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 Bonding in Homogenous Catalysis â€“ Seen Through the Eyes of Vibrational Spectroscopy. , 2024, , 622-648.		0
2	Pivotal role of water molecules in the photodegradation of pymetrozine: New insights for developing green pesticides. Journal of Hazardous Materials, 2022, 423, 127197.	12.4	7
3	Analysis of spectator chemical bonds in SN2@C and @Si reaction mechanisms in the gas phase. Chemical Physics Letters, 2022, 787, 139282.	2.6	3
4	Structural study of 1- and 2-naphthol: new insights into the non-covalent Hâ€“H interaction in cis-1-naphthol. Physical Chemistry Chemical Physics, 2022, 24, 3722-3732.	2.8	7
5	Capturing Individual Hydrogen Bond Strengths in Ices via Periodic Local Vibrational Mode Theory: Beyond the Lattice Energy Picture. Journal of Chemical Theory and Computation, 2022, 18, 562-579.	5.3	17
6	LModeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis. Journal of Chemical Theory and Computation, 2022, 18, 1821-1837.	5.3	16
7	BF3â€“Catalyzed Dielsâ€“Alder Reaction between Butadiene and Methyl Acrylate in Aqueous Solutionâ€”An URVA and Local Vibrational Mode Study. Catalysts, 2022, 12, 415.	3.5	3
8	Unusual Intramolecular Motion of ReH₉^{2â€“} in K₂ReH₉ Crystal: Circle Dance and Three-Arm Turnstile Mechanisms Revealed by Computational Studies. Inorganic Chemistry, 2022, 61, 1041-1050.	4.0	2
9	Allosteric control of ACE2 peptidase domain dynamics. Organic and Biomolecular Chemistry, 2022, 20, 3605-3618.	2.8	3
10	Uranium: The Nuclear Fuel Cycle and Beyond. International Journal of Molecular Sciences, 2022, 23, 4655.	4.1	18
11	Bonding in nitrile photo-dissociating ruthenium drug candidatesâ€”A local vibrational mode study. Journal of Chemical Physics, 2022, 157, .	3.0	6
12	SSnet: A Deep Learning Approach for Protein-Ligand Interaction Prediction. International Journal of Molecular Sciences, 2021, 22, 1392.	4.1	29
13	Exceptionally Long Covalent CC Bondsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 950.	3.8	26
14	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
15	Describing Polytopal Rearrangement Processes of Octacoordinate Structures. I. Renewed Insights into Fluxionality of the Rhenium Polyhydride Complex ReH₅(PPh₃)₂(Pyridine). Inorganic Chemistry, 2021, 60, 2492-2502.	4.0	6
16	Systematic Detection and Characterization of Hydrogen Bonding in Proteins via Local Vibrational Modes. Journal of Physical Chemistry B, 2021, 125, 2551-2565.	2.6	15
17	Theoretical Insights into [NHC]Au(I) Catalyzed Hydroalkoxylation of Allenes: A Unified Reaction Valley Approach Study. Journal of Organic Chemistry, 2021, 86, 5714-5726.	3.2	11
18	A revised formulation of the generalized subsystem vibrational analysis (GSVA). Theoretical Chemistry Accounts, 2021, 140, 31.	1.4	6

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19	Hydrogen Bonding in Natural and Unnatural Base Pairsâ€"A Local Vibrational Mode Study. Molecules, 2021, 26, 2268.	3.8	26
20	Assessing the Intrinsic Strengths of Ionâ€"Solvent and Solventâ€"Solvent Interactions for Hydrated Mg2+ Clusters. Inorganics, 2021, 9, 31.	2.7	5
21	Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering. Journal of Chemical Information and Modeling, 2021, 61, 2159-2174.	5.4	5
22	Halogen Bonding Involving I2 and d8 Transition-Metal Pincer Complexes. Crystals, 2021, 11, 373.	2.2	14
23	Vibrational Analysis of Benziodoxoles and Benziodazolotetrazoles. Physchem, 2021, 1, 45-68.	1.1	5
24	Generative adversarial networks for transition state geometry prediction. Journal of Chemical Physics, 2021, 155, 024116.	3.0	21
25	Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€Type Iodine Compounds. ChemPlusChem, 2021, 86, 1199-1210.	2.8	5
26	On the formation of CN bonds in Titanâ€™s atmosphereâ€"a unified reaction valley approach study. Journal of Molecular Modeling, 2021, 27, 320.	1.8	2
27	Comment on â€œExploring nature and predicting strength of hydrogen bonds: A correlation analysis between <scp>atomsâ€inâ€molecules</scp> descriptors, binding energies, and energy components of <scp>symmetryâ€adapted</scp> perturbation theoryâ€. Journal of Computational Chemistry, 2021, 42, 516-521.	3.3	9
28	Metalâ€"Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	2.9	26
29	PyVibMS: a PyMOL plugin for visualizing vibrations in molecules and solids. Journal of Molecular Modeling, 2020, 26, 290.	1.8	14
30	Modeling Hydrogen Release from Water with Borane and Alane Catalysts: A Unified Reaction Valley Approach. Journal of Physical Chemistry A, 2020, 124, 8978-8993.	2.5	12
31	Equilibrium Geometries, Adiabatic Excitation Energies and Intrinsic C=C/Câ€"H Bond Strengths of Ethylene in Lowest Singlet Excited States Described by TDDFT. Symmetry, 2020, 12, 1545.	2.2	5
32	Local Vibrational Mode Analysis of Ï€â€"Hole Interactions between Aryl Donors and Small Molecule Acceptors. Crystals, 2020, 10, 556.	2.2	22
33	Peritectic phase transition of benzene and acetonitrile into a cocrystal relevant to Titan, Saturn's moon. Chemical Communications, 2020, 56, 13520-13523.	4.1	11
34	Characterizing the Metalâ€"Ligand Bond Strength via Vibrational Spectroscopy: The Metalâ€"Ligand Electronic Parameter (MLEP). Topics in Organometallic Chemistry, 2020, , 227-269.	0.7	3
35	Local vibrational mode analysis of ionâ€"solvent and solventâ€"solvent interactions for hydrated Ca2+ clusters. Journal of Chemical Physics, 2020, 153, 224303.	3.0	14
36	Critical assessment of the FeC and CO bond strength in carboxymyoglobin: a QM/MM local vibrational mode study. Journal of Molecular Modeling, 2020, 26, 281.	1.8	24

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37	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
38	Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1480.	14.6	85
39	Computational analysis of vibrational frequencies and rovibrational spectroscopic constants of hydrogen sulfide dimer using MP2 and CCSD(T). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118540.	3.9	14
40	Chelation-Assisted Selective Etching Construction of Hierarchical Polyoxometalate-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 5550-5557.	6.7	43
41	Describing Polytopal Rearrangements of Fluxional Molecules with Curvilinear Coordinates Derived from Normal Vibrational Modes: A Conceptual Extension of Cremerâ€“Pople Puckering Coordinates. Journal of Chemical Theory and Computation, 2020, 16, 3162-3193.	5.3	8
42	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
43	Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA)â€”A Review. Catalysts, 2020, 10, 691.	3.5	20
44	Quantitative assessment of intramolecular hydrogen bonds in neutral histidine. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	20
45	Crystal structure of 1-propanethiolâ€“Co2(dobdc) from laboratory X-ray powder diffraction data. Powder Diffraction, 2020, 35, 3-6.	0.2	1
46	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	5
47	A Critical Evaluation of Vibrational Stark Effect (VSE) Probes with the Local Vibrational Mode Theory. Sensors, 2020, 20, 2358.	3.8	29
48	Systematic description of molecular deformations with Cremerâ€“Pople puckering and deformation coordinates utilizing analytic derivatives: Applied to cycloheptane, cyclooctane, and cyclo[18]carbon. Journal of Chemical Physics, 2020, 152, 154107.	3.0	16
49	Metalâ€“ring interactions in actinide sandwich compounds: A combined normalized elimination of the small component and local vibrational mode study. Molecular Physics, 2020, 118, e1768314.	1.7	14
50	Calculation of contact densities and MÃ¶ssbauer isomer shifts utilising the Dirac-exact two-component normalised elimination of the small component (2c-NESC) method. Molecular Physics, 2019, 117, 1164-1171.	1.7	10
51	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. Journal of Physical Chemistry A, 2019, 123, 7087-7103.	2.5	32
52	Pushing 3câ€“4e Bonds to the Limit: A Coupled Cluster Study of Stepwise Fluorination of First-Row Atoms. Inorganic Chemistry, 2019, 58, 14777-14789.	4.0	16
53	Preface: Dieter Cremer's scientific journey. Molecular Physics, 2019, 117, 1047-1058.	1.7	3
54	Correlation between molecular acidity (pKa) and vibrational spectroscopy. Journal of Molecular Modeling, 2019, 25, 48.	1.8	8

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55	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
56	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
57	Quantitative Assessment of Bâˆ’Bâˆ’B, Bâˆ’H_bâˆ’B, and Bâˆ’H_t Bonds: From BH₃ to B₁₂H₁₂^{2â€“}. ChemPhysChem, 2019, 20, 1967-1977.	2.1	30
58	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
59	A Continuum from Halogen Bonds to Covalent Bonds: Where Do Î»3 Iodanes Fit?. Inorganics, 2019, 7, 47.	2.7	39
60	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
61	New mechanistic insights into the Claisen rearrangement of chorismate â€“ a Unified Reaction Valley Approach study. Molecular Physics, 2019, 117, 1172-1192.	1.7	22
62	Odd-even effect of the number of free valence electrons on the electronic structure properties of gold-thiolate clusters. Molecular Physics, 2019, 117, 1442-1450.	1.7	5
63	Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis. Journal of Chemical Theory and Computation, 2018, 14, 2558-2569.	5.3	23
64	Gold(I)-assisted catalysis â€“ a comprehensive view on the [3,3]-sigmatropic rearrangement of allyl acetate. Molecular Physics, 2018, 116, 611-630.	1.7	18
65	Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. Journal of Computational Chemistry, 2018, 39, 293-306.	3.3	11
66	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. Molecules, 2018, 23, 2763.	3.8	84
67	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
68	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
69	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
70	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
71	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
72	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

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73	Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502.	4.0	91
74	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. Journal of Physical Chemistry A, 2017, 121, 8086-8096.	2.5	15
75	Strengthening of hydrogen bonding with the push-pull effect. Chemical Physics Letters, 2017, 685, 251-258.	2.6	58
76	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 6845-6862.	2.5	95
77	Systematic Coupled Cluster Study of Noncovalent Interactions Involving Halogens, Chalcogens, and Pnicogens. Journal of Physical Chemistry A, 2017, 121, 9544-9556.	2.5	72
78	C₂ in a Box: Determining Its Intrinsic Bond Strength for the X¹Σ_g⁺ Ground State. Chemistry - A European Journal, 2016, 22, 4087-4099.	3.3	120
79	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
80	Super-pnicogen bonding in the radical anion of the fluorophosphine dimer. Chemical Physics Letters, 2016, 662, 182-187.	2.6	49
81	A Reaction Valley Investigation of the Cycloaddition of 1,3-Dipoles with the Dipolarophiles Ethene and Acetylene: Solution of a Mechanistic Puzzle. Journal of Physical Chemistry A, 2016, 120, 8400-8418.	2.5	21
82	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
83	Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. Journal of Organic Chemistry, 2016, 81, 9669-9686.	3.2	56
84	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
85	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
86	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
87	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
88	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
89	Direct Measure of Metalâ€“Ligand Bonding Replacing the Tolman Electronic Parameter. Inorganic Chemistry, 2016, 55, 2332-2344.	4.0	85
90	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

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91	Analytical energy gradient for the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2015, 142, 214106.	3.0	39
92	Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. Journal of Physical Chemistry A, 2015, 119, 9541-9556.	2.5	54
93	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
94	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
95	Pseudorotational Landscape of Sevenâ€Membered Rings: The Most Stable Chair and Twistâ€Boat Conformers of Îµâ€Caprolactone. Chemistry - A European Journal, 2014, 20, 14084-14089.	3.3	12
96	Description of Bond Pseudorotation, Bond Pseudolibration, and Ring Pseudoinversion Processes Caused by the Pseudo-Jahnâ€"Teller Effect: Fluoro Derivatives of the Cyclopropane Radical Cation. Australian Journal of Chemistry, 2014, 67, 435.	0.9	21
97	The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	23
98	Properties of local vibrational modes: the infrared intensity. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	43
99	New Approach to Tolmanâ€™s Electronic Parameter Based on Local Vibrational Modes. Inorganic Chemistry, 2014, 53, 478-495.	4.0	61
100	Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. Journal of Physical Chemistry A, 2014, 118, 223-237.	2.5	67
101	Calculation of response properties with the normalized elimination of the small component method. International Journal of Quantum Chemistry, 2014, 114, 993-1005.	2.0	23
102	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
103	Enediynes, enyneâ€allenes, their reactions, and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 285-324.	14.6	32
104	Are carbonâ€"halogen double and triple bonds possible?. International Journal of Quantum Chemistry, 2014, 114, 1060-1072.	2.0	41
105	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
106	Exploring Bonding in Heavy Atom Chemistry with Dirac-Exact Methods. Current Inorganic Chemistry, 2014, 3, 220-234.	0.2	1
107	Relativistic Calculation of Hyperfine Parameters of Mercury Compounds. Current Inorganic Chemistry, 2014, 3, 284-290.	0.2	5
108	Identification of the Strongest Bonds in Chemistry. Journal of Physical Chemistry A, 2013, 117, 8981-8995.	2.5	140

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109	Relating normal vibrational modes to local vibrational modes: benzene and naphthalene. Journal of Molecular Modeling, 2013, 19, 2865-2877.	1.8	35
110	Description of local and global shape properties of protein helices. Journal of Molecular Modeling, 2013, 19, 2901-2911.	1.8	14
111	Nearly Degenerate Isomers of C(BH)₂: Cumulene, Carbene, or Carbone?. Chemistry - A European Journal, 2013, 19, 15941-15954.	3.3	25
112	From configuration interaction to coupled cluster theory: The quadratic configuration interaction approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 482-503.	14.6	19
113	Improved Predictorâ€“Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27
114	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
115	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
116	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. Chirality, 2013, 25, 185-196.	2.6	25
117	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
118	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
119	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
120	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
121	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
122	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
123	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
124	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
125	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. International Journal of Quantum Chemistry, 2012, 112, 3174-3187.	2.0	121
126	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

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127	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
128	Reaction path Hamiltonian and the unified reaction valley approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 531-556.	14.6	47
129	An improved algorithm for the normalized elimination of the small-component method. Theoretical Chemistry Accounts, 2011, 130, 633-644.	1.4	41
130	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
131	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
132	A stunning example for a spontaneous reaction with a complex mechanism: the vinylideneâ€“acetylene cycloaddition reaction. Molecular Physics, 2010, 108, 2667-2685.	1.7	22
133	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
134	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
135	Description and recognition of regular and distorted secondary structures in proteins using the automated protein structure analysis method. Proteins: Structure, Function and Bioinformatics, 2009, 76, 418-438.	2.6	10
136	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
137	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
138	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
139	Efficient density-functional theory integrations by locally augmented radial grids. Journal of Chemical Physics, 2007, 127, 164113.	3.0	53
140	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
141	Calculation and analysis of NMR spinâ€“spin coupling constants. Physical Chemistry Chemical Physics, 2007, 9, 2791-2816.	2.8	95
142	A QM/MM Study of the Bergman Reaction of Dynemicin A in the Minor Groove of DNA. Journal of Physical Chemistry B, 2007, 111, 8321-8328.	2.6	16
143	Finding the Transition State of Quasi-Barrierless Reactions by a Growing String Method for Newton Trajectories:â€‰ Application to the Dissociation of Methylenecyclopropene and Cyclopropane. Journal of Physical Chemistry A, 2007, 111, 11287-11293.	2.5	22
144	The Reactivity of Calicheamicin Î³₁^I in the Minor Groove of DNA: The Decisive Role of the Environment. Chemistry - A European Journal, 2007, 13, 9256-9269.	3.3	12

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145	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
146	Analysis of long-range NMR spinâ€“spin coupling in polyenes and the Ï€-mechanism. Physical Chemistry Chemical Physics, 2005, 7, 452-462.	2.8	17
147	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
148	Decomposition of nuclear magnetic resonance spinâ€“spin coupling constants into active and passive orbital contributions. Journal of Chemical Physics, 2004, 120, 9952-9968.	3.0	16
149	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
150	Revision of the Dissociation Energies of Mercury Chalcogenides?Unusual Types of Mercury Bonding. ChemPhysChem, 2004, 5, 1547-1557.	2.1	48
151	Systematic strategy for decoding the NMR spinâ€“spin coupling mechanism: the J-OC-PSP method. Magnetic Resonance in Chemistry, 2004, 42, S138-S157.	1.9	13
152	Analysis of the spin-dipole transmission mechanism for NMR spinâ€“spin coupling constants using orbital contributions, spin polarization, and spin-dipole energy density distribution. Chemical Physics Letters, 2004, 387, 415-427.	2.6	24
153	Analysis of the NMR through-space coupling mechanism between 19F atoms. Chemical Physics Letters, 2004, 394, 5-13.	2.6	40
154	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
155	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
156	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
157	One-electron versus electronâ€“electron interaction contributions to the spinâ€“spin coupling mechanism in nuclear magnetic resonance spectroscopy: Analysis of basic electronic effects. Journal of Chemical Physics, 2004, 121, 12217.	3.0	9
158	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
159	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
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