Elfi Kraka

List of Publications by Year
in descending order

258	13,426	18482 62	32842 100
papers	citations	h-index	g-index

265	265	265	6870
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Chemical Bonds without Bonding Electron Density ? Does the Difference Electron-Density Analysis Suffice for a Description of the Chemical Bond?. Angewandte Chemie International Edition in English, 1984, 23, 627-628.	4.4	1,276
2	Nuclear magnetic resonance spinâ€“spin coupling constants from coupled perturbed density functional theory. Journal of Chemical Physics, 2000, 113, 3530-3547.	3.0	311
3	Density functional theory: coverage of dynamic and non-dynamic electron correlation effects. Molecular Physics, 2001, 99, 1899-1940.	1.7	281
4	Analytical evaluation of energy gradients in quadratic configuration interaction theory. Chemical Physics Letters, 1988, 150, 280-286.	2.6	218
5	Helium chemistry: theoretical predictions and experimental challenge. Journal of the American Chemical Society, 1987, 109, 5917-5934.	13.7	207
6	Electron correlation and the self-interaction error of density functional theory. Molecular Physics, 2002, 100, 1771-1790.	1.7	202
7	A new way of analyzing vibrational spectra. I. Derivation of adiabatic internal modes. International Journal of Quantum Chemistry, 1998, 67, 1-9.	2.0	198
8	MÃ¸llerâ€“Plesset perturbation theory: from small molecule methods to methods for thousands of atoms. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 509-530.	14.6	171
9	CCSD(T) Investigation of the Bergman Cyclization of Enediyne. Relative Stability of o-, m-, and p-Didehydrobenzene. Journal of the American Chemical Society, 1994, 116, 4929-4936.	13.7	168
10	Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650.	3.0	161
11	Computational Analysis of the Mechanism of Chemical Reactions in Terms of Reaction Phases: Hidden Intermediates and Hidden Transition States. Accounts of Chemical Research, 2010, 43, 591-601.	15.6	160
12	Stabilities and nature of the attractive interactions in HeBeO, NeBeO, and ArBeO and a comparison with analogs NGLiF, NGBN, and NGLiH (NG = He, Ar). A theoretical investigation. Journal of the American Chemical Society, 1988, 110, 8007-8016.	13.7	158
13	The impact of the self-interaction error on the density functional theory description of dissociating radical cations: Ionic and covalent dissociation limits. Journal of Chemical Physics, 2004, 120, 524-539.	3.0	141
14	Identification of the Strongest Bonds in Chemistry. Journal of Physical Chemistry A, 2013, 117, 8981-8995.	2.5	140
15	The combination of density functional theory with multi-configuration methods â€“ CAS-DFT. Chemical Physics Letters, 2000, 316, 569-577.	2.6	139
16	Can density functional theory describe multi-reference systems? Investigation of carbenes and organic biradicals. Physical Chemistry Chemical Physics, 2000, 2, 2091-2103.	2.8	135
17	Strength of the Pnicogen Bond in Complexes Involving Group Va Elements N, P, and As. Journal of Physical Chemistry A, 2015, 119, 1642-1656.	2.5	132
18	A new way of analyzing vibrational spectra. III. Characterization of normal vibrational modes in terms of internal vibrational modes. International Journal of Quantum Chemistry, 1998, 67, 29-40.	2.0	128

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19	The intrinsic strength of the halogen bond: electrostatic and covalent contributions described by coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 33031-33046.	2.8	128
20	Bâ€“HÂ·Â·Â·Ï€ Interaction: A New Type of Nonclassical Hydrogen Bonding. Journal of the American Chemical Society, 2016, 138, 4334-4337.	13.7	126
21	Some Thoughts about Bond Energies, Bond Lengths, and Force Constants. Journal of Molecular Modeling, 2000, 6, 396-412.	1.8	124
22	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. International Journal of Quantum Chemistry, 2012, 112, 3174-3187.	2.0	121
23	C₂ in a Box: Determining Its Intrinsic Bond Strength for the X¹Î£_g⁺ Ground State. Chemistry - A European Journal, 2016, 22, 4087-4099.	3.3	120
24	Some thoughts about the stability and reliability of commonly used exchange?correlation functionals ? coverage of dynamic and nondynamic correlation effects. Theoretical Chemistry Accounts, 2002, 107, 291-303.	1.4	116
25	Relating normal vibrational modes to local vibrational modes with the help of an adiabatic connection scheme. Journal of Chemical Physics, 2012, 137, 084114.	3.0	113
26	Development of a CAS-DFT method covering non-dynamical and dynamical electron correlation in a balanced way. Molecular Physics, 2005, 103, 279-308.	1.7	109
27	Effect of the self-interaction error for three-electron bonds: On the development of new exchange-correlation functionals. Physical Chemistry Chemical Physics, 2004, 6, 1096-1112.	2.8	107
28	Light noble gas chemistry: structures, stabilities, and bonding of helium, neon, and argon compounds. Journal of the American Chemical Society, 1990, 112, 4240-4256.	13.7	103
29	Density functional theory for open-shell singlet biradicals. Chemical Physics Letters, 1998, 288, 593-602.	2.6	103
30	Characterization of CF Bonds with Multipleâ€Bond Character: Bond Lengths, Stretching Force Constants, and Bond Dissociation Energies. ChemPhysChem, 2009, 10, 686-698.	2.1	103
31	A new way of analyzing vibrational spectra. II. Comparison of internal mode frequencies. International Journal of Quantum Chemistry, 1998, 67, 11-27.	2.0	100
32	Helium bonding in singly and doubly charged first-row diatomic cations HeXn+ (X = Li-Ne; n = 1,2). The Journal of Physical Chemistry, 1989, 93, 3397-3410.	2.9	99
33	Calculation and analysis of NMR spinâ€“spin coupling constants. Physical Chemistry Chemical Physics, 2007, 9, 2791-2816.	2.8	95
34	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 6845-6862.	2.5	95
35	Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502.	4.0	91
36	A new way of analyzing vibrational spectra. IV. Application and testing of adiabatic modes within the concept of the characterization of normal modes. International Journal of Quantum Chemistry, 1998, 67, 41-55.	2.0	90

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37	On the diagnostic value of (Åœ2) in Kohn-Sham density functional theory. Molecular Physics, 2001, 99, 981-989.	1.7	89
38	Reâ€evaluation of the bond lengthâ€“bond strength rule: The stronger bond is not always the shorter bond. Journal of Computational Chemistry, 2016, 37, 130-142.	3.3	88
39	Direct Measure of Metalâ€“Ligand Bonding Replacing the Tolman Electronic Parameter. Inorganic Chemistry, 2016, 55, 2332-2344.	4.0	85
40	Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?. Journal of Chemical Theory and Computation, 2017, 13, 55-76.	5.3	85
41	Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1480.	14.6	85
42	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. Molecules, 2018, 23, 2763.	3.8	84
43	Solvated Silylium Cations:Â Structure Determination by NMR Spectroscopy and the NMR/Ab Initio/IGLO Method. Journal of the American Chemical Society, 1996, 118, 5120-5131.	13.7	81
44	Long-range and short-range Coulomb correlation effects as simulated by Hartree-Fock, local density approximation, and generalized gradient approximation exchange functionals. Theoretical Chemistry Accounts, 2003, 109, 22-35.	1.4	81
45	Neon and argon bonding in first-row cations NeX+ and ArX+ (X = Li-Ne). The Journal of Physical Chemistry, 1989, 93, 3410-3418.	2.9	80
46	The chemistry of the noble gas elements helium, neon, and argon â€” Experimental facts and theoretical predictions. Structure and Bonding, 1990, , 17-95.	1.0	77
47	Analytical Energy Gradients in MÃ¸ller-Plesset Perturbation and Quadratic Configuration Interaction Methods: Theory and Application. Advances in Quantum Chemistry, 1992, 23, 205-299.	0.8	76
48	Calculation of NMR Chemical Shifts â€” The Third Dimension of Quantum Chemistry. Israel Journal of Chemistry, 1993, 33, 369-385.	2.3	74
49	Vibrational Spectrum ofm-Benzyne:Â A Matrix Isolation and Computational Studyâ€. Journal of the American Chemical Society, 2002, 124, 13072-13079.	13.7	74
50	Transition from metal-ligand bonding to halogen bonding involving a metal as halogen acceptor a study of Cu, Ag, Au, Pt, and Hg complexes. Chemical Physics Letters, 2017, 681, 56-63.	2.6	74
51	Systematic Coupled Cluster Study of Noncovalent Interactions Involving Halogens, Chalcogens, and Pnicogens. Journal of Physical Chemistry A, 2017, 121, 9544-9556.	2.5	72
52	A CCSD(T) and DFT investigation of m-benzyne and 4-hydroxy-m-benzyne. Chemical Physics Letters, 1997, 268, 313-320.	2.6	70
53	Calculation of puckered rings with analytical gradients. The Journal of Physical Chemistry, 1990, 94, 5502-5509.	2.9	69
54	Development and application of the analytical energy gradient for the normalized elimination of the small component method. Journal of Chemical Physics, 2011, 134, 244117.	3.0	68

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55	Generalization of the Tolman electronic parameter: the metalâ€“ligand electronic parameter and the intrinsic strength of the metalâ€“ligand bond. Dalton Transactions, 2017, 46, 8323-8338.	3.3	68
56	1H-Bicyclo[3.1.0]hexa-3,5-dien-2-one. A strained 1,3-bridged cyclopropene. Journal of the American Chemical Society, 1991, 113, 5311-5322.	13.7	67
57	Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. Journal of Physical Chemistry A, 2014, 118, 223-237.	2.5	67
58	Bonding in Mercury Molecules Described by the Normalized Elimination of the Small Component and Coupled Cluster Theory. ChemPhysChem, 2008, 9, 2510-2521.	2.1	66
59	Quantitative Assessment of the Multiplicity of Carbonâ€“Halogen Bonds: Carbenium and Halonium Ions with F, Cl, Br, and I. Journal of Physical Chemistry A, 2014, 118, 1948-1963.	2.5	66
60	Theoretical determination of molecular structure and conformation. Journal of Molecular Structure, 1981, 75, 225-240.	3.6	65
61	Influence of the self-interaction error on the structure of the DFT exchange hole. Chemical Physics Letters, 2002, 352, 469-478.	2.6	65
62	Sumâ€overâ€states density functional perturbation theory: Prediction of reliable 13C, 15N, and 17O nuclear magnetic resonance chemical shifts. Journal of Chemical Physics, 1996, 105, 8995-9006.	3.0	64
63	Thepara-didehydropyridine,para-didehydropyridinium, and related biradicals?a contribution to the chemistry of enediyne antitumor drugs. Journal of Computational Chemistry, 2001, 22, 216-229.	3.3	64
64	Extension of the Karplus Relationship for NMR Spinâ^'Spin Coupling Constants to Nonplanar Ring Systems: Pseudorotation of Cyclopentane. Journal of Physical Chemistry A, 2002, 106, 657-667.	2.5	63
65	Avoiding singularity problems associated with meta-GGA (generalized gradient approximation) exchange and correlation functionals containing the kinetic energy density. Journal of Chemical Physics, 2007, 127, 214103.	3.0	62
66	New Approach to Tolmanâ€™s Electronic Parameter Based on Local Vibrational Modes. Inorganic Chemistry, 2014, 53, 478-495.	4.0	61
67	Theoretical determination of molecular structure and conformation. 7. Stereoselectivity of the ozonolysis reaction. Journal of the American Chemical Society, 1981, 103, 3619-3626.	13.7	60
68	Calculation of indirect nuclear spinâ€“spin coupling constants within the regular approximation for relativistic effects. Journal of Chemical Physics, 2004, 120, 11407-11422.	3.0	60
69	Strengthening of hydrogen bonding with the push-pull effect. Chemical Physics Letters, 2017, 685, 251-258.	2.6	58
70	Extension of the Karplus Relationship for NMR Spin-Spin Coupling Constants to Nonplanar Ring Systems: Pseudorotation of Tetrahydrofuran. International Journal of Molecular Sciences, 2003, 4, 158-192.	4.1	57
71	Theoretical Determination of Molecular Structure and Conformation. XI. The Puckering of Oxolanes. Israel Journal of Chemistry, 1983, 23, 72-84.	2.3	56
72	Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. Journal of Organic Chemistry, 2016, 81, 9669-9686.	3.2	56

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73	Theoretical determination of molecular structure and conformation. 8. Energetics of the ozonolysis reaction. Primary ozonide vs. carbonyl oxide control of stereochemistry. Journal of the American Chemical Society, 1981, 103, 3627-3633.	13.7	55
74	What correlation effects are covered by density functional theory?. Molecular Physics, 2000, 98, 1639-1658.	1.7	55
75	Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. Journal of Physical Chemistry A, 2015, 119, 9541-9556.	2.5	54
76	Theoretical determination of molecular structure and conformation. III. The pseudorotation surface of 1,2,3â€trioxolane and 1,2,4â€trioxolane. Journal of Chemical Physics, 1979, 70, 1898-1910.	3.0	53
77	Efficient density-functional theory integrations by locally augmented radial grids. Journal of Chemical Physics, 2007, 127, 164113.	3.0	53
78	Structure and stability of fluorine-substituted benzene-argon complexes: The decisive role of exchange-repulsion and dispersion interactions. Journal of Chemical Physics, 2001, 115, 6018-6029.	3.0	52
79	Prediction of Nitrogen and Oxygen NMR Chemical Shifts in Organic Compounds by Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 16881-16891.	2.9	51
80	Analysis of the Transmission Mechanism of NMR Spinâ^'Spin Coupling Constants Using Fermi Contact Spin Density Distribution, Partial Spin Polarization, and Orbital Currents:â€‰ XHn Molecules. Journal of Physical Chemistry A, 2003, 107, 7043-7056.	2.5	51
81	The self-interaction error and the description of non-dynamic electron correlation in density functional theory. Theoretical Chemistry Accounts, 2009, 123, 171-182.	1.4	51
82	Spin-orbit coupling calculations with the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2013, 139, 014106.	3.0	51
83	p-Benzyne. Angewandte Chemie - International Edition, 1998, 37, 955-958.	13.8	50
84	A General Definition of Ring Substituent Positions. Israel Journal of Chemistry, 1980, 20, 12-19.	2.3	49
85	The expectation value of the spin operator Åœ2 as a diagnostic tool in coupled cluster theory. Chemical Physics Letters, 2000, 324, 389-402.	2.6	49
86	Super-pnicogen bonding in the radical anion of the fluorophosphine dimer. Chemical Physics Letters, 2016, 662, 182-187.	2.6	49
87	On the physical meaning of the ZORA Hamiltonian. Molecular Physics, 2003, 101, 2295-2302.	1.7	48
88	Revision of the Dissociation Energies of Mercury Chalcogenides?Unusual Types of Mercury Bonding. ChemPhysChem, 2004, 5, 1547-1557.	2.1	48
89	Implementation of analytical energy gradients at third- and fourth-order MÃ¸ller-Plesset perturbation theory. Chemical Physics Letters, 1987, 138, 131-140.	2.6	47
90	Reaction path Hamiltonian and the unified reaction valley approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 531-556.	14.6	47

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91	The mechanism of a barrierless reaction: hidden transition state and hidden intermediates in the reaction of methylene with ethene. Molecular Physics, 2007, 105, 2697-2717.	1.7	45
92	Diracâ€exact relativistic methods: the normalized elimination of the small component method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 436-467.	14.6	45
93	From strong to weak NF bonds: on the design of a new class of fluorinating agents. Physical Chemistry Chemical Physics, 2018, 20, 23913-23927.	2.8	45
94	Analytical differentiation of the energy contribution due to triple excitations in fourth-order MÃ¸ller-Plesset perturbation theory. Chemical Physics Letters, 1988, 153, 303-308.	2.6	44
95	Development, Implementation, and Application of an Analytic Second Derivative Formalism for the Normalized Elimination of the Small Component Method. Journal of Chemical Theory and Computation, 2012, 8, 2617-2629.	5.3	44
96	Properties of local vibrational modes: the infrared intensity. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	43
97	Chelation-Assisted Selective Etching Construction of Hierarchical Polyoxometalate-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 5550-5557.	6.7	43
98	On the r0- and re-structures of H2O2. Journal of Molecular Spectroscopy, 1979, 74, 480-482.	1.2	42
99	An improved algorithm for the normalized elimination of the small-component method. Theoretical Chemistry Accounts, 2011, 130, 633-644.	1.4	41
100	Are carbonâ€"halogen double and triple bonds possible?. International Journal of Quantum Chemistry, 2014, 114, 1060-1072.	2.0	41
101	11,11-Dimethyl-1,6-methano[10]annuleneâ€"An Annulene with an Ultralong CC Bond or a Fluxional Molecule?. Journal of Physical Chemistry A, 2015, 119, 1666-1682.	2.5	41
102	A New Method for Describing the Mechanism of a Chemical Reaction Based on the Unified Reaction Valley Approach. Journal of Chemical Theory and Computation, 2016, 12, 650-663.	5.3	41
103	Analysis of the NMR through-space coupling mechanism between 19F atoms. Chemical Physics Letters, 2004, 394, 5-13.	2.6	40
104	Analytic Calculation of Isotropic Hyperfine Structure Constants Using the Normalized Elimination of the Small Component Formalism. Journal of Physical Chemistry A, 2012, 116, 3481-3486.	2.5	40
105	Analytic Calculation of Contact Densities and MÃ¶ssbauer Isomer Shifts Using the Normalized Elimination of the Small-Component Formalism. Journal of Chemical Theory and Computation, 2012, 8, 875-882.	5.3	40
106	Rational Design in Catalysis: A Mechanistic Study of Î²-Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley. Inorganic Chemistry, 2016, 55, 8636-8645.	4.0	40
107	The mechanism of the reaction FH + H2C=CH2â†'H3Câ€"CFH2. Investigation of hidden intermediates with the unified reaction valley approach. Physical Chemistry Chemical Physics, 2001, 3, 674-687.	2.8	39
108	Analytical energy gradient for the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2015, 142, 214106.	3.0	39

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109	A Continuum from Halogen Bonds to Covalent Bonds: Where Do Î»3 Iodanes Fit?. Inorganics, 2019, 7, 47.	2.7	39
110	Structure, stabilization energies and chemical shifts of the cyclobutenyl cation. Does it have ?aromatic? homocyclopropenium ion character? Anab initio study. Journal of Physical Organic Chemistry, 1993, 6, 445-464.	1.9	37
111	Extraordinary Mechanism of the Dielsâ€“Alder Reaction: Investigation of Stereochemistry, Charge Transfer, Charge Polarization, and Biradicaloid Formation. Journal of Physical Chemistry A, 2016, 120, 1097-1111.	2.5	37
112	Peculiar Structure of the HOOO-Anion. Journal of the American Chemical Society, 2002, 124, 8462-8470.	13.7	36
113	New Way of Describing Static and Dynamic Deformations of the Jahnâ€“Teller Type in Ring Molecules. Journal of Physical Chemistry A, 2011, 115, 8731-8742.	2.5	36
114	Analysis of coupled cluster and quadratic configuration interaction theory in terms of sixth-order perturbation theory. International Journal of Quantum Chemistry, 1991, 40, 43-70.	2.0	35
115	Homolytic dissociation energies from GVB-LSDC calculations. Chemical Physics, 1992, 161, 149-153.	1.9	35
116	Investigation of the NMR Spinâ^'Spin Coupling Constants across the Hydrogen Bonds in Ubiquitin:Â The Nature of the Hydrogen Bond as Reflected by the Coupling Mechanism. Journal of the American Chemical Society, 2004, 126, 5093-5107.	13.7	35
117	Relating normal vibrational modes to local vibrational modes: benzene and naphthalene. Journal of Molecular Modeling, 2013, 19, 2865-2877.	1.8	35
118	Structures, stabilities, and bonding in CBe2, C2Be, and C2Be2. Journal of the American Chemical Society, 1986, 108, 5732-5737.	13.7	34
119	New insights into Feâ€“H$$_{2}$$ and Feâ€“H$$^{-}$$ bonding of a [NiFe] hydrogenase mimic: a local vibrational mode study. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	34
120	A new way of studying chemical reactions: a hand-in-hand URVA and QTAIM approach. Physical Chemistry Chemical Physics, 2019, 21, 15007-15018.	2.8	33
121	Theoretical determination of molecular structure and conformation. Computational and Theoretical Chemistry, 1984, 110, 277-291.	1.5	32
122	Structure of the chlorobenzeneâ€“argon dimer: Microwave spectrum andab initioanalysis. Journal of Chemical Physics, 2000, 113, 9051-9059.	3.0	32
123	Can One Assess theÏ€ Character of a Câ€“C Bond with the Help of the NMR Spinâ€“Spin Coupling Constants?. ChemPhysChem, 2004, 5, 349-366.	2.1	32
124	Relativistically corrected hyperfine structure constants calculated with the regular approximation applied to correlation corrected ab initio theory. Journal of Chemical Physics, 2004, 121, 5618-5622.	3.0	32
125	Enediynes, enyneâ€allenes, their reactions, and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 285-324.	14.6	32
126	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. Journal of Physical Chemistry A, 2019, 123, 7087-7103.	2.5	32

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127	In Situ Measure of Intrinsic Bond Strength in Crystalline Structures: Local Vibrational Mode Theory for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 1761-1776.	5.3	32
128	Puckered Structures of 1,3-Dihydro-1,3-diboretes and Bicyclobutane-2,4-dione: Nonplanar HÃ¼ckel 2Ï€-Electron Aromatic Molecules. Angewandte Chemie International Edition in English, 1984, 23, 374-375.	4.4	31
129	Analysis of multipath transmission of spinâ€“spin coupling constants in cyclic compounds with the help of partially spin-polarized orbital contributions. Physical Chemistry Chemical Physics, 2003, 5, 4541-4550.	2.8	31
130	Calculation of electric properties using regular approximations to relativistic effects: The polarizabilities of RuO4, OsO4, and HsO4 (Z=108). Journal of Chemical Physics, 2003, 119, 1412-1420.	3.0	31
131	Energetics and Mechanism of the Hydrogenation of XH_n for Group IV to Group VII Elements X. Journal of Chemical Theory and Computation, 2012, 8, 4931-4943.	5.3	30
132	Quantitative Assessment of Bâ^'Bâ^'B, Bâ^'H_bâ^'B, and Bâ^'H_t Bonds: From BH₃ to B₁₂H₁₂^{2â^'}. ChemPhysChem, 2019, 20, 1967-1977.	2.1	30
133	Nature of the Si(SiMe3)3+ Cation in Aromatic Solvents. Organometallics, 1996, 15, 5495-5501.	2.3	29
134	Structure, Vibrational Spectra, and Unimolecular Dissociation of Gaseous 1-Fluoro-1-phenethyl Cations. Journal of Physical Chemistry A, 2008, 112, 10774-10783.	2.5	29
135	Solving the Pericyclicâ€“Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. Journal of Organic Chemistry, 2016, 81, 404-414.	3.2	29
136	A Critical Evaluation of Vibrational Stark Effect (VSE) Probes with the Local Vibrational Mode Theory. Sensors, 2020, 20, 2358.	3.8	29
137	SSnet: A Deep Learning Approach for Protein-Ligand Interaction Prediction. International Journal of Molecular Sciences, 2021, 22, 1392.	4.1	29
138	Electric field gradients and nuclear quadrupole coupling constants of isonitriles obtained from Moeller-Plesset and quadratic configuration interaction calculations. The Journal of Physical Chemistry, 1992, 96, 3239-3245.	2.9	28
139	Sixth-order many-body perturbation theory. I. Basic theory and derivation of the energy formula. International Journal of Quantum Chemistry, 1996, 59, 15-29.	2.0	28
140	Mechanism and dynamics of organic reactions: 1,2-H shift in methylchlorocarbene. Journal of Physical Organic Chemistry, 2002, 15, 431-447.	1.9	28
141	Removal of Mercury from the Environment: A Quantum-Chemical Study with the Normalized Elimination of the Small Component Method. Inorganic Chemistry, 2013, 52, 2497-2504.	4.0	28
142	Insights into the mechanisms of chemical reactions. Reaction paths for chemical reactions. Faraday Discussions of the Chemical Society, 1987, 84, 427.	2.2	27
143	New Approach for Determining the Conformational Features of Pseudorotating Ring Molecules Utilizing Calculated and Measured NMR Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2003, 107, 1797-1810.	2.5	27
144	Improved Predictorâ€“Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27

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145	Calculations of electric dipole moments and static dipole polarizabilities based on the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2016, 145, 184104.	3.0	27
146	Calculations of atomic magnetic nuclear shielding constants based on the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2017, 146, 134109.	3.0	27
147	The Peculiar Role of the Au₃ Unit in Au_m Clusters: Ï*f*-Aromaticity of the Au₅Zn⁺ Ion. Inorganic Chemistry, 2017, 56, 5793-5803.	4.0	27
148	Local vibrational force constants â€“ From the assessment of empirical force constants to the description of bonding in large systems. Chemical Physics Letters, 2020, 748, 137337.	2.6	27
149	Predicting Potential SARS-COV-2 Drugsâ€”In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. International Journal of Molecular Sciences, 2021, 22, 1573.	4.1	27
150	Theoretical determination of molecular structure and conformation. IV. Electronic effects 1979, 70, 1911-1927.	3.0	26
151	Diabatic ordering of vibrational normal modes in reaction valley studies. Journal of Computational Chemistry, 1997, 18, 1282-1294.	3.3	26
152	Relativistically corrected electric field gradients calculated with the normalized elimination of the small component formalism. Journal of Chemical Physics, 2012, 137, 054113.	3.0	26
153	Analytic calculation of second-order electric response properties with the normalized elimination of the small component (NESC) method. Journal of Chemical Physics, 2012, 137, 084108.	3.0	26
154	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
155	Metalâ€“Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	2.9	26
156	In Situ Assessment of Intrinsic Strength of X-Iâ‹¯OA-Type Halogen Bonds in Molecular Crystals with Periodic Local Vibrational Mode Theory. Molecules, 2020, 25, 1589.	3.8	26
157	Exceptionally Long Covalent CC Bondsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 950.	3.8	26
158	Hydrogen Bonding in Natural and Unnatural Base Pairsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 2268.	3.8	26
159	Bonding in radon hexafluoride: An unusual relativistic problem?. Physical Chemistry Chemical Physics, 2003, 5, 1103-1105.	2.8	25
160	Bondpseudorotation, Jahnâ€Teller, and pseudoâ€Jahnâ€Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. International Journal of Quantum Chemistry, 2012, 112, 3277-3288.	2.0	25
161	Nearly Degenerate Isomers of C(BH)₂: Cumulene, Carbene, or Carbone?. Chemistry - A European Journal, 2013, 19, 15941-15954.	3.3	25
162	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. Chirality, 2013, 25, 185-196.	2.6	25

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163	Dimesitylketone O-oxide: verification of an unusually stable carbonyl oxide by NMR chemical shift calculations. Chemical Physics Letters, 1996, 260, 43-50.	2.6	24
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