Wolfram Koch

List of Publications by Year
in descending order

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177 papers	9,481 citations	57758 44 h-index	60623 81 g-index
188 all docs	188 docs citations	188 times ranked	6816 citing authors

#	Article	IF	Citations
1	On the parameterization of the local correlation functional. What is Becke-3-LYP?. Chemical Physics Letters, 1997, 268, 345-351.	2.6	865
2	The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces. Theoretical Chemistry Accounts, 1998, 99, 95-99.	1.4	805
3	A Comparative Computational Study of Cationic Coinage Metalâ˜Ethylene Complexes (C2H4)M+ (M = Cu,) Tj ETQq1 1 0.784314 rgBT /	2.9	209
4	Helium chemistry: theoretical predictions and experimental challenge. Journal of the American Chemical Society, 1987, 109, 5917-5934.	13.7	207
5	How Does Fe+ Activate Câ˜C and Câ˜H Bonds in Ethane? A Theoretical Investigation Using Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6236-6242.	2.9	163
6	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
7	The performance of densityâ€functional/Hartreeâ€“Fock hybrid methods: Cationic transitionâ€metal methyl complexes MCH+3 (M=Scâ€“Cu,La,Hfâ€“Au). Journal of Chemical Physics, 1995, 102, 4931-4941.	3.0	150
8	Relativistic Effects on Bonding in Cationic Transition-Metal-Carbene Complexes: A Density-Functional Study. Journal of the American Chemical Society, 1995, 117, 495-500.	13.7	146
9	SiOH+/HSiO+ and SiOH./HSiO.: gas-phase generation and characterization. A combined neutralization-reionization mass spectrometry and ab initio molecular orbital study. Journal of the American Chemical Society, 1991, 113, 5970-5975.	13.7	136
10	The tert-butyl cation (C4H9+) potential energy surface. Journal of the American Chemical Society, 1993, 115, 259-270.	13.7	126
11	The performance of density functional/Hartree-Fock hybrid methods: the bonding in cationic first-row transition metal methylene complexes. Chemical Physics Letters, 1995, 240, 245-252.	2.6	117
12	Experimental and Theoretical Studies of Gold(I) Complexes Au(L)+ (L = H2O, CO, NH3, C2H4, C3H6, C4H6,) Tj ETQq0 0 0 rgBT /Overlock	2.3	113
13	A Theoretical View on Co+-Mediated Câ˜C and Câ˜H Bond Activations in Ethane. Journal of the American Chemical Society, 1996, 118, 9932-9940.	13.7	104
14	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
15	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
16	On the accuracy of density functionals and their basis set dependence: An extensive study on the main group homonuclear diatomic molecules Li2 to Br2. Journal of Computational Chemistry, 1995, 16, 576-585.	3.3	98
17	RÃ¶ntgenstrukturuntersuchung von Î±â€²(Trimethylsilyl)benzyllithiumÂ·Tetramethylendiamin [C ₆ H ₅ CH(SiMe ₃)LiÂ·TMEDA] und Î±â€²(Phenylthio)â€benzyllithiumÂ·3 Tetrahydrofuran [C ₆ H ₅ CH(SPh)LiÂ·(THF) ₃] â€“ zwei zentralâ€chirale Benzyllithiumâ€Verbindungen. Chemische Berichte, 1991, 124, 543-549.	0.2	95
18	Î±â€Oxygenâ€Substituted Organolithium Compounds and Their Carbenoid Nature: Calculations of the Configurational Stability and of LiCH₂OH Model Structures, Crystal Structure of Diphenyl(trimethylsilyloxy)methyllithium Â· 3 THF, and the Stereochemistry of the (Reverse) Brook Rearrangement. Chemische Berichte, 1992, 125, 2265-2273.	0.2	92

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19	Definitive characterization of the C3H7+ potential energy surface. Journal of the American Chemical Society, 1989, 111, 3479-3480.	13.7	87
20	Observation of the Hammick Intermediate:Â Reduction of the Pyridine-2-ylid Ion in the Gas Phaseâ€. Journal of the American Chemical Society, 1996, 118, 11898-11904.	13.7	84
21	Theory Predicts Triplet Ground-State Organic Silylenes. Journal of the American Chemical Society, 1999, 121, 2623-2624.	13.7	82
22	Substituent effects on neutral and ionized carbon-carbon and carbon-oxygen double bonds and their implications for the stability order of keto/enol tautomers. Journal of the American Chemical Society, 1986, 108, 593-600.	13.7	80
23	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
24	The metal-ligand bond strengths in cationic gold(I) complexes. Application of approximate density functional theory. Chemical Physics Letters, 1995, 236, 194-200.	2.6	79
25	How do coinage metal ions bind to benzene?. Molecular Physics, 1999, 96, 583-591.	1.7	79
26	An ab initio molecular orbital study of the structures and energetics of the neutral and cationic CuO2 and CuNO molecules in the gas phase. Journal of Chemical Physics, 1994, 101, 3898-3905.	3.0	74
27	Relativistic Effects in Cationic Gold(I) Complexes: A Comparative Study of ab Initio Pseudopotential and Density Functional Methods. Organometallics, 1995, 14, 1284-1291.	2.3	73
28	Are there neutral helium compounds which are stable in their ground state?. Chemical Physics Letters, 1986, 132, 330-333.	2.6	70
29	How Unstable are Thiosulfoxides? An ab Initio MO Study of Various Disulfanes RSSR (R = H, Me, Pr, All), Their Branched Isomers R2SS, and the Related Transition States1,2. Journal of the American Chemical Society, 1997, 119, 1990-1996.	13.7	67
30	Structural and Energetical Characterization of Reactive Intermediates Derived from Toluene-Cr(CO)3. Chemistry - A European Journal, 1999, 5, 537-545.	3.3	67
31	The C4H7+ cation. A theoretical investigation. Journal of the American Chemical Society, 1988, 110, 7325-7328.	13.7	59
32	Relativistic effects in the cationic platinum carbene PtCH+2. Journal of Chemical Physics, 1996, 104, 4642-4651.	3.0	58
33	Equilibrium Isotope Effects in Cationic Transition-Metal(I) Ethene Complexes M(C2X4)+with M = Cu, Ag, Au and X = H, D. Organometallics, 2000, 19, 2608-2615.	2.3	58
34	An approximate method for treating spin-orbit effects in platinum. Chemical Physics Letters, 1995, 245, 509-518.	2.6	56
35	Distortion toward bridging accompanying hyperconjugation in a simple tertiary alkyl carbocation. Journal of the American Chemical Society, 1991, 113, 3990-3992.	13.7	55
36	Donor-acceptor interaction and the peculiar structures of dications. Journal of the American Chemical Society, 1986, 108, 5808-5817.	13.7	54

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37	s-Indacene: A Delocalized, Formally Antiaromatic 12 ? Electron System. Angewandte Chemie International Edition in English, 1994, 33, 1192-1194.	4.4	53
38	The ArF+ cation. Is it stable enough to be isolated in a salt?. Journal of the American Chemical Society, 1989, 111, 31-33.	13.7	50
39	The energetical and structural properties of FeO+. An application of multireference perturbation theory. Chemical Physics Letters, 1993, 211, 242-248.	2.6	50
40	Mechanistic Details of the Fe+-Mediated C?C and C?H Bond Activations in Propane: A Theoretical Investigation. Helvetica Chimica Acta, 1996, 79, 1939-1956.	1.6	49
41	Theoretical refinement of the pentaborane (B5H11) structure. Application of IGLO chemical shift calculations. Inorganic Chemistry, 1990, 29, 153-155.	4.0	48
42	The Cl2O2+ Cation:â€‰ Preparation and Structural Investigation of Cl2O2+SbF6- and Cl2O2+Sb2F11-. Journal of the American Chemical Society, 1999, 121, 4379-4384.	13.7	47
43	Hyperconjugative distortions and the cyclopentyl cation structure. Journal of the American Chemical Society, 1989, 111, 5475-5477.	13.7	46
44	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. Chemical Physics Letters, 1997, 278, 391-397.	2.6	45
45	A Mo/llerâ€“Plesset study of the electron affinities of the diatomic hydrides XH (X=Li, B, Be, C, N, O). Journal of Chemical Physics, 1986, 84, 3224-3229.	3.0	44
46	Mechanism of the Fe+ Mediated Cï£¿C and Cï£¿H Bond Activations in Ethane from a Theoretical Viewpoint. Angewandte Chemie International Edition in English, 1995, 34, 2282-2285.	4.4	43
47	Energy Storage as Part of a Secure Energy Supply. ChemBioEng Reviews, 2017, 4, 144-210.	4.4	42
48	Structures and energies of isomeric cyclopentenyl cations. Resolution of the question of anchimeric assistance in cyclopenten-4-yl solvolysis. Journal of the American Chemical Society, 1987, 109, 6953-6957.	13.7	41
49	Quantum chemical study on the equilibrium geometries of S3and Sâ^'3, The electron affinity of S3and the low lying electronic states of Sâ^'3. Journal of Chemical Physics, 1995, 102, 6159-6167.	3.0	40
50	The 7-Norbornadienyl Cation: An NMR/IGLO Validation of its ab initio Structure. Angewandte Chemie International Edition in English, 1989, 28, 1042-1044.	4.4	38
51	Homoconjugation in 7-boranorbornene and 7-boranorbornadiene: comparison with the isoelectronic 7-norbornenyl and 7-norbornadienyl cations. Journal of the American Chemical Society, 1992, 114, 7897-7901.	13.7	38
52	Theoretical investigation of the structures and electron affinities of cyanato and thiocyanato isomers, 2-azallyl, and methanimine. The Journal of Physical Chemistry, 1987, 91, 49-53.	2.9	37
53	A theoretical study of the reaction of ketene radical cation with ethylene: nucleophilic addition or concerted [2 + 1] cycloaddition?. Journal of the American Chemical Society, 1988, 110, 6332-6336.	13.7	37
54	Structure of the 2-norbornyl cation. Journal of the American Chemical Society, 1989, 111, 1527-1528.	13.7	37

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55	The low lying electronic states of Oâ˜3. Journal of Chemical Physics, 1993, 99, 1271-1277.	3.0	37
56	Experimental evidence for the existence of the protonitronium dication (HONO2+) in the gas phase and ab initio molecular orbital calculations of its potential energy surface. Journal of the American Chemical Society, 1993, 115, 6312-6316.	13.7	36
57	Mechanism of the Ta+-Mediated Activation of the Câ˜H Bond in Methane. Organometallics, 1997, 16, 5244-5251.	2.3	36
58	A Quantum Chemical View on the Mechanism of the Ta+-Mediated Coupling of Carbon Dioxide with Methane. Organometallics, 1998, 17, 2344-2351.	2.3	35
59	Structures, stabilities, and bonding in CBe2, C2Be, and C2Be2. Journal of the American Chemical Society, 1986, 108, 5732-5737.	13.7	34
60	Double-bond geometry in norbornene, sesquinorbornenes, and related compounds: a high-level quantum chemical investigation. The Journal of Physical Chemistry, 1993, 97, 10021-10027.	2.9	34
61	CF22+ and CF2+, two unusually stable dications with carbon-fluorine double bonding. Chemical Physics Letters, 1985, 114, 178-181.	2.6	33
62	Structure of the 2-butyl cation. Hydrogen bridged or methyl bridged?. Journal of the American Chemical Society, 1990, 112, 4064-4066.	13.7	33
63	The TpZnâ€“OH/CS2 reaction: theoretical and preparative visualization of an essential bioinorganic reaction path. Chemical Communications, 2000, , 647-648.	4.1	32
64	Combined experimental and ab initio molecular orbital studies on gaseous OHn2+ species (n = 1â€“4). International Journal of Mass Spectrometry and Ion Processes, 1985, 67, 305-306.	1.8	31
65	Mindo/3 and mndo calculations of closed- and open-shell cations containing C, H, N, and O. Journal of Computational Chemistry, 1986, 7, 93-104.	3.3	31
66	The prop-2-yl cation is chiral. Journal of the Chemical Society Chemical Communications, 1989, , 1098-1099.	2.0	31
67	Crossed-Beam Study of Co+(3F4)+Propane: Experiment and Density Functional Theory. Chemistry - A European Journal, 2000, 6, 2232-2245.	3.3	31
68	Theoretical investigations of small multiply charged cations. III. NeN2+. Journal of Chemical Physics, 1990, 92, 2464-2468.	3.0	30
69	Experimental and Theoretical IR Spectra of the 2-Norbornyl Cation. Angewandte Chemie International Edition in English, 1990, 29, 183-185.	4.4	29
70	Spectroscopic Properties of Se2â˜2and Seâ˜2in Cancrinite. Journal of Solid State Chemistry, 1996, 126, 50-54.	2.9	29
71	Ground- and excited-state properties of neutral and anionic selenium dimers and trimers. Physical Review A, 1996, 54, 1979-1993.	2.5	29
72	Gas-phase characterization of the neutral and cationic Si2O2 molecules. A combined experimental and ab initio study. Chemical Physics Letters, 1994, 225, 404-409.	2.6	28

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73	Experimental and theoretical studies on the charge stripping from CH3X+ and CH2XH+? ions (X = F, Cl,) Tj ETQq1 1 0.784314 rgBT /Ove	2.0	27
74	Towards an accurate gold carbonyl binding energy in AuCO+: Basis set convergence and a comparison between density functional and conventional methods. Journal of Chemical Physics, 1998, 108, 3876-3885.	3.0	27
75	Synergy of Theory and Experiment in the Remote Functionalization of Aliphatic Nitriles by â€œBareâ€•Fe(I) and Co(I) Cations in the Gas Phaseâ€. Organometallics, 1997, 16, 3135-3147.	2.3	26
76	Structure and bonding of the remarkable donor-acceptor complexes XBeO (X = NH3, NMe3, CO, N2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.7	26
77	Mass spectrometric and quantum mechanical analysis of gas-phase formation, structure, and decomposition of various b2 ions and their specifically deuterated analogs. Journal of the American Society for Mass Spectrometry, 1998, 9, 1002-1011.	2.8	25
78	Experimental and Theoretical Studies of Small Organic Dications, Molecules with Highly Remarkable Properties. , 1987, , 413-465.		25
79	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25
80	Hydrogen substituted by helium(+): theoretical investigations on the structures and stabilities of He2O2+, He2N2+, and He2C2+. Journal of the Chemical Society Chemical Communications, 1986, , 1095.	2.0	24
81	The CH2+ dication: Metastable or not? A combined theoretical and experimental investigation. Chemical Physics Letters, 1987, 142, 147-152.	2.6	24
82	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. Chemical Physics Letters, 1997, 273, 164-170.	2.6	24
83	Theoretical and experimental studies on the ground state potential energy surface of C2H4O dications. International Journal of Mass Spectrometry and Ion Processes, 1985, 63, 59-82.	1.8	23
84	Experimental and theoretical studies on SiHn2+dications (n= 1â€“5)1. Journal of the Chemical Society Perkin Transactions II, 1986, , 757-760.	0.9	23
85	Confirmation of the H-bridged structure of the 2-butyl cation by comparison of experimental and ab initio IR frequencies. Journal of the Chemical Society Chemical Communications, 1991, , 671-674.	2.0	23
86	Combined experimental and theoretical study of the C-H bond strength and the gas phase acidity of triacetylene, C6H2, and the electron affinity of the C6H. radical. Chemical Physics Letters, 1994, 229, 429-434.	2.6	23
87	CS2Fixation by Carbonic Anhydrase Model SystemsA New Substrate in the Catalytic Cycle. Inorganic Chemistry, 2001, 40, 1006-1013.	4.0	23
88	ChlorophyllaRadical Ions:Â A Density Functional Study. Journal of Physical Chemistry B, 2002, 106, 5281-5288.	2.6	23
89	Theoretical Investigations on Fluorine-Substituted Ethylene Dications C2HnF4-n2+(n = 0-4). Journal of Computational Chemistry, 1986, 7, 406-416.	3.3	21
90	The NHn2+ (n = 1â˜4) dications. A theoretical investigation. International Journal of Mass Spectrometry and Ion Processes, 1986, 68, 49-56.	1.8	21

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91	Electronic spectrum ofS2â^, the electron affinity ofS2, and the binding energies of neutral and anionicS3clusters. Physical Review A, 1995, 52, 1024-1038.	2.5	21
92	Theoretical investigations of small multiply charged cations. II. CNen+ (1â‰nâ‰4). Journal of Chemical Physics, 1987, 86, 5617-5624.	3.0	20
93	Theoretical investigations of small multiply charged cations. I. SiH2+. Journal of Chemical Physics, 1986, 84, 2703-2706.	3.0	19
94	Experimentelles und theoretisches IRâ€Spektrum des 2â€Norbornylâ€Kations. Angewandte Chemie, 1990, 102, 198-200.	2.0	19
95	The lowâ€lying electronic states of protonated C2, CCH+. Journal of Chemical Physics, 1990, 93, 8021-8028.	3.0	19
96	Quantum chemical predictions of the electron affinities of carbon-hydrogen clusters C2nHÂ·, the CH binding energies and the gas phase acidities of polyacetylenes C2nH2forn= 1â€“3. Molecular Physics, 1995, 84, 691-706.	1.7	19
97	Interaction of the Fe+cation with heavy noble gas atoms. Journal of Chemical Physics, 1995, 103, 4551-4561.	3.0	19
98	Density functional study on the mechanism of the Simmonsâ€“Smith reaction. Journal of the Chemical Society Perkin Transactions II, 1996, , 877-881.	0.9	19
99	Massâ€Spectrometric and GAUSSIAN2 Studies of the Diazene (HNNH) and Isodiazene (H₂NN) Molecules and Their Radical Cations. Chemische Berichte, 1993, 126, 2753-2758.	0.2	18
100	A Theoretician's View of the C-F Bond Activation Mediated by the Lanthanide Cations Ce+ and Ho+. Chemistry - A European Journal, 1999, 5, 312-319.	3.3	18
101	A quantum chemical investigation of the unimolecular chemistry of the formic acid radical cation and some of its isomers. International Journal of Mass Spectrometry and Ion Processes, 1986, 73, 187-196.	1.8	17
102	A CASSCF-CI study of the ground and low-lying excited electronic states of C2H+2. Chemical Physics Letters, 1993, 212, 631-636.	2.6	17
103	Combined quantum chemical and mass spectrometric study of [Si,C,H3,O]+isomers. Journal of the Chemical Society Perkin Transactions II, 1996, , 2389-2399.	0.9	17
104	Density Functional Investigation of Reactive Intermediates Derived from Alkyne-Co2(CO)6 Complexes. Chemistry - A European Journal, 2001, 7, 5325-5332.	3.3	17
105	Bacteriochlorophyll a radical cation and anionâ€”calculation of isotropic hyperfine coupling constants by density functional methods. Physical Chemistry Chemical Physics, 2000, 2, 4772-4778.	2.8	16
106	On the regioselectivity of nucleophilic additions to anisole-Cr(CO)3 and related complexes: a density functional study. New Journal of Chemistry, 2001, 25, 446-450.	2.8	16
107	The valence isomers of (CH)8 and (SiH)8: Anab initio MO study. Journal of Computational Chemistry, 1994, 15, 1151-1162.	3.3	15
108	Structural and Energetical Characterization of the Methylbutadieneâ€“Fe(CO)3 Isomers and Related Reactive Intermediates with Quantum Chemical Methods. European Journal of Inorganic Chemistry, 1999, 1999, 1869-1880.	2.0	15

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109	Fluorination effect on the structural properties in benzocyclobutenes and benzocyclobutadienes. International Journal of Quantum Chemistry, 1993, 48, 319-332.	2.0	14
110	Fluorination effect on the structural properties of selected benzocyclopropenes. Journal of the Chemical Society Perkin Transactions II, 1993, , 2195.	0.9	14
111	Structure and stability of the CF32+ dication. International Journal of Mass Spectrometry, 1999, 185-187, 701-706.	1.5	14
112	Ab initio molecular orbital study of the CH3N2+ potential energy surface. Journal of the American Chemical Society, 1986, 108, 5400-5403.	13.7	13
113	1(9)-Homocubene and 9-Homocubylidene: Theoretical Investigation of Structures, Energies, and Rearrangement Reactions. Angewandte Chemie International Edition in English, 1994, 33, 668-670.	4.4	13
114	The tellurium dimer and its anion. Molecular Physics, 1997, 92, 463-470.	1.7	13
115	A study of the low-lying states of CaAr+ and CaKr+. Chemical Physics Letters, 1998, 286, 131-137.	2.6	13
116	The electronic ground state of the NeAr2+ dication. A complete active space SCF/multi-reference CI study. Chemical Physics Letters, 1993, 203, 205-210.	2.6	12
117	Ab initio molecular orbital study on R3SiCO+/R3SiOC+ (R = H or CH3). International Journal of Mass Spectrometry and Ion Processes, 1993, 127, 183-190.	1.8	12
118	Experimental and ab initio molecular orbital studies on CH3O2+.cntdot. dications. Journal of the American Chemical Society, 1985, 107, 2256-2260.	13.7	11
119	Mechanismus der Fe⁺â€vermittelten Câ€Câ€•und Câ€Hâ€Bindungsaktivierung in Ethan aus theoretischer Sicht. Angewandte Chemie, 1995, 107, 2430-2432.	2.0	11
120	The CCl4 dication revisited. International Journal of Mass Spectrometry and Ion Processes, 1986, 72, 313-315.	1.8	10
121	Theoretical predictions of metastable ions with short carbon-helium bonds. International Journal of Mass Spectrometry and Ion Processes, 1986, 74, 133-136.	1.8	10
122	The singlet-triplet splitting of the low-lying electronic states of H2O2+ and a comparison with isoelectronic CH2 and CH22+. Chemical Physics Letters, 1987, 138, 503-508.	2.6	10
123	Evidence that the chlorine fluoride cation (Cl2F+) has an asymmetric bent (Cs) Cl-Cl-F+ structure. Inorganic Chemistry, 1990, 29, 4513-4517.	4.0	10
124	Ground-state potentials for Co+/rare-gas interactions. Molecular Physics, 1996, 89, 473-488.	1.7	10
125	On the origin of the different activation energies for hydrogen additions at the C and O centres of Rî—¸CO+ ions (R = H, CH3): A theoretical interpretation. Chemical Physics Letters, 1984, 105, 490-494.	2.6	9
126	Structures and stabilities of ion/dipole complexes. Computational and Theoretical Chemistry, 1984, 110, 49-59.	1.5	9

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127	Ab initio investigation of the potential energy surfaces of C2H2F2 and C2H2F2+. Journal of Computational Chemistry, 1985, 6, 189-199.	3.3	9
128	Experimental and Theoretical Studies of the Gas-Phase Reactions of "Bare" Iron(I) with Tetralin. Organometallics, 1995, 14, 4409-4414.	2.3	9
129	Heat of formation of the CF2++ dication: a theoretical estimate. International Journal of Mass Spectrometry, 2000, 201, 269-275.	1.5	9
130	Theoretical and experimental studies on the tetrafluoroethylene dication. Journal of the Chemical Society Chemical Communications, 1984, , 1187.	2.0	8
131	Ab initio molecular orbital studies of CH2O2+2 isomers. Chemical Physics Letters, 1986, 125, 443-446.	2.6	8
132	The structures and energies of SiHn2+dications (n= 1â€“5). Journal of the Chemical Society Chemical Communications, 1985, , 1119-1121.	2.0	7
133	The Origin of the Remarkable Regioselectivity of Fe‹sup›+‹/sup›â€Mediated Dehydrogenation in Benzocycloalkenes. Chemistry - A European Journal, 1997, 3, 1315-1323.	3.3	7
134	Quantum Chemical Investigation of the Initial Steps of the Yttrium-Mediated Polymerization of Ethene and Propene. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2000, 626, 392-399.	1.2	7
135	Neutral and cationic hof structures. Chemical Physics Letters, 1984, 105, 659-662.	2.6	6
136	On the formation of doubly charged cation radicals from acetyl and 1-hydroxyvinyl cations in the gas phase. A combined experimental and ab initio study. International Journal of Mass Spectrometry and Ion Processes, 1985, 67, 171-177.	1.8	6
137	Structures and stabilities of C6H3â¨¥6 isomers: an ab initio molecular orbital study. Chemical Physics Letters, 1985, 113, 145-150.	2.6	6
138	Theoretical investigations of the low-lying electronic states of the HeC2+ dication. Chemical Physics Letters, 1987, 139, 149-154.	2.6	6
139	Theoretical challenge to the X-ray structure determination of dichloronitronium ion (â€œinorganic) Tj ETQq1 1 0.784314 rgBT /Overlo	2.6	6
140	Why Does Cp2YH Catalyze the Polymerization of Ethene but Not of Propene?. Organometallics, 2002, 21, 1861-1869.	2.3	6
141	Ten years of Analytical and Bioanalytical Chemistry. Analytical and Bioanalytical Chemistry, 2012, 402, 1-1.	3.7	6
142	Experimental and theoretical evidence for the existence of a stable ketene dication in the gas phase. Journal of the Chemical Society Chemical Communications, 1984, , 1679.	2.0	5
143	Propella[3.4] prismane and its congeners: A MO-theoretical study. Journal of Computational Chemistry, 1995, 16, 31-36.	3.3	5
144	Economical treatments of relativistic effects and electron correlation in WH6. Journal of Computational Chemistry, 1998, 19, 1604-1611.	3.3	5

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145	Gas phase ion chemistry: a fruitful playground for the interplay between experiment and theory. International Journal of Mass Spectrometry, 2000, 201, ix-x.	1.5	5
146	The electronic spectrum of selenium sulfide â€" a theoretical study. Physical Chemistry Chemical Physics, 2000, 2, 2219-2225.	2.8	5
147	The future of academic publishing: TheÂchemistsâ€™ point of view. Information Services and Use, 2015, 35, 137-140.	0.2	5
148	Ethics and chemistry: the role of learned societies, as exemplified by the German chemical societies. Toxicological and Environmental Chemistry, 2016, 98, 1060-1066.	1.2	5
149	The TiP double bond in [Cp2Tip(SiH3)2]. A theoretical investigation. Chemical Physics Letters, 1991, 180, 109-113.	2.6	4
150	FromChem. Eur. J.toChemSusChem: All from ChemPubSoc Europe. ChemSusChem, 2009, 2, 5-5.	6.8	4
151	Introducingâ€¦ Advisory Editors and New Author Profiles at Angewandte Chemie. Angewandte Chemie - International Edition, 2021, 60, 16720-16722.	13.8	4
152	Massenspektrometrischer Nachweis von Aminoacetylen sowie seinem Monoâ€•und Dikation. Angewandte Chemie, 1986, 98, 834-835.	2.0	3
153	A possible explanation why doubly charged NeN2+, but no NeC2+ and NeO2+ were observed in charge-stripping mass spectrometry. International Journal of Mass Spectrometry and Ion Processes, 1988, 82, 335-338.	1.8	3
154	FromChem. Eur. J.toChemSusChem: All from ChemPubSoc Europe. Chemistry - A European Journal, 2009, 15, 11-11.	3.3	3
155	Excellent, Valuable, and Entertaining. Angewandte Chemie - International Edition, 2008, 47, 7170-7170.	13.8	2
156	Exzellent, wertvoll und unterhaltsam. Angewandte Chemie, 2008, 120, 7282-7282.	2.0	2
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