for Hermitian and Non-Hermitian Electronic Systems under Time-Reversal Symmetry. Symmetry, 2021, 13, 808.	1.1	2
9	Paulingâ€™s Conceptions of Hybridization and Resonance in Modern Quantum Chemistry. Molecules, 2021, 26, 4110.	1.7	11
10	NBO/NRT Two-State Theory of Bond-Shift Spectral Excitation. Molecules, 2020, 25, 4052.	1.7	9
11	Substituted Ortho-Benzynes: Properties of the Triple Bond. Journal of Organic Chemistry, 2020, 85, 9905-9914.	1.7	6
12	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
13	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
14	NBO 7.0: New vistas in localized and delocalized chemical bonding theory. Journal of Computational Chemistry, 2019, 40, 2234-2241.	1.5	249
15	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
16	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
17	Resonance Theory Reboot. Journal of the American Chemical Society, 2019, 141, 4156-4166.	6.6	45
18	To Be or Not to Be: Demystifying the 2ndâ€‰Quantized Picture of Complex Electronic Configuration Patterns in Chemistry with Natural Polyâ€‰Electron Population Analysis. Journal of Computational Chemistry, 2019, 40, 1509-1520.	1.5	7

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19	Resonance Natural Bond Orbitals: Efficient Semilocalized Orbitals for Computing and Visualizing Reactive Chemical Processes. Journal of Chemical Theory and Computation, 2019, 15, 916-921.	2.3	13
20	Natural Bond Orbital Theory of Pseudo-Jahnâ€“Teller Effects. Journal of Physical Chemistry A, 2018, 122, 4490-4498.	1.1	11
21	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
22	The role of hyperconjugation in the unusual conformation of thymine: A natural bond orbital analysis. Computational and Theoretical Chemistry, 2018, 1130, 58-62.	1.1	7
23	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
24	Efficient evaluation of poly-electron populations in natural bond orbital analysis. Chemical Physics Letters, 2018, 711, 23-26.	1.2	12
25	Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners. Inorganic Chemistry, 2018, 57, 7851-7859.	1.9	3
26	Natural resonance theory of chemical reactivity, with illustrative application to intramolecular Claisen rearrangement. Tetrahedron, 2018, 74, 4799-4804.	1.0	7
27	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
28	Why Do Cumulene Ketones Kink?. Journal of Organic Chemistry, 2017, 82, 12238-12245.	1.7	10
29	Polyion Covalency: Exotic Species from the Unexplored World of Electrostatically Shielded Molecular Ion Chemistry. Angewandte Chemie, 2017, 129, 14769-14773.	1.6	7
30	Predicting the Ionic Product of Water. Scientific Reports, 2017, 7, 10244.	1.6	40
31	Insight into the Mechanism of the Michael Reaction. ChemPhysChem, 2016, 17, 2022-2034.	1.0	26
32	Spectroscopic Evidence for Clusters of Likeâ€Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. ChemPhysChem, 2016, 17, 458-462.	1.0	115
33	18â€electron rule and the 3c/4e hyperbonding saturation limit. Journal of Computational Chemistry, 2016, 37, 237-241.	1.5	20
34	Spectroscopic Evidence for Clusters of Likeâ€Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. ChemPhysChem, 2016, 17, 447-447.	1.0	1
35	What is NBO analysis and how is it useful?. International Reviews in Physical Chemistry, 2016, 35, 399-440.	0.9	585
36	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 /Over	1.3	19

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37	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie, 2015, 127, 2636-2638.	1.6	17
38	Resonance Character of Copper/Silver/Gold Bonding in Small Moleculeâ‹…â‹…â‹…Mï£¿X (X=F, Cl, Br,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	23
39	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie - International Edition, 2015, 54, 2600-2602.	7.2	42
40	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
41	Rabbit ears concepts of water lone pairs: a reply to comments of Hiberty, Danovich, and Shaik. Chemistry Education Research and Practice, 2015, 16, 694-696.	1.4	6
42	Rabbit-ears hybrids, VSEPR sterics, and other orbital anachronisms. Chemistry Education Research and Practice, 2014, 15, 417-434.	1.4	52
43	Antiâ€Electrostatic Hydrogen Bonds. Angewandte Chemie - International Edition, 2014, 53, 11214-11217.	7.2	171
44	Kinetics and Mechanism of Water Cluster Equilibria. Journal of Physical Chemistry B, 2014, 118, 7792-7798.	1.2	15
45	What is a hydrogen bond? Resonance covalency in the supramolecular domain. Chemistry Education Research and Practice, 2014, 15, 276-285.	1.4	97
46	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
47	Addendum: Antiâ€Electrostatic Hydrogen Bonds. Angewandte Chemie - International Edition, 2014, 53, 12992-12992.	7.2	16
48	Quantum Cluster Equilibrium. Letters in Mathematical Physics, 2014, , 77-96.	0.4	7
49	NBO 6.0: Natural bond orbital analysis program. Journal of Computational Chemistry, 2013, 34, 1429-1437.	1.5	1,269
50	Natural Bondâ€“Bond Polarizability: A HÃ¼ckel-Like Electronic Delocalization Index. Journal of Organic Chemistry, 2013, 78, 1844-1850.	1.7	6
51	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
52	3c/4e ÏƒÌ‚-Type Long-Bonding: A Novel Transitional Motif toward the Metallic Delocalization Limit. Inorganic Chemistry, 2013, 52, 5154-5166.	1.9	48
53	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
54	Comments on â€œIs It Time To Retire the Hybrid Atomic Orbital?â€• Journal of Chemical Education, 2012, 89, 570-572.	1.1	23

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55	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
56	Natural bond orbital analysis: A critical overview of relationships to alternative bonding perspectives. Journal of Computational Chemistry, 2012, 33, 2363-2379.	1.5	515
57	Natural bond orbital methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 1-42.	6.2	1,153
58	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
59	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
60	The Nature of the Siliconâ€“Oxygen Bond. Organometallics, 2011, 30, 5815-5824.	1.1	135
61	Isotopeâ€sensitive Degenerate [1,3]â€Hydrogen Migration versus Competitive Enolâ€“Keto Tautomerization. Chemistry - A European Journal, 2009, 15, 11815-11819.	1.7	7
62	Radical hydrogen bonding: Origin of stability of radical-molecule complexes. Journal of Chemical Physics, 2007, 127, 164102.	1.2	49
63	The ABCs of Multiple Bonding. Science, 2007, 318, 746-746.	6.0	3
64	Characterization of the Methoxy Carbonyl Radical Formed via Photolysis of Methyl Chloroformate at 193.3 nm. Journal of Physical Chemistry A, 2007, 111, 1762-1770.	1.1	10
65	CHEMISTRY: High Bond Orders in Metal-Metal Bonding. Science, 2007, 316, 61-63.	6.0	81
66	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
67	Valence and extra-valence orbitals in main group and transition metal bonding. Journal of Computational Chemistry, 2007, 28, 198-203.	1.5	46
68	Determination of the Conformation of 2-Hydroxy- and 2-Aminobenzoic Acid Dimers Using 13C NMR and Density Functional Theory/Natural Bond Order Analysis:â€‰ The Central Importance of the Carboxylic Acid Carbon. Journal of Physical Chemistry A, 2006, 110, 8832-8839.	1.1	8
69	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
70	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
71	Comments on Purser's Article: "Lewis Structures are Models for Predicting Molecular Structure, Not Electronic Structure". Journal of Chemical Education, 2005, 82, 527.	1.1	6
72	Resonance Character of Hydrogenâ€bonding Interactions in Water and Other Hâ€bonded Species. Advances in Protein Chemistry, 2005, 72, 121-155.	4.4	53

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73	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
74	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
75	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
76	Tests of quantum cluster equilibrium (QCE)-based computational methods for describing formic acid clustering. Molecular Physics, 2003, 101, 1147-1153.	0.8	8
77	Supramolecular bonding. , 2003, , 579-709.		0
78	Nuclear motion and Breitâ€"Pauli corrections to the diamagnetism of atomic helium. Journal of Chemical Physics, 2002, 117, 3243-3247.	1.2	15
79	Quantum Cluster Equilibrium Theory of Liquids: Isotopically substituted QCE/3-21G Model Water. Zeitschrift Fur Physikalische Chemie, 2002, 216, .	1.4	21
80	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
81	Experimental and theoretical spin-spin coupling constants for [15N] formamide. Molecular Physics, 2002, 100, 2807-2814.	0.8	7
82	Trans-Hydrogen-Bondh2JNNandh1JNHCouplings in the DNA Aâ^'T Base Pair:Â Natural Bond Orbital Analysis. Journal of the American Chemical Society, 2002, 124, 1190-1191.	6.6	43
83	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
84	Die molekulare Zusammensetzung des flï¿½ï¿½ssigen Schwefels. Angewandte Chemie, 2002, 114, 3331-3335.	1.6	2
85	Molecular Composition of Liquid Sulfur. Angewandte Chemie - International Edition, 2002, 41, 3199-3202.	7.2	26
86	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
87	NATURAL BOND ORBITALS AND EXTENSIONS OF LOCALIZED BONDING CONCEPTS. Chemistry Education Research and Practice, 2001, 2, 91-104.	1.4	732
88	A new twist on molecular shape. Nature, 2001, 411, 539-541.	13.7	234
89	Natural resonance theory. I. General formalism. Journal of Computational Chemistry, 2000, 21, 411-413.	1.5	11
90	Diamagnetism of helium. Journal of Chemical Physics, 2000, 113, 8667-8670.	1.2	28

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91	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
92	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
93	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
94	Natural steric analysis of internal rotation barriers. International Journal of Quantum Chemistry, 1999, 72, 269-280.	1.0	179
95	Chemical Bonding as a Superposition Phenomenon. Journal of Chemical Education, 1999, 76, 1141.	1.1	42
96	Origin of Methyl Internal Rotation Barriers. Accounts of Chemical Research, 1999, 32, 983-993.	7.6	113
97	Quantum cluster equilibrium theory of liquids: molecular clusters and thermodynamics of liquid ethanol. Molecular Physics, 1999, 97, 465-477.	0.8	75
98	Natural steric analysis of internal rotation barriers. , 1999, 72, 269.		2
99	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	5
100	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
101	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
102	Natural resonance theory: I. General formalism. Journal of Computational Chemistry, 1998, 19, 593-609.	1.5	621
103	Natural resonance theory: II. Natural bond order and valency. Journal of Computational Chemistry, 1998, 19, 610-627.	1.5	480
104	Natural resonance theory: III. Chemical applications. Journal of Computational Chemistry, 1998, 19, 628-646.	1.5	460
105	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
106	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
107	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
108	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

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109	Quantum cluster equilibrium theory of liquids: General theory and computer implementation. Journal of Chemical Physics, 1998, 109, 367-372.	1.2	153
110	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
111	Ab initioand regularized force fields of haloethanes: CH3CH2Cl, CH3CHCl2, CH3CF2Cl, and CH3CFCl2. Journal of Chemical Physics, 1998, 109, 7286-7299.	1.2	15
112	Quantum cluster equilibrium theory of liquids: Illustrative application to water. Journal of Chemical Physics, 1998, 109, 373-384.	1.2	107
113	Natural resonance theory: II. Natural bond order and valency. , 1998, 19, 610.		1
114	Natural resonance theory: I. General formalism. , 1998, 19, 593.		13
115	Natural resonance theory: II. Natural bond order and valency. Journal of Computational Chemistry, 1998, 19, 610-627.	1.5	19
116	Natural resonance theory: III. Chemical applications. , 1998, 19, 628.		3
117	Solvent and concentration dependence of the hydroxyl chemical shift of methanol. Molecular Physics, 1998, 93, 145-151.	0.8	54
118	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
119	Theoretical study of hydrogen bonding in liquid and gaseous N-methylformamide. Journal of Chemical Physics, 1997, 107, 499-507.	1.2	99
120	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
121	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
122	Natural steric analysis:Ab initiovan der Waals radii of atoms and ions. Journal of Chemical Physics, 1997, 107, 5422-5432.	1.2	173
123	Natural bond orbital analysis of steric interactions. Journal of Chemical Physics, 1997, 107, 5406-5421.	1.2	257
124	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
125	Constraints on the values of force constants for molecular force field models based on ab initio calculations. Journal of Molecular Structure, 1997, 410-411, 457-461.	1.8	2
126	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

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127	Threshold photoionization spectra of benzyl radical: Cation vibrational states and ab initio calculations. Journal of Chemical Physics, 1996, 104, 8886-8895.	1.2	31
128	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
129	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
130	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
131	Temperature dependence of hydrogen bonding in neat, liquid formamide. Journal of Chemical Physics, 1995, 103, 3636-3642.	1.2	49
132	Experimental and theoretical studies of hydrogen bonding in neat, liquid formamide. Journal of Chemical Physics, 1995, 102, 5118-5125.	1.2	85
133	Ab Initio Calculations of Protium/Deuterium Fractionation Factors in O2H5+ Clusters. The Journal of Physical Chemistry, 1995, 99, 8013-8016.	2.9	15
134	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
135	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
136	Common Textbook and Teaching Misrepresentations of Lewis Structures. Journal of Chemical Education, 1995, 72, 583.	1.1	57
137	Understanding barriers to internal rotation in substituted toluenes and their cations. Journal of Chemical Physics, 1995, 102, 6787-6805.	1.2	110
138	Structure of Magnesium Cluster Grignard Reagents. Inorganic Chemistry, 1995, 34, 2980-2983.	1.9	43
139	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
140	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
141	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
142	Use of Hueckel Methodology with ab Initio Molecular Orbitals: Polarizabilities and Prediction of Organic Reactions. Journal of the American Chemical Society, 1994, 116, 1579-1580.	6.6	13
143	The role of delocalization in benzene. Journal of the American Chemical Society, 1993, 115, 10952-10957.	6.6	100
144	Boron oxides:Ab initiostudies with natural bond orbital analysis. Journal of Chemical Physics, 1993, 98, 1329-1335.	1.2	37

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145	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
146	Natural bond orbitals in multiconfigurational expansions: Local treatment of electron correlation in molecules. Journal of Chemical Physics, 1992, 97, 1095-1108.	1.2	25
147	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
148	Natural Bond Orbital Analysis of Internal Rotation Barriers and Related Phenomena. Israel Journal of Chemistry, 1991, 31, 277-285.	1.0	179
149	Photoelectron spectroscopy of free radicals with cmâ¯1 resolution: The benzyl cation. Journal of Chemical Physics, 1991, 95, 8665-8668.	1.2	56
150	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
151	Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. Chemical Reviews, 1988, 88, 899-926.	23.0	15,946
152	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
153	Some remarks on nonorthogonal orbitals in quantum chemistry. Computational and Theoretical Chemistry, 1988, 165, 189-202.	1.5	70
154	Transferability of natural bond orbitals. Journal of the American Chemical Society, 1988, 110, 368-372.	6.6	65
155	The 2Ag excited state of (CO)+2. Journal of Chemical Physics, 1988, 88, 1467-1468.	1.2	8
156	The Natural Bond Orbital Lewis Structure Concept for Molecules, Radicals, and Radical Ions. , 1988, , 227-236.		392
157	Torsion-vibration interactions in hydrogen peroxide. 2. Natural bond orbital analysis. The Journal of Physical Chemistry, 1988, 92, 4306-4313.	2.9	24
158	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
159	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
160	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
161	Eine C‹sub›sp‹/sub›‹sup›3‹/sup›â€gebundene Methylgruppe in ekliptischer Konformation; experimenteller und theoretischer Nachweis von Cï£¿H â€¦ Oâ€Wasserstoffbrücken. Angewandte Chemie, 1987, 99, 1216-1218.	1.6	29
162	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

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163	On the role of d orbitals in sulfur hexafluoride. Journal of the American Chemical Society, 1986, 108, 3586-3593.	6.6	168
164	Torsion-vibration interactions in overtone excited states of hydrogen peroxide. The Journal of Physical Chemistry, 1986, 90, 6405-6408.	2.9	29
165	Theoretical studies of O2?:(H2O)n clusters. Journal of Computational Chemistry, 1986, 7, 294-305.	1.5	31
166	Some remarks on the Câ€“H bond dipole moment. Journal of Chemical Physics, 1986, 84, 2428-2430.	1.2	42
167	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
168	Natural localized molecular orbitals. Journal of Chemical Physics, 1985, 83, 1736-1740.	1.2	2,019
169	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
170	A theoretical model of bonding in hyperlithiated carbon compounds. Journal of the American Chemical Society, 1985, 107, 1919-1921.	6.6	58
171	Natural population analysis. Journal of Chemical Physics, 1985, 83, 735-746.	1.2	8,757
172	Natural bond orbital analysis of nearâ€Hartreeâ€“Fock water dimer. Journal of Chemical Physics, 1983, 78, 4066-4073.	1.2	2,775
173	Mass polarization and Breit-Pauli corrections for the polarizability of helium-4. The Journal of Physical Chemistry, 1982, 86, 1111-1116.	2.9	23
174	Coupling of internal rotations in propanelike molecules. International Journal of Quantum Chemistry, 1982, 21, 487-509.	1.0	16
175	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
176	Complex-coordinate calculations with complex basis sets. Physical Review A, 1981, 24, 1254-1259.	1.0	12
177	Criteria of accuracy of resonance eigenvalues. International Journal of Quantum Chemistry, 1980, 17, 1201-1211.	1.0	26
178	Antisymmetrization effects in bondâ€orbital models of internal rotation barriers. Journal of Chemical Physics, 1980, 72, 2866-2868.	1.2	39
179	Natural hybrid orbitals. Journal of the American Chemical Society, 1980, 102, 7211-7218.	6.6	4,505
180	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

#	Article	IF	Citations
181	Natural hybrid orbitals: Ab initio SCF and CI results for CO and NiCO. International Journal of Quantum Chemistry, 1980, 18, 201-209.	1.0	4
182	Variation-perturbation approach to complex eigenvalues of resonance states. The Journal of Physical Chemistry, 1979, 83, 1517-1520.	2.9	4
183	Electron-correlation effects in the positions and widths of two-electron autoionizing resonances. Physical Review A, 1979, 20, 27-31.	1.0	35
184	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
185	Complex-coordinate studies of helium autoionizing resonances. International Journal of Quantum Chemistry, 1978, 14, 727-736.	1.0	61
186	Resonance properties of complex-rotated hamiltonians. Molecular Physics, 1978, 36, 1613-1630.	0.8	369
187	Geometrical Aspects of Equilibrium Thermodynamics. Theoretical Chemistry, 1978, 3, 15-54.	0.2	5
188	Bivariational calculations of bounds on complex-frequency polarizabilities. Journal of Chemical Physics, 1978, 68, 2915.	1.2	5
189	On the dipole moment of three identical spherical atoms. Molecular Physics, 1978, 35, 1205-1210.	0.8	20
190	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
191	G+Kâ€‰1Î£+g doubleâ€minimum excited state of H2. Journal of Chemical Physics, 1977, 66, 303-305.	1.2	12
192	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
193	Conceptual model of "through-bonds" interactions. Journal of the American Chemical Society, 1976, 98, 4392-4393.	6.6	56
194	The principle of maximum overlap. Journal of the American Chemical Society, 1976, 98, 3745-3749.	6.6	25
195	Metric geometry of equilibrium thermodynamics. V. Aspects of heterogeneous equilibrium. Journal of Chemical Physics, 1976, 65, 559-564.	1.2	105
196	Geometric representation of equilibrium thermodynamics. Accounts of Chemical Research, 1976, 9, 236-240.	7.6	24
197	Moment-theory investigations of photoabsorption and dispersion profiles in atoms and ions. Physical Review A, 1976, 14, 1042-1056.	1.0	133
198	Dynamic polarizabilities of twoâ€electron atoms, with rigorous upper and lower bounds. Journal of Chemical Physics, 1976, 65, 4913-4926.	1.2	136

#	Article	IF	Citations
199	Partitioning Technique for Determinantal Equations. , 1976, , 307-314.		1
200	Bounds to the lifetime of the Ar XVII2ÂS3state. Physical Review A, 1975, 11, 442-445.	1.0	12
201	Metric geometry of equilibrium thermodynamics. Journal of Chemical Physics, 1975, 63, 2479-2483.	1.2	560
202	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
203	Metric geometry of equilibrium thermodynamics. II. Scaling, homogeneity, and generalized Gibbsâ€"Duhem relations. Journal of Chemical Physics, 1975, 63, 2484-2487.	1.2	179
204	Metric geometry of equilibrium thermodynamics. IV. Vectorâ€algebraic evaluation of thermodynamic derivatives. Journal of Chemical Physics, 1975, 63, 2496-2501.	1.2	86
205	Dipole oscillator strengths, with rigorous limits of error, for He andLi+. Physical Review A, 1974, 9, 118-128.	1.0	66
206	Relative accuracy of length and velocity forms in oscillator-strength calculations. Physical Review A, 1974, 10, 1457-1463.	1.0	25
207	Lower Bounds to Expectation Values: Two-Electron Atoms. Canadian Journal of Chemistry, 1973, 51, 260-264.	0.6	14
208	Variational calculation of continuum corrections to overlap. Journal of Chemical Physics, 1973, 59, 355-362.	1.2	19
209	Variational Wavefunctions for H2+. Journal of Chemical Physics, 1972, 56, 3798-3801.	1.2	8
210	Upper and Lower Bounds to Excited States of Twoâ€Electron Atoms. Journal of Chemical Physics, 1972, 57, 1738-1745.	1.2	5
211	Upper and Lower Bounds to Quantum-Mechanical Properties. Advances in Quantum Chemistry, 1972, , 299-331.	0.4	80
212	Dickinson Energy of H2+. Journal of Chemical Physics, 1971, 54, 530-532.	1.2	13
213	On a formula of Braun and Rebane for variational bounds to overlap. International Journal of Quantum Chemistry, 1971, 5, 215-220.	1.0	7
214	Calculation of Upper and Lower Bounds to Oscillator Strengths. Journal of Chemical Physics, 1971, 54, 1874-1881.	1.2	61
215	Remarks on the calculation of upper and lower limits to quantum-mechanical properties. International Journal of Quantum Chemistry, 1971, 5, 721-728.	1.0	5
216	Criteria of Accuracy of Approximate Wavefunctions. Journal of Mathematical Physics, 1970, 11, 2127-2138.	0.5	69

#	Article	IF	Citations
217	Variational Upper and Lower Bounds to Dipole Transition Moments. Physical Review Letters, 1970, 25, 907-909.	2.9	27
218	Variational Extensions of Lower Bounds to Expectation Values. Physical Review A, 1970, 1, 122-124.	1.0	17
219	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
220	New Formulas for Lower Bounds to Expectation Values. Physical Review, 1969, 183, 142-147.	2.7	24
221	Inequalities for Multipole Dispersion Interactions. Journal of Chemical Physics, 1969, 50, 4136-4137.	1.2	12
222	Remark on lower bounds to eigenvalues. International Journal of Quantum Chemistry, 1969, 3, 371-373.	1.0	7
223	Upper and lower bounds to quantum-mechanical sum rules. Journal of Physics A, 1968, 1, 655-660.	1.6	14
224	Lower bounds to expectation values. Journal of Physics A, 1968, 1, 305-313.	1.6	25
225	Improved lower bounds to expectation values. Journal of Physics A, 1968, 1, 535-538.	1.6	11
226	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
227	Reduced Density Matrices of Atoms and Molecules. II. On the Nâ€Representability Problem. Journal of Chemical Physics, 1967, 47, 2298-2311.	1.2	97
228	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
229	Can a Wanzlick-like equilibrium exist between dicoordinate borylenes and diborenes?. Chemical Science, 0, , .	3.7	3