Frank Weinhold

List of Publications by Year in Descending Order

251 papers	49,885 citations	67 h-index	223 g-index
277 ext. papers	53,336 ext. citations	6.4 avg, IF	7.72 L-index

#	Paper	IF	Citations
251	Anti-Electrostatic Pi-Hole Bonding: How Covalency Conquers Coulombics.. *Molecules*, **2022**, 27,	4.8	1
250	Chlorine dioxide: An exception that proves the rules of localized chemical bonding.. *Journal of Chemical Physics*, **2022**, 156, 124303	3.9	2
249	6 Natural bond orbital theory: Discovering chemistry with NBO7 **2021**, 129-156		4
248	Comment on "Superposition of Waves or Densities: Which Is the Nature of Chemical Resonance?" [J. Comput. Chem. 2021, 42, 412-417]. *Journal of Computational Chemistry*, **2021**, 42, 1338-1340	3.5	2
247	Time-Conjugation in a Unified Quantum Theory for Hermitian and Non-Hermitian Electronic Systems under Time-Reversal Symmetry. *Symmetry*, **2021**, 13, 808	2.7	1
246	Sulfur Tetrahydride and Allied Superhydride Clusters: When Resonance Takes Precedence. *Chemistry - A European Journal*, **2021**, 27, 6748-6759	4.8	
245	Pauling's Conceptions of Hybridization and Resonance in Modern Quantum Chemistry. *Molecules*, **2021**, 26,	4.8	3
244	Substituted -Benzynes: Properties of the Triple Bond. *Journal of Organic Chemistry*, **2020**, 85, 9905-9914	4.2	2
243	NBO/NRT Two-State Theory of Bond-Shift Spectral Excitation. *Molecules*, **2020**, 25,	4.8	5
242	NBO 7.0: New vistas in localized and delocalized chemical bonding theory. *Journal of Computational Chemistry*, **2019**, 40, 2234-2241	3.5	85
241	What Is the Nature of Supramolecular Bonding? Comprehensive NBO/NRT Picture of Halogen and Pnicogen Bonding in RPH□F/FI Complexes (R = CH, OH, CF, CN, NO). *Molecules*, **2019**, 24,	4.8	12
240	Efficient optimization of natural resonance theory weightings and bond orders by gram-based convex programming. *Journal of Computational Chemistry*, **2019**, 40, 2028-2035	3.5	45
239	Resonance Theory Reboot. *Journal of the American Chemical Society*, **2019**, 141, 4156-4166	16.4	26
238	To Be or Not to Be: Demystifying the 2nd-Quantized Picture of Complex Electronic Configuration Patterns in Chemistry with Natural Poly-Electron Population Analysis. *Journal of Computational Chemistry*, **2019**, 40, 1509-1520	3.5	5
237	Comment on "Observation of alkaline earth complexes M(CO) (M = Ca, Sr, or Ba) that mimic transition metals". *Science*, **2019**, 365,	33.3	25
236	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
235	Resonance Natural Bond Orbitals: Efficient Semilocalized Orbitals for Computing and Visualizing Reactive Chemical Processes. *Journal of Chemical Theory and Computation*, **2019**, 15, 916-921	6.4	8

234	Natural Bond Orbital Theory of Pseudo-Jahn-Teller Effects. *Journal of Physical Chemistry A*, **2018**, 122, 4490-4498	2.8	7
233	Theoretical Prediction of Robust Second-Row Oxyanion Clusters in the Metastable Domain of Antielectrostatic Hydrogen Bonding. *Inorganic Chemistry*, **2018**, 57, 2035-2044	5.1	31
232	The role of hyperconjugation in the unusual conformation of thymine: A natural bond orbital analysis. *Computational and Theoretical Chemistry*, **2018**, 1130, 58-62	2	6
231	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	5.1	1
230	Natural resonance theory of chemical reactivity, with illustrative application to intramolecular Claisen rearrangement. *Tetrahedron*, **2018**, 74, 4799-4804	2.4	5
229	Comment on "Natural Bond Orbitals and the Nature of the Hydrogen Bond". *Journal of Physical Chemistry A*, **2018**, 122, 724-732	2.8	26
228	Efficient evaluation of poly-electron populations in natural bond orbital analysis. *Chemical Physics Letters*, **2018**, 711, 23-26	2.5	7
227	Polyion Covalency: Exotic Species from the Unexplored World of Electrostatically Shielded Molecular Ion Chemistry. *Angewandte Chemie - International Edition*, **2017**, 56, 14577-14581	16.4	21
226	Why Do Cumulene Ketones Kink?. *Journal of Organic Chemistry*, **2017**, 82, 12238-12245	4.2	9
225	Polyion Covalency: Exotic Species from the Unexplored World of Electrostatically Shielded Molecular Ion Chemistry. *Angewandte Chemie*, **2017**, 129, 14769-14773	3.6	7
224	Predicting the Ionic Product of Water. *Scientific Reports*, **2017**, 7, 10244	4.9	23
223	Appendix A: What's under the Hood? **2016**, 297-299		
222	Appendix E: Atomic Units (a.u.) and Conversion Factors **2016**, 307-308		
221	Appendix B: Orbital Graphics: The NBOView Orbital Plotter **2016**, 300-301		
220	Appendix C: Digging at the Details **2016**, 302-303		
219	Excited State Chemistry **2016**, 252-296		
218	Electrons in Atoms **2016**, 10-33		
217	Atoms in Molecules **2016**, 34-50		

216	Hybrids and Bonds in Molecules **2016**, 51-91		
215	Resonance Delocalization Corrections **2016**, 92-134		1
214	Steric and Electrostatic Effects **2016**, 135-154		
213	Nuclear and Electronic Spin Effects **2016**, 155-175		
212	Coordination and Hyperbonding **2016**, 176-208		
211	Intermolecular Interactions **2016**, 209-230		1
210	Transition State Species and Chemical Reactions **2016**, 231-251		
209	18-electron rule and the 3c/4e hyperbonding saturation limit. *Journal of Computational Chemistry*, **2016**, 37, 237-41	3.5	14
208	Spectroscopic Evidence for Clusters of Like-Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. *ChemPhysChem*, **2016**, 17, 447-447	3.2	1
207	What is NBO analysis and how is it useful?. *International Reviews in Physical Chemistry*, **2016**, 35, 399-4407		375
206	3c/4e [small sigma, Greek, circumflex]-type long-bonding competes with bonding in noble-gas hydrides HNgY (Ng = He, Ne, Ar, Kr, Xe, Rn; Y = F, Cl, Br, I): a NBO/NRT perspective. *Physical Chemistry Chemical Physics*, **2016**, 18, 8015-26	3.6	14
205	Insight into the Mechanism of the Michael Reaction. *ChemPhysChem*, **2016**, 17, 2022-34	3.2	19
204	Spectroscopic Evidence for Clusters of Like-Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. *ChemPhysChem*, **2016**, 17, 458-62	3.2	100
203	Appendix D: What if Something goes Wrong? **2016**, 304-306		
202	Bonding Analysis of TM(cAAC)2 (TM = Cu, Ag, and Au) and the Importance of Reference State. *Organometallics*, **2015**, 34, 3442-3449	3.8	36
201	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	2.1	4
200	Improved General Understanding of the Hydrogen-Bonding Phenomena: A Reply. *Angewandte Chemie*, **2015**, 127, 2636-2638	3.6	16
199	Resonance Character of Copper/Silver/Gold Bonding in Small Molecule???M-X (X=F, Cl, Br, CH3, CF3) Complexes. *ChemPhysChem*, **2015**, 16, 2424-31	3.2	18

198	Improved general understanding of the hydrogen-bonding phenomena: a reply. *Angewandte Chemie - International Edition*, **2015**, 54, 2600-2	16.4	38
197	The NBO View of Chemical Bonding **2014**, 91-120		40
196	Rabbit-ears hybrids, VSEPR sterics, and other orbital anachronisms. *Chemistry Education Research and Practice*, **2014**, 15, 417-434	2.1	38
195	Anti-Electrostatic Hydrogen Bonds. *Angewandte Chemie*, **2014**, 126, 11396-11399	3.6	69
194	Anti-electrostatic hydrogen bonds. *Angewandte Chemie - International Edition*, **2014**, 53, 11214-7	16.4	146
193	Kinetics and mechanism of water cluster equilibria. *Journal of Physical Chemistry B*, **2014**, 118, 7792-8	3.4	14
192	What is a hydrogen bond? Resonance covalency in the supramolecular domain. *Chemistry Education Research and Practice*, **2014**, 15, 276-285	2.1	82
191	Bay-type H···H "bonding" in cis-2-butene and related species: QTAIM versus NBO description. *Journal of Computational Chemistry*, **2014**, 35, 1499-508	3.5	54
190	Addendum: Anti-Electrostatic Hydrogen Bonds. *Angewandte Chemie - International Edition*, **2014**, 53, 12992-12992	16.4	14
189	Addendum: Anti-Electrostatic Hydrogen Bonds. *Angewandte Chemie*, **2014**, 126, 13207-13207	3.6	11
188	Quantum Cluster Equilibrium. *Letters in Mathematical Physics*, **2014**, 77-96	0.2	6
187	NBO 6.0: natural bond orbital analysis program. *Journal of Computational Chemistry*, **2013**, 34, 1429-37	3.5	916
186	Natural bond-bond polarizability: a Hückel-like electronic delocalization index. *Journal of Organic Chemistry*, **2013**, 78, 1844-50	4.2	6
185	Hyperconjugative interactions in permethylated siloxanes and ethers: the nature of the SiO bond. *Journal of the American Chemical Society*, **2013**, 135, 5762-7	16.4	75
184	3c/4e π-type long-bonding: a novel transitional motif toward the metallic delocalization limit. *Inorganic Chemistry*, **2013**, 52, 5154-66	5.1	40
183	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, 4670-82	16.4	17
182	Comments on "Is It Time To Retire the Hybrid Atomic Orbital?" *Journal of Chemical Education*, **2012**, 89, 570-572	2.4	20
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177	**2012**,		394
176	Natural Bond Orbitals and Lewis-Like Structures of Copper Blue Proteins **2011**, 77-89		1
175	The Nature of the Silicon□Oxygen Bond. *Organometallics*, **2011**, 30, 5815-5824	3.8	110
174	Hyperfine-shifted 13C resonance assignments in an iron-sulfur protein with quantum chemical verification: aliphatic C-H□□S 3-center-4-electron interactions. *Journal of the American Chemical Society*, **2011**, 133, 1310-6	16.4	28
173	Isotope-sensitive degenerate [1,3]-hydrogen migration versus competitive enol-keto tautomerization. *Chemistry - A European Journal*, **2009**, 15, 11815-9	4.8	7
172	Natural hybrid orbitals: Ab initio SCF and CI results for CO and NiCO. *International Journal of Quantum Chemistry*, **2009**, 18, 201-209	2.1	3
171	Remarks on the calculation of upper and lower limits to quantum-mechanical properties. *International Journal of Quantum Chemistry*, **2009**, 5, 721-728	2.1	5
170	Further Aspects of Thermodynamic Geometry **2008**, 421-463		
169	**2008**,		6
168	Characterization of the methoxy carbonyl radical formed via photolysis of methyl chloroformate at 193.3 nm. *Journal of Physical Chemistry A*, **2007**, 111, 1762-70	2.8	8
167	Chemistry. High bond orders in metal-metal bonding. *Science*, **2007**, 316, 61-3	33.3	65
166	News from the Periodic Table: An Introduction to "Periodicity Symbols, Tables, and Models for Higher-Order Valency and Donor□Acceptor Kinships". *Journal of Chemical Education*, **2007**, 84, 1145	2.4	21
165	Valence and extra-valence orbitals in main group and transition metal bonding. *Journal of Computational Chemistry*, **2007**, 28, 198-203	3.5	43
164	Radical hydrogen bonding: origin of stability of radical-molecule complexes. *Journal of Chemical Physics*, **2007**, 127, 164102	3.9	43
163	The ABCs of multiple bonding. *Science*, **2007**, 318, 746; author reply 746	33.3	3

162	Determination of the conformation of 2-hydroxy- and 2-aminobenzoic acid dimers using 13C NMR and density functional theory/natural bond order analysis: the central importance of the carboxylic acid carbon. *Journal of Physical Chemistry A*, **2006**, 110, 8832-9	2.8	8
161	Origin of trans-bent geometries in maximally bonded transition metal and main group molecules. *Journal of the American Chemical Society*, **2006**, 128, 7335-45	16.4	90
160	Resonance bonding patterns of peroxide chemistry: cyclic three-center hyperbonding in "phosphadioxirane" intermediates. *Journal of the American Chemical Society*, **2006**, 128, 11850-9	16.4	19
159	Comments on Purser's Article: "Lewis Structures are Models for Predicting Molecular Structure, Not Electronic Structure". *Journal of Chemical Education*, **2005**, 82, 527	2.4	5
158	Resonance Character of Hydrogen-bonding Interactions in Water and Other H-bonded Species. *Advances in Protein Chemistry*, **2005**, 72, 121-55		50
157	Natural Bond Orbital Analysis of Photochemical Excitation, With Illustrative Applications to Vinoxy Radical. *Molecular and Supramolecular Photochemistry*, **2005**, 393-476		4
156	Blue-Shifted and Red-Shifted Hydrogen Bonds in Hypervalent Rare-Gas FRgHIIIY Sandwiches. *Journal of Physical Chemistry A*, **2004**, 108, 4720-4730	2.8	67
155	Supramolecular bonding **2003**, 579-709		
154	Rebuttal to the BickelhauptBaerends Case for Steric Repulsion Causing the Staggered Conformation of Ethane. *Angewandte Chemie*, **2003**, 115, 4320-4326	3.6	39
153	Rebuttal to the BickelhauptBaerends Case for Steric Repulsion Causing the Staggered Conformation of Ethane. *Angewandte Chemie - International Edition*, **2003**, 42, 4188-4194	16.4	145
152	Electronic basis of improper hydrogen bonding: a subtle balance of hyperconjugation and rehybridization. *Journal of the American Chemical Society*, **2003**, 125, 5973-87	16.4	644
151	Tests of quantum cluster equilibrium (QCE)-based computational methods for describing formic acid clustering. *Molecular Physics*, **2003**, 101, 1147-1153	1.7	8
150	Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective **2003**,		1289
149	Die molekulare Zusammensetzung des flüssigen Schwefels. *Angewandte Chemie*, **2002**, 114, 3331-3335	3.6	2
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147	Nuclear motion and BreitPauli corrections to the diamagnetism of atomic helium. *Journal of Chemical Physics*, **2002**, 117, 3243-3247	3.9	12
146	Quantum Cluster Equilibrium Theory of Liquids: Isotopically substituted QCE/3-21G Model Water. *Zeitschrift Fur Physikalische Chemie*, **2002**, 216,	3.1	19
145	Quantum chemical calculations on structural models of the catalytic site of chymotrypsin: comparison of calculated results with experimental data from NMR spectroscopy. *Journal of the American Chemical Society*, **2002**, 124, 14373-81	16.4	23

144	Experimental and theoretical spin-spin coupling constants for [15N] formamide. *Molecular Physics*, **2002**, 100, 2807-2814	1.7	7
143	Trans-hydrogen-bond (h2)J(NN) and (h1)J(NH) couplings in the DNA A-T base pair: natural bond orbital analysis. *Journal of the American Chemical Society*, **2002**, 124, 1190-1	16.4	41
142	Collagen stability: 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, 2497-505	16.4	276
141	Natural J-coupling analysis: interpretation of scalar J-couplings in terms of natural bond orbitals. *Journal of the American Chemical Society*, **2001**, 123, 12026-36	16.4	93
140	NATURAL BOND ORBITALS AND EXTENSIONS OF LOCALIZED BONDING CONCEPTS. *Chemistry Education Research and Practice*, **2001**, 2, 91-104	2.1	582
139	Natural resonance theory. I. General formalism. *Journal of Computational Chemistry*, **2000**, 21, 411-413	3.5	10
138	Diamagnetism of helium. *Journal of Chemical Physics*, **2000**, 113, 8667-8670	3.9	25
137	Quantum cluster equilibrium theory of liquids: light and heavy QCE/3-21G model water. *Physical Chemistry Chemical Physics*, **2000**, 2, 1613-1619	3.6	24
136	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	1.7	38
135	Quantum cluster equilibrium theory of liquids: Freezing of QCE/3-21G water to tetrakaidecahedral Bucky-ice *Journal of Chemical Physics*, **1999**, 110, 508-515	3.9	67
134	Natural steric analysis of internal rotation barriers. *International Journal of Quantum Chemistry*, **1999**, 72, 269-280	2.1	159
133	Chemical Bonding as a Superposition Phenomenon. *Journal of Chemical Education*, **1999**, 76, 1141	2.4	34
132	Origin of Methyl Internal Rotation Barriers. *Accounts of Chemical Research*, **1999**, 32, 983-993	24.3	107
131	Quantum cluster equilibrium theory of liquids: molecular clusters and thermodynamics of liquid ethanol. *Molecular Physics*, **1999**, 97, 465-477	1.7	66
130	Natural steric analysis of internal rotation barriers **1999**, 72, 269		1
129	Quantum cluster equilibrium theory of liquids part I: Molecular clusters and thermodynamics of liquid ammonia. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 197-204		26
128	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		24
127	Natural resonance theory: I. General formalism. *Journal of Computational Chemistry*, **1998**, 19, 593-609	3.5	549

126	Natural resonance theory: II. Natural bond order and valency. *Journal of Computational Chemistry*, **1998**, 19, 610-627	3.5	432
125	Natural resonance theory: III. Chemical applications. *Journal of Computational Chemistry*, **1998**, 19, 628-646	3.5	416
124	Quantum Cluster Equilibrium Theory of Liquids: Temperature Dependence of Hydrogen Bonding in Liquid N-Methylacetamide Studied by IR Spectra. *Journal of Physical Chemistry B*, **1998**, 102, 9312-9318	3.4	99
123	Inadequacies of the Point-Dipole Approximation for Describing Electron□Nuclear Interactions in Paramagnetic Proteins: 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	3.4	26
122	NMR Investigations of Clostridium pasteurianum Rubredoxin. Origin of Hyperfine 1H, 2H, 13C, and 15N NMR Chemical Shifts in Iron□Sulfur Proteins As Determined by Comparison of Experimental Data with Hybrid Density Functional Calculations□ *Journal of the American Chemical Society*, **1998**, 120, 4806-4814	16.4	86
121	Protonation of Rhenium Alkyne Complexes Produces □3-Allyl Rhenium Complexes via Observable 1-Metallacyclopropene Intermediates. *Journal of the American Chemical Society*, **1998**, 120, 12500-12511	16.4	57
120	Quantum cluster equilibrium theory of liquids: General theory and computer implementation. *Journal of Chemical Physics*, **1998**, 109, 367-372	3.9	124
119	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	3.9	27
118	Ab initio and regularized force fields of haloethanes: CH3CH2Cl, CH3CHCl2, CH3CF2Cl, and CH3CFCl2. *Journal of Chemical Physics*, **1998**, 109, 7286-7299	3.9	14
117	Quantum cluster equilibrium theory of liquids: Illustrative application to water. *Journal of Chemical Physics*, **1998**, 109, 373-384	3.9	90
116	Solvent and concentration dependence of the hydroxyl chemical shift of methanol. *Molecular Physics*, **1998**, 93, 145-151	1.7	45
115	Natural resonance theory: II. Natural bond order and valency **1998**, 19, 610		1
114	Natural resonance theory: I. General formalism **1998**, 19, 593		13
113	Natural resonance theory: II. Natural bond order and valency **1998**, 19, 610		19
112	Natural resonance theory: III. Chemical applications **1998**, 19, 628		3
111	High Harmonic Generation Spectra of Neutral Helium by the Complex-Scaled (t,t?) Method: Role of Dynamical Electron Correlation. *Physical Review Letters*, **1997**, 78, 2100-2103	7.4	51
110	Theoretical study of hydrogen bonding in liquid and gaseous N-methylformamide. *Journal of Chemical Physics*, **1997**, 107, 499-507	3.9	89
109	Natural chemical shielding analysis of nuclear magnetic resonance shielding tensors from gauge-including atomic orbital calculations. *Journal of Chemical Physics*, **1997**, 107, 1173-1184	3.9	216

108	Structure of Liquid N-Methylacetamide: Temperature Dependence of NMR Chemical Shifts and Quadrupole Coupling Constants. *Journal of Physical Chemistry A*, **1997**, 101, 8861-8870	2.8	58
107	Natural steric analysis: Ab initio van der Waals radii of atoms and ions. *Journal of Chemical Physics*, **1997**, 107, 5422-5432	3.9	146
106	Natural bond orbital analysis of steric interactions. *Journal of Chemical Physics*, **1997**, 107, 5406-5421	3.9	228
105	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		199
104	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	3.4	1
103	Effective O-17 quadrupole moments for the calibrated computation of quadrupole coupling parameters at different levels of theory. *Journal of Chemical Physics*, **1996**, 105, 8223-8230	3.9	29
102	Threshold photoionization spectra of benzyl radical: Cation vibrational states and ab initio calculations. *Journal of Chemical Physics*, **1996**, 104, 8886-8895	3.9	29
101	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	3	2
100	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	3.9	114
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96	Ab Initio Calculations of Protium/Deuterium Fractionation Factors in O2H5+ Clusters. *The Journal of Physical Chemistry*, **1995**, 99, 8013-8016		15
95	Theoretical Studies of Protium/Deuterium Fractionation Factors and Cooperative Hydrogen Bonding in Peptides. *Journal of the American Chemical Society*, **1995**, 117, 9619-9624	16.4	40
94	Structure and spectroscopy of (HCN)n clusters: Cooperative and electronic delocalization effects in CH???N hydrogen bonding. *Journal of Chemical Physics*, **1995**, 103, 333-347	3.9	210
93	Common Textbook and Teaching Misrepresentations of Lewis Structures. *Journal of Chemical Education*, **1995**, 72, 583	2.4	52
92	Understanding barriers to internal rotation in substituted toluenes and their cations. *Journal of Chemical Physics*, **1995**, 102, 6787-6805	3.9	101
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90	Joint treatment of ab initio and experimental data in molecular force field calculations with Tikhonov□ method of regularization. *Journal of Chemical Physics*, **1994**, 100, 1414-1424	3.9	46
89	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, 519-42	3	42
88	Estimates of phi and psi torsion angles in proteins from one-, two- and three-bond nuclear spin-spin couplings: application to staphylococcal nuclease. *Journal of Biomolecular NMR*, **1994**, 4, 543-51	3	28
87	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	16.4	13
86	The role of delocalization in benzene. *Journal of the American Chemical Society*, **1993**, 115, 10952-10957	16.4	85
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84	Calculation of nuclear spin-spin coupling constants with ab initio molecular orbital wave functions. *The Journal of Physical Chemistry*, **1993**, 97, 11657-11665		23
83	Natural bond orbitals in multiconfigurational expansions: Local treatment of electron correlation in molecules. *Journal of Chemical Physics*, **1992**, 97, 1095-1108	3.9	25
82	Structures of the aluminum oxides studied by ab initio methods with natural bond orbital analysis. *Journal of Chemical Physics*, **1992**, 97, 3420-3430	3.9	52
81	Photoelectron spectroscopy of free radicals with cm□ resolution: The benzyl cation. *Journal of Chemical Physics*, **1991**, 95, 8665-8668	3.9	53
80	Natural Bond Orbital Analysis of Internal Rotation Barriers and Related Phenomena. *Israel Journal of Chemistry*, **1991**, 31, 277-285	3.4	160
79	Experimental and theoretical study of the relaxation of vibrationally excited HF by NO and CO. *Journal of Chemical Physics*, **1989**, 91, 1688-1696	3.9	12
78	Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. *Chemical Reviews*, **1988**, 88, 899-926	68.1	14317
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76	Some remarks on nonorthogonal orbitals in quantum chemistry. *Computational and Theoretical Chemistry*, **1988**, 165, 189-202		65
75	Transferability of natural bond orbitals. *Journal of the American Chemical Society*, **1988**, 110, 368-372	16.4	57
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73	The Natural Bond Orbital Lewis Structure Concept for Molecules, Radicals, and Radical Ions **1988**, 227-236		333

72	Torsion-vibration interactions in hydrogen peroxide. 2. Natural bond orbital analysis. *The Journal of Physical Chemistry*, **1988**, 92, 4306-4313		23
71	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		30
70	Photodissociation of (CO)+2: Theoretical studies of ground 2Bu and excited 2Bg potential energy surfaces. *Journal of Chemical Physics*, **1987**, 87, 392-410	3.9	33
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68	Eine Csp3-gebundene Methylgruppe in ekliptischer Konformation; experimenteller und theoretischer Nachweis von C?H O-Wasserstoffbrücken. *Angewandte Chemie*, **1987**, 99, 1216-1218	3.6	21
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