Frank Jensen

List of Publications by Year
in descending order

195 papers	10,890 citations	28242 55 h-index	34964 98 g-index
217 all docs	217 docs citations	217 times ranked	9306 citing authors

#	Article	IF	Citations
1	A spin correction procedure for unrestricted Hartree-Fock and MÃ¸ller-Plesset wavefunctions for singlet diradicals and polyradicals. Chemical Physics Letters, 1988, 149, 537-542.	1.2	720
2	Polarization consistent basis sets: Principles. Journal of Chemical Physics, 2001, 115, 9113-9125.	1.2	571
3	Measurement and laser control of attosecond charge migration in ionized iodoacetylene. Science, 2015, 350, 790-795.	6.0	463
4	Polarization consistent basis sets. II. Estimating the Kohnâ€“Sham basis set limit. Journal of Chemical Physics, 2002, 116, 7372-7379.	1.2	369
5	Basis Set Convergence of Nuclear Magnetic Shielding Constants Calculated by Density Functional Methods. Journal of Chemical Theory and Computation, 2008, 4, 719-727.	2.3	320
6	Polarization consistent basis sets. III. The importance of diffuse functions. Journal of Chemical Physics, 2002, 117, 9234-9240.	1.2	295
7	Structure and stability of C24 and B12N12 isomers. Chemical Physics Letters, 1993, 201, 89-96.	1.2	265
8	Segmented Contracted Basis Sets Optimized for Nuclear Magnetic Shielding. Journal of Chemical Theory and Computation, 2015, 11, 132-138.	2.3	235
9	Unifying General and Segmented Contracted Basis Sets. Segmented Polarization Consistent Basis Sets. Journal of Chemical Theory and Computation, 2014, 10, 1074-1085.	2.3	232
10	Towards An Understanding of the Mechanism of Electron-Capture Dissociation: A Historical Perspective and Modern Ideas. European Journal of Mass Spectrometry, 2002, 8, 337-349.	0.5	227
11	The Basis Set Convergence of Spinâ^'Spin Coupling Constants Calculated by Density Functional Methods. Journal of Chemical Theory and Computation, 2006, 2, 1360-1369.	2.3	223
12	Dissociative capture of hot (3â€“13 eV) electrons by polypeptide polycations: an efficient process accompanied by secondary fragmentation. Chemical Physics Letters, 2002, 356, 201-206.	1.2	184
13	Polarization consistent basis sets. V. The elements Siâ€“Cl. Journal of Chemical Physics, 2004, 121, 3463-3470.	1.2	181
14	Solvent-dependent singlet oxygen lifetimes: temperature effects implicate tunneling and charge-transfer interactions. Physical Chemistry Chemical Physics, 2016, 18, 22946-22961.	1.3	174
15	Atomic orbital basis sets. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 273-295.	6.2	165
16	Estimating the Hartreeâ€”Fock limit from finite basis set calculations. Theoretical Chemistry Accounts, 2005, 113, 267-273.	0.5	148
17	Structure and stability of complexes of glycine and glycine methyl analogs with H+, Li+, and Na+. Journal of the American Chemical Society, 1992, 114, 9533-9537.	6.6	147
18	Reaction of Organic Sulfides with Singlet Oxygen. A Revised Mechanism. Journal of the American Chemical Society, 1998, 120, 4439-4449.	6.6	134

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19	The dipole moment of carbon monoxide. Journal of Chemical Physics, 1991, 94, 6660-6663.	1.2	130
20	Pyrrolo-Annelated Tetrathiafulvalenes:Â The Parent Systems. Journal of Organic Chemistry, 2000, 65, 5794-5805.	1.7	129
21	The optimum contraction of basis sets for calculating spinâ€“spin coupling constants. Theoretical Chemistry Accounts, 2010, 126, 371-382.	0.5	125
22	Synthesis, computational study and cytotoxic activity of new 4-hydroxycoumarin derivatives. European Journal of Medicinal Chemistry, 2008, 43, 694-706.	2.6	117
23	Cross-trienamines in Asymmetric Organocatalysis. Journal of the American Chemical Society, 2012, 134, 12943-12946.	6.6	117
24	Polarization Consistent Basis Sets. 4:â€‰ The Elements He, Li, Be, B, Ne, Na, Mg, Al, and Ar. Journal of Physical Chemistry A, 2007, 111, 11198-11204.	1.1	105
25	Overview of Theoretical and Computational Methods Applied to the Oxygenâ€“Organic Molecule Photosystem. Photochemistry and Photobiology, 2006, 82, 1136.	1.3	104
26	Describing Anions by Density Functional Theory: Fractional Electron Affinity. Journal of Chemical Theory and Computation, 2010, 6, 2726-2735.	2.3	104
27	Phenyl Radical, Cation, and Anion. The Tripletâ^'Singlet Gap and Higher Excited States of the Phenyl Cation. Journal of the American Chemical Society, 1997, 119, 8083-8088.	6.6	103
28	Transition structures for the Claisen rearrangement. Journal of the American Chemical Society, 1988, 110, 2314-2315.	6.6	98
29	Reaction of 4-phenyl-1,2,4-triazoline-3,5-dione with substituted butadienes. A nonconcerted Diels-Alder reaction. Journal of the American Chemical Society, 1987, 109, 6376-6385.	6.6	97
30	Enantioselective Formal [4+2] Cycloadditions to 3â€Nitroindoles by Trienamine Catalysis: Synthesis of Chiral Dihydrocarbazoles. Angewandte Chemie - International Edition, 2016, 55, 1020-1024.	7.2	94
31	Polarization consistent basis sets. IV. The basis set convergence of equilibrium geometries, harmonic vibrational frequencies, and intensities. Journal of Chemical Physics, 2003, 118, 2459.	1.2	93
32	New extended .pi.-electron donors. Tetrathiafulvalene systems with heterocyclic spacer groups. Journal of the American Chemical Society, 1992, 114, 5035-5039.	6.6	92
33	Organocatalytic Asymmetric 1,6â€Addition/1,4â€Addition Sequence to 2,4â€Dienals for the Synthesis of Chiral Chromans. Angewandte Chemie - International Edition, 2015, 54, 8203-8207.	7.2	92
34	Anticancer thiopyrano[2,3-d][1,3]thiazol-2-ones with norbornane moiety. Synthesis, cytotoxicity, physico-chemical properties, and computational studies. Bioorganic and Medicinal Chemistry, 2006, 14, 5230-5240.	1.4	90
35	Supramolecular Receptor Design: Anion-Triggered Binding of C60. Angewandte Chemie - International Edition, 2006, 45, 6848-6853.	7.2	90
36	A remarkable large effect of spin contamination on calculated vibrational frequencies. Chemical Physics Letters, 1990, 169, 519-528.	1.2	87

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37	Synthesis of 5â€(1,2,3â€Triazolâ€4â€yl)â€2â€²â€deoxyuridines by a Click Chemistry Approach: Stacking of Triazoles in the Major Groove Gives Increased Nucleic Acid Duplex Stability. ChemBioChem, 2007, 8, 2106-2116.	1.3	81
38	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. International Journal of Quantum Chemistry, 2007, 107, 1390-1395.	1.0	81
39	The basis set convergence of the Hartreeâ€“Fock energy for H2. Journal of Chemical Physics, 1999, 110, 6601-6605.	1.2	80
40	Enantioselective Formal [4+2] Cycloadditions to 3â€Nitroindoles by Trienamine Catalysis: Synthesis of Chiral Dihydrocarbazoles. Angewandte Chemie, 2016, 128, 1032-1036.	1.6	80
41	Optimization of augmentation functions for correlated calculations of spin-spin coupling constants and related properties. Journal of Chemical Physics, 2008, 129, 064111.	1.2	78
42	The magnitude of intramolecular basis set superposition error. Chemical Physics Letters, 1996, 261, 633-636.	1.2	76
43	Theoretical Investigations and Density Functional Theory Based Quantitative Structureâ€“Activity Relationships Model for Novel Cytotoxic Platinum(IV) Complexes. Journal of Medicinal Chemistry, 2013, 56, 330-344.	2.9	76
44	Locating transition structures by mode following: A comparison of six methods on the Ar8 Lennardâ€Jones potential. Journal of Chemical Physics, 1995, 102, 6706-6718.	1.2	73
45	Transition states from empirical force fields. Theoretical Chemistry Accounts, 2003, 109, 1-7.	0.5	71
46	Pyrrolo Annelated Tetrathiafulvalenes:Â The Parent Systems. Organic Letters, 1999, 1, 1291-1294.	2.4	70
47	Structure factors for tunneling ionization rates of molecules. Physical Review A, 2013, 87, .	1.0	70
48	Observation of laser-induced electronic structure in oriented polyatomic molecules. Nature Communications, 2015, 6, 7039.	5.8	68
49	An Atomic Counterpoise Method for Estimating Inter- and Intramolecular Basis Set Superposition Errors. Journal of Chemical Theory and Computation, 2010, 6, 100-106.	2.3	66
50	Crown ether annelated tetrathiafulvalenes. 2. Journal of Organic Chemistry, 1993, 58, 1359-1366.	1.7	65
51	Force Field Modeling of Amino Acid Conformational Energies. Journal of Chemical Theory and Computation, 2007, 3, 1774-1788.	2.3	65
52	Electron capture dissociation of weakly bound polypeptide polycationic complexes. Rapid Communications in Mass Spectrometry, 2002, 16, 2260-2265.	0.7	64
53	Steric Effects in SN2 Reactions. The Influence of Microsolvation. Journal of Physical Chemistry A, 2001, 105, 3259-3268.	1.1	62
54	Gradient extremal bifurcation and turning points: An application to the H2CO potential energy surface. Journal of Chemical Physics, 1996, 104, 8025-8031.	1.2	61

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55	Probing Basis Set Requirements for Calculating Core Ionization and Core Excitation Spectroscopy by the Î” Self-Consistent-Field Approach. Journal of Chemical Theory and Computation, 2019, 15, 325-337.	2.3	58
56	Two Classes of Alongside Charge-Transfer Interactions Defined in One [2]Catenane. Journal of the American Chemical Society, 2007, 129, 7354-7363.	6.6	54
57	Do rotational barriers dictate the regioselectivity in the ene reactions of singlet oxygen and triazolinedione with alkenes?. Journal of the American Chemical Society, 1991, 113, 3180-3181.	6.6	53
58	Influence of basis sets and electron correlation on theoretically predicted infrared intensities. The Journal of Physical Chemistry, 1989, 93, 4495-4502.	2.9	52
59	Transition State Looseness and Î±-Secondary Kinetic Isotope Effects. Journal of the American Chemical Society, 1997, 119, 227-232.	6.6	52
60	Synthesis of ent-BE-43547A1 reveals a potent hypoxia-selective anticancer agent and uncovers the biosynthetic origin of the APD-CLD natural products. Nature Chemistry, 2017, 9, 264-272.	6.6	52
61	A theoretical study of steric effects in SN2 reactions. Chemical Physics Letters, 1992, 196, 368-376.	1.2	50
62	A Novel Class of Bis- and Tris-Chelate Diam(m)inebis(dicarboxylato)platinum(IV) Complexes as Potential Anticancer Prodrugs. Journal of Medicinal Chemistry, 2014, 57, 6751-6764.	2.9	49
63	A Theoretical Study of the Allene Effect in [1,n] Sigmatropic Hydrogen Shifts. Journal of the American Chemical Society, 1995, 117, 7487-7492.	6.6	46
64	Comprehensive Analysis of Energy Minima of the 20 Natural Amino Acids. Journal of Physical Chemistry A, 2014, 118, 7876-7891.	1.1	46
65	Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model. Journal of Chemical Physics, 2010, 133, 044104.	1.2	44
66	Polarization consistent basis sets. VII. The elements K, Ca, Ga, Ge, As, Se, Br, and Kr. Journal of Chemical Physics, 2012, 136, 114107.	1.2	44
67	Structure and spectra of chlorine oxide dimers. The Journal of Physical Chemistry, 1990, 94, 2235-2237.	2.9	43
68	The stability of cage and ring isomers for carbon and boron nitride clusters. Chemical Physics Letters, 1993, 209, 417-422.	1.2	43
69	Electrostatic Potential of Insulin: Exploring the Limitations of Density Functional Theory and Force Field Methods. Journal of Chemical Theory and Computation, 2013, 9, 3978-3985.	2.3	42
70	Role of Multi-Electron Effects in the Asymmetry of Strong-Field Ionization and Fragmentation of Polar Molecules: The Methyl Halide Series. Journal of Physical Chemistry A, 2015, 119, 11772-11782.	1.1	42
71	Locating minima on seams of intersecting potential energy surfaces. An application to transition structure modeling. Journal of the American Chemical Society, 1992, 114, 1596-1603.	6.6	40
72	Correlated transition structure for the 1,5-sigmatropic hydrogen shift. Journal of the American Chemical Society, 1987, 109, 3139-3140.	6.6	38

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73	The basis set convergence of the Hartree-Fock energy for H 3 + , Li 2 and N 2. Theoretical Chemistry Accounts, 2000, 104, 484-490.	0.5	38
74	Reaction of organic sulfides with singlet oxygen. A theoretical study including electron correlation. Journal of Organic Chemistry, 1992, 57, 6478-6487.	1.7	36
75	Efficient RNA-targeting by the introduction of aromatic stacking in the duplex major groove via 5-(1-phenyl-1,2,3-triazol-4-yl)-2â€²-deoxyuridines. Bioorganic and Medicinal Chemistry, 2010, 18, 4702-4710.	1.4	36
76	Duplex and Triplex Formation of Mixed Pyrimidine Oligonucleotides with Stacking of Phenyl-triazole Moieties in the Major Groove. Journal of Organic Chemistry, 2011, 76, 6177-6187.	1.7	35
77	Kinetic Isotope Effects and Transition State Geometries. A Theoretical Investigation of E2 Model Systems. Journal of Organic Chemistry, 1997, 62, 253-260.	1.7	33
78	Chemistry of singlet oxygen. 49. Photooxidation of thiiranes. Journal of the American Chemical Society, 1987, 109, 1478-1485.	6.6	31
79	Energies and properties of ions involved in electrophilic halogenations: singlet and triplet states of halogen cations (X+, X3+, and X42+) and hydrohalonium ions (HX2+ and H2X+). Journal of the American Chemical Society, 1990, 112, 3922-3926.	6.6	31
80	C24: Ring or fullerene?. Journal of Chemical Physics, 1998, 108, 3213-3217.	1.2	31
81	Transition structure modeling by intersecting potential energy surfaces. Journal of Computational Chemistry, 1994, 15, 1199-1216.	1.5	30
82	The effect of different density functional methods on basis set parameters. Chemical Physics Letters, 2005, 402, 510-513.	1.2	30
83	Systematic Improvement of Potential-Derived Atomic Multipoles and Redundancy of the Electrostatic Parameter Space. Journal of Chemical Theory and Computation, 2014, 10, 5493-5504.	2.3	30
84	The accuracy of local MP2 methods for conformational energies. Molecular Physics, 2008, 106, 1899-1906.	0.8	29
85	Organocatalytic Asymmetric 1,6â€Addition/1,4â€Addition Sequence to 2,4â€Dienals for the Synthesis of Chiral Chromans. Angewandte Chemie, 2015, 127, 8321-8325.	1.6	29
86	Enantioselective Organocatalytic Cascade Approach to Different Classes of Benzofused Acetals. Chemistry - A European Journal, 2016, 22, 16810-16818.	1.7	28
87	Attosecond transient absorption spectroscopy of molecular nitrogen: Vibrational coherences in the bâ€² 1Î£+u state. Chemical Physics Letters, 2017, 683, 408-415.	1.2	28
88	How Large is the Elephant in the Density Functional Theory Room?. Journal of Physical Chemistry A, 2017, 121, 6104-6107.	1.1	28
89	Inference of Transition State Geometries from Kinetic Isotope Effects: An Ab Initio Study of an E2 Model System. Journal of the American Chemical Society, 1994, 116, 9302-9310.	6.6	27
90	Method Calibration or Data Fitting?. Journal of Chemical Theory and Computation, 2018, 14, 4651-4661.	2.3	27

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91	Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. Journal of Chemical Theory and Computation, 2012, 8, 4425-4433.	2.3	26
92	Polarization consistent basis sets. VIII. The transition metals Sc-Zn. Journal of Chemical Physics, 2013, 138, 014107.	1.2	26
93	Application of the weak-field asymptotic theory to tunneling ionization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:math>. Physical Review A, 2014, 89, .	1.0	26
94	On the accuracy of numerical Hartree?Fock energies. Theoretical Chemistry Accounts, 2005, 113, 187-190.	0.5	25
95	Reaction of singlet oxygen with organic sulfides. A theoretical study. Journal of the American Chemical Society, 1988, 110, 2368-2375.	6.6	24
96	Photomagnetic Switching of Heterometallic Complexes [M(dmf)₄(H₂O)₃(Î¼â€CN)Fe(CN)₅]â‹…H₂O (M=Nd,) Tj ETQq0 0 0 rg Journal, 2010, 16, 7215-7223.	1.7	24
97	Dynamic resolution of 2-cyclohexylidene acetaldehydes through organocatalytic dienamine [4+2] cycloaddition. Chemical Communications, 2016, 52, 7153-7156.	2.2	24
98	Squeezing the [Cuâˆ’OHÂ·Â·Â·H2Oâˆ’Cu]3+ Bridge by Cryptate Encapsulation. Inorganic Chemistry, 2005, 44, 5987-5989.	1.9	23
99	Controlled formation and topologies of thiophenolate-based macrocycles: rings, cylinders and bowls. Dalton Transactions, 2006, , 108-120.	1.6	23
100	On the photostability of peptides after selective photoexcitation of the backbone: prompt versus slow dissociation. Physical Chemistry Chemical Physics, 2014, 16, 15831-15838.	1.3	22
101	Development of polarization consistent basis sets for spin-spin coupling constant calculations for the atoms Li, Be, Na, and Mg. Journal of Chemical Physics, 2018, 149, 044117.	1.2	22
102	Describing Molecular Polarizability by a Bond Capacity Model. Journal of Chemical Theory and Computation, 2019, 15, 3093-3107.	2.3	22
103	The walk rearrangement in bicyclo[2.1.0]pent-2-ene. An MCSCF study. Journal of the American Chemical Society, 1989, 111, 4643-4647.	6.6	20
104	Improved radical stabilization energies. Journal of Organic Chemistry, 1991, 56, 884-885.	1.7	20
105	Harmonic Vibrational Analysis in Delocalized Internal Coordinates. Journal of Chemical Theory and Computation, 2011, 7, 223-230.	2.3	20
106	Modeling the Effect of Solvents on Nonradiative Singlet Oxygen Deactivation: Going beyond Weak Coupling in Intermolecular Electronic-to-Vibrational Energy Transfer. Journal of Physical Chemistry B, 2020, 124, 2245-2254.	1.2	20
107	CHEMISTRY OF SINGLET OXYGENâ€”48. ISOLATION and STRUCTURE OF THE PRIMARY PRODUCT OF PHOTOOXYGENATION OF 3,5â€Dâ€tâ€BUTYL CATECHOL. Photochemistry and Photobiology, 1987, 46, 325-330.	1.3	19
108	A general procedure for obtaining wave functions obeying the virial theorem. Journal of Computational Chemistry, 1991, 12, 1089-1096.	1.5	19

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109	Using force fields methods for locating transition structures. Journal of Chemical Physics, 2003, 119, 8804-8808.	1.2	19
110	Basis Set and Correlation Effects on Transition State Geometries and Kinetic Isotope Effects. The Journal of Physical Chemistry, 1996, 100, 16892-16898.	2.9	18
111	Stationary points on the H 2 CO potential energy surface: dependence on theoretical level. Theoretical Chemistry Accounts, 1998, 99, 295-300.	0.5	18
112	The basis set convergence of the density functional energy for H2. Chemical Physics Letters, 2000, 317, 400-403.	1.2	18
113	Probing basis set requirements for calculating hyperfine coupling constants. Journal of Chemical Physics, 2019, 151, 174107.	1.2	18
114	AM1 calculations of substituent effects in retro-Diels-Alder reactions. Journal of Organic Chemistry, 1990, 55, 1034-1040.	1.7	17
115	Ring Strain Effects on the Interconversion of Intermediates in the Reaction of Organic Sulfides with Singlet Oxygen. Journal of Organic Chemistry, 1996, 61, 4107-4110.	1.7	17
116	Donor strength of Ï€-extended tetrathiafulvalenes: ionisation energies vs. oxidation potentials. A joint theoretical and experimental study. Journal of Materials Chemistry, 2004, 14, 1768-1773.	6.7	17
117	Modeling chemical reactions for conformationally mobile systems with force field methods. Journal of Chemical Physics, 2003, 118, 3523-3531.	1.2	16
118	Searching the Force Field Electrostatic Multipole Parameter Space. Journal of Chemical Theory and Computation, 2016, 12, 1824-1832.	2.3	16
119	Structural Investigation of Yeâ€™elimite, Ca₄Al₆O₁₂SO₄, by ²⁷Al MAS and MQMAS NMR at Different Magnetic Fields. Journal of Physical Chemistry C, 2018, 122, 12077-12089.	1.5	16
120	Decay Rate Measurement of the First Vibrationally Excited State of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>MgH</mml:mi><mml:mo mathvariant="bold">+</mml:mo></mml:msup></mml:math>in a Cryogenic Paul Trap. Physical Review Letters, 2013, 111, 053002.	2.9	15
121	Accelerating Kohnâ€Sham response theory using density fitting and the auxiliaryâ€densityâ€matrix method. International Journal of Quantum Chemistry, 2018, 118, e25639.	1.0	15
122	MNDO calculations on tetrathiafulvalenes. Synthetic Metals, 1989, 32, 179-190.	2.1	14
123	Experimental andab InitioComputational Evidence for New Peroxidic Intermediates (Iminopersulfinic) Tj ETQq1 1 0.784314 rgBT /Over American Chemical Society, 1997, 119, 4380-4387.	6.6	14
124	Ab initio study of the nucleophilic ring opening of ethylene oxide. Connection between secondary kinetic isotope effects and transition structures. Journal of the Chemical Society Perkin Transactions II, 1994, , 871.	0.9	13
125	DFT study of the structure and spectral behavior of new pt(II) complexes with 5â€methylâ€5(4â€pyridyl)hydantoin. International Journal of Quantum Chemistry, 2009, 109, 826-836.	1.0	13
126	Conformational Interconversions of Amino Acid Derivatives. Journal of Chemical Theory and Computation, 2016, 12, 694-705.	2.3	13

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127	Structure factors for tunneling ionization rates of molecules: General Hartree-Fock-based integral representation. Physical Review A, 2017, 96, .	1.0	13
128	Probing the Importance of Charge Flux in Force Field Modeling. Journal of Chemical Theory and Computation, 2017, 13, 3715-3721.	2.3	13
129	Probing Basis Set Requirements for Calculating Core Ionization and Core Excitation Spectra Using Correlated Wave Function Methods. Journal of Chemical Theory and Computation, 2021, 17, 2832-2842.	2.3	13
130	Interaction of Amyloid-Î²-(1â€“42) Peptide and Its Aggregates with Lipid/Water Interfaces Probed by Vibrational Sum-Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 11208-11218.	1.2	13
131	Laser-induced Coulomb-explosion imaging of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml dimer: The effect of non-Coulombic interactions. Physical Review A, 2020, 102, .	1.0	13
132	Influence of Substituents on Kinetic Isotope Effects. Journal of the American Chemical Society, 1996, 118, 10577-10583.	6.6	12
133	Experimental and Computational Evidence for the Formation of Iminopersulfinic Acids. Journal of Organic Chemistry, 1998, 63, 3397-3402.	1.7	12
134	The same number of optimized parameters scheme for determining intermolecular interaction energies. Journal of Chemical Physics, 2015, 142, 114116.	1.2	12
135	Structure factors for tunneling ionization rates of molecules: General grid-based methodology and convergence studies. Journal of Chemical Physics, 2018, 149, 164107.	1.2	12
136	Conformations of Glycolic Acid.. Acta Chemica Scandinavica, 1997, 51, 439-441.	0.7	12
137	The structure of higher homologues of 1,6,6aÎ»4-trithiapentalenes the question of no-bond-single-bond-resonance in five sulfuratom homologues. Tetrahedron, 2003, 59, 10255-10259.	1.0	11
138	Contracted basis sets for density functional calculations: Segmented versus general contraction. Journal of Chemical Physics, 2005, 122, 074111.	1.2	11
139	The primary photo-dissociation dynamics of carboxylate anions in aqueous solution: decarboxylation. Physical Chemistry Chemical Physics, 2019, 21, 7358-7366.	1.3	11
140	Tungsten Iodide Clusters as Singlet Oxygen Photosensitizers: Exploring the Domain of Resonant Energy Transfer at 1 eV. Journal of Physical Chemistry A, 2019, 123, 1730-1739.	1.1	11
141	Nucleophilic tele-substitution in 2-chloro-3-formylindoles via ring openingâ€“ring closure. Journal of the Chemical Society Chemical Communications, 1988, , 1583-1584.	2.0	10
142	The calculation of electric dipole moments from the polarization propagator. Theory and application. Journal of Chemical Physics, 1989, 91, 364-367.	1.2	10
143	Using atomic charges to model molecular polarization. Physical Chemistry Chemical Physics, 2022, 24, 1926-1943.	1.3	10
144	Influence of the chalcogenocarbonyl group on the structure of heterocyclic analogues of Î²-tricarbonyl compounds. Synthesis and structural features of Schiff bases derived from 3-formyl-4-thio(seleno)coumarin. Journal of the Chemical Society Perkin Transactions II, 1993, , 2423-2428.	0.9	9

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145	A Novel Zeolite-Induced Population of a Planar Viologen Conformation. New Viologen Charge Transfer Complexes and Alkene/Viologen/Zeolite Arrays. Journal of Physical Chemistry B, 2004, 108, 4673-4678.	1.2	9
146	Searching Peptide Conformational Space. Journal of Chemical Theory and Computation, 2011, 7, 1783-1790.	2.3	9
147	Analysis of energy-optimized Gaussian basis sets for condensed phase density functional calculations. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	9
148	Molecular Dynamics Using Nonvariational Polarizable Force Fields: Theory, Periodic Boundary Conditions Implementation, and Application to the Bond Capacity Model. Journal of Chemical Theory and Computation, 2019, 15, 6213-6224.	2.3	9
149	Synthesis and Inhibiting Activity of Some 4-Hydroxycoumarin Derivatives on HIV-1 Protease. ISRN Pharmaceutics, 2011, 2011, 1-9.	1.0	8
150	Using valence bond methods to estimate intramolecular basis set superposition errors. Journal of Chemical Physics, 2017, 146, .	1.2	8
151	Local decomposition of imaginary polarizabilities and dispersion coefficients. Physical Chemistry Chemical Physics, 2017, 19, 20241-20250.	1.3	8
152	Including implicit solvation in the bond capacity polarization model. Journal of Chemical Physics, 2019, 151, 114118.	1.2	8
153	Structure, DFT based investigations on vibrational and nonlinear optical behavior of a new guanidinium cobalt thiocyanate complex. Structural Chemistry, 2020, 31, 103-114.	1.0	8
154	The primary photo-dissociation dynamics of lactate in aqueous solution: decarboxylation prevents dehydroxylation. Physical Chemistry Chemical Physics, 2021, 23, 4555-4568.	1.3	8
155	Force Field Modelling of Conformational Energies. Molecular Simulation, 2004, 30, 801-806.	0.9	7
156	Synthesis and evaluation of galacto-noeurostegine and its 2-deoxy analogue as glycosidase inhibitors. Organic and Biomolecular Chemistry, 2015, 13, 7979-7992.	1.5	7
157	The primary photo-dissociation dynamics of amino acids in aqueous solution: breaking the C_{Î±}-bond. Physical Chemistry Chemical Physics, 2020, 22, 2307-2318.	1.3	7
158	Reactivity of Î±,Ï‰-Dihydrofluoropolyethers toward OH Predicted by Multiconformer Transition State Theory and the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2020, 124, 3460-3470.	1.1	7
159	Geometry Dependence of Spinâ€“Orbit Coupling in Complexes of Molecular Oxygen with Atoms, H2, or Organic Molecules. Journal of Physical Chemistry A, 2022, , .	1.1	7
160	The magnitude of pseudo-potential errors for density functional calculations. Chemical Physics Letters, 2005, 406, 501-503.	1.2	6
161	Locating seam minima for macromolecular systems. Theoretical Chemistry Accounts, 2009, 123, 477-485.	0.5	6
162	Predicting largeâ€scale conformational changes in proteins using energyâ€weighted normal modes. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2778-2793.	1.5	6

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163	Protonation of aqueous alanine by photoionization of water. Physical Chemistry Chemical Physics, 2017, 19, 1560-1570.	1.3	6
164	Experimental and Theoretical Studies on the Reduction of CO2 to CO with Chloro(methyl)disilane Components from the Direct Process. Synlett, 2017, 28, 2439-2444.	1.0	6
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