Dieter Cremer

List of Publications by Year
in descending order

Version: 2024-02-01

130 papers	9,011 citations	38742 50 h-index	45317 90 g-index
136 all docs	136 docs citations	136 times ranked	5216 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	Theoretical determination of molecular structure and conformation. 15. Three-membered rings: bent bonds, ring strain, and surface delocalization. Journal of the American Chemical Society, 1985, 107, 3800-3810.	13.7	239
5	Electron correlation and the self-interaction error of density functional theory. Molecular Physics, 2002, 100, 1771-1790.	1.7	202
6	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
7	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
8	Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650.	3.0	161
9	Theoretical determination of molecular structure and conformation. 20. Reevaluation of the strain energies of cyclopropane and cyclobutane carbon-carbon and carbon-hydrogen bond energies, 1,3 interactions, and .sigma.-aromaticity. Journal of the American Chemical Society, 1986, 108, 7467-7477.	13.7	155
10	Identification of the Strongest Bonds in Chemistry. Journal of Physical Chemistry A, 2013, 117, 8981-8995.	2.5	140
11	From Molecular Vibrations to Bonding, Chemical Reactions, and Reaction Mechanism. Current Organic Chemistry, 2010, 14, 1524-1560.	1.6	139
12	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
13	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
14	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
15	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
16	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
17	Some Thoughts about Bond Energies, Bond Lengths, and Force Constants. Journal of Molecular Modeling, 2000, 6, 396-412.	1.8	124
18	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. International Journal of Quantum Chemistry, 2012, 112, 3174-3187.	2.0	121

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19	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
20	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
21	Theoretical determination of molecular structure and conformation. 16. Substituted cyclopropanes - an electron density model of substituent-ring interactions. Journal of the American Chemical Society, 1985, 107, 3811-3819.	13.7	114
22	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
23	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
24	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
25	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
26	Sixth-Order MÃ¸llerâ^'Plesset Perturbation TheoryOn the Convergence of the MPn Series. The Journal of Physical Chemistry, 1996, 100, 6173-6188.	2.9	95
27	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 6845-6862.	2.5	95
28	Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502.	4.0	91
29	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
30	On the diagnostic value of (Åœ2) in Kohn-Sham density functional theory. Molecular Physics, 2001, 99, 981-989.	1.7	89
31	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
32	Direct Measure of Metalâ€“Ligand Bonding Replacing the Tolman Electronic Parameter. Inorganic Chemistry, 2016, 55, 2332-2344.	4.0	85
33	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
34	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
35	Pros and cons of Ïƒ -aromaticity. Tetrahedron, 1988, 44, 7427-7454.	1.9	77
36	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

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37	Unified Reaction Valley Approach Mechanism of the Reaction CH3+ H2â† CH4+ H. Journal of Physical Chemistry A, 1997, 101, 1742-1757.	2.5	73
38	New developments in the analysis of vibrational spectra On the use of adiabatic internal vibrational modes. Theoretical and Computational Chemistry, 1998, , 259-327.	0.4	71
39	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
40	Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. Journal of Physical Chemistry A, 2014, 118, 223-237.	2.5	67
41	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
42	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
43	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
44	New Approach to Tolmanâ€™s Electronic Parameter Based on Local Vibrational Modes. Inorganic Chemistry, 2014, 53, 478-495.	4.0	61
45	Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. Journal of Organic Chemistry, 2016, 81, 9669-9686.	3.2	56
46	What correlation effects are covered by density functional theory?. Molecular Physics, 2000, 98, 1639-1658.	1.7	55
47	Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. Journal of Physical Chemistry A, 2015, 119, 9541-9556.	2.5	54
48	Efficient density-functional theory integrations by locally augmented radial grids. Journal of Chemical Physics, 2007, 127, 164113.	3.0	53
49	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
50	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
51	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
52	p-Benzyne. Angewandte Chemie - International Edition, 1998, 37, 955-958.	13.8	50
53	Super-pnicogen bonding in the radical anion of the fluorophosphine dimer. Chemical Physics Letters, 2016, 662, 182-187.	2.6	49
54	Analysis of coupled cluster methods. II. What is the best way to account for triple excitations in coupled cluster theory?. Theoretica Chimica Acta, 1993, 85, 305-323.	0.8	48

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55	On the physical meaning of the ZORA Hamiltonian. Molecular Physics, 2003, 101, 2295-2302.	1.7	48
56	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
57	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
58	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
59	Representation of the exact relativistic electronic Hamiltonian within the regular approximation. Journal of Chemical Physics, 2003, 119, 11526-11540.	3.0	43
60	Properties of local vibrational modes: the infrared intensity. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	43
61	Description of an unusual hydrogen bond between carborane and a phenyl group. Journal of Organometallic Chemistry, 2018, 865, 114-127.	1.8	42
62	An improved algorithm for the normalized elimination of the small-component method. Theoretical Chemistry Accounts, 2011, 130, 633-644.	1.4	41
63	Are carbonâ€"halogen double and triple bonds possible?. International Journal of Quantum Chemistry, 2014, 114, 1060-1072.	2.0	41
64	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
65	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
66	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
67	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
68	Accurate determination of the binding energy of the formic acid dimer: The importance of geometry relaxation. Journal of Chemical Physics, 2014, 140, 084315.	3.0	39
69	Analytical energy gradient for the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2015, 142, 214106.	3.0	39
70	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
71	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
72	Analytic energy derivatives for regular approximations of relativistic effects applicable to methods with and without correlation corrections. Journal of Chemical Physics, 2003, 118, 6741-6750.	3.0	36

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73	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
74	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
75	Photochemistry of p-Benzoquinone Diazide Carboxylic Acids:â€‰ Formation of 2,4-Didehydrophenols. Journal of the American Chemical Society, 1997, 119, 10660-10672.	13.7	34
76	Quantum Chemical Descriptions of FOOF:Â The Unsolved Problem of Predicting Its Equilibrium Geometry. Journal of Physical Chemistry A, 2001, 105, 3269-3276.	2.5	33
77	Structure of the chlorobenzeneâ€“argon dimer: Microwave spectrum andab initioanalysis. Journal of Chemical Physics, 2000, 113, 9051-9059.	3.0	32
78	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
79	Enediynes, enyneâ€allenes, their reactions, and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 285-324.	14.6	32
80	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
81	Kleine Ringe, 78. Triâ€tertâ€butyl(trimethylsilyl)cyclobutadien und Triâ€tertâ€butyl(trimethylsilyl)tetrahedran. Chemische Berichte, 1994, 127, 173-189.	0.2	31
82	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
83	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
84	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
85	Convergence behavior of the Mï¿½ller-Plesset perturbation series: Use of Feenberg scaling for the exclusion of backdoor intruder states. International Journal of Quantum Chemistry, 2000, 76, 306-330.	2.0	29
86	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
87	Sixth-order many-body perturbation theory. IV. Improvement of the Mï¿½ller-Plesset correlation energy series by using Padï¿½, Feenberg, and other approximations up to sixth order. International Journal of Quantum Chemistry, 1996, 59, 71-95.	2.0	28
88	Mechanism and dynamics of organic reactions: 1,2-H shift in methylchlorocarbene. Journal of Physical Organic Chemistry, 2002, 15, 431-447.	1.9	28
89	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
90	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

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91	The Peculiar Role of the Au₃ Unit in Au_m Clusters: Ïƒ-Aromaticity of the Au₅Zn⁺ Ion. Inorganic Chemistry, 2017, 56, 5793-5803.	4.0	27
92	Diabatic ordering of vibrational normal modes in reaction valley studies. Journal of Computational Chemistry, 1997, 18, 1282-1294.	3.3	26
93	Photochemistry of Butatriene â^' Spectroscopic Evidence for the Existence of Allenylcarbeneâ€. Journal of Physical Chemistry A, 2000, 104, 3819-3825.	2.5	26
94	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
95	Bonding in radon hexafluoride: An unusual relativistic problem?. Physical Chemistry Chemical Physics, 2003, 5, 1103-1105.	2.8	25
96	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
97	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. Chirality, 2013, 25, 185-196.	2.6	25
98	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
99	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
100	Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis. Journal of Chemical Theory and Computation, 2018, 14, 2558-2569.	5.3	23
101	2,4-Didehydrophenol?First Proof of ameta-Aryne by IR Spectroscopy. Angewandte Chemie International Edition in English, 1992, 31, 1230-1233.	4.4	22
102	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
103	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
104	Sixth-order many-body perturbation theory. II. Implementation and application. International Journal of Quantum Chemistry, 1996, 59, 31-55.	2.0	21
105	Relativistically corrected nuclear magnetic resonance chemical shifts calculated with the normalized elimination of the small component using an effective potential-NMR chemical shifts of molybdenum and tungsten. Journal of Chemical Physics, 2003, 119, 701-712.	3.0	21
106	Bonding in the ClOO(2Aâ€³) and BrOO(2Aâ€³) radical: Nonrelativistic single-reference versus relativistic multi-reference descriptions in density functional theory. Physical Chemistry Chemical Physics, 2003, 5, 2320-2326.	2.8	20
107	Vibrational Properties of the Isotopomers of the Water Dimer Derived from Experiment and Computations. Australian Journal of Chemistry, 2014, 67, 426.	0.9	20
108	General and Theoretical Aspects of the Cyclopropyl Group. , 0, , 43-137.		19

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109	Sixth-order many-body perturbation theory. III. Correlation energies of size-extensive MP6 methods. International Journal of Quantum Chemistry, 1996, 59, 57-69.	2.0	19
110	Comparison of CCSDT- n methods with coupled-cluster theory with single and double excitations and coupled-cluster theory with single, double, and triple excitations in terms of many-body perturbation theory - what is the most effective triple-excitation method?. Theoretical Chemistry Accounts, 2001, 105, 182-196.	1.4	19
111	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
112	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
113	Application of quadratic CI with singles, doubles, and triples (QCISDT): An attractive alternative to CCSDT. International Journal of Quantum Chemistry, 1996, 57, 157-172.	2.0	16
114	Analysis of fourth-order MÃ¸ller-Plesset limit energies: the importance of three-electron correlation effects. Theoretical Chemistry Accounts, 2000, 105, 110-122.	1.4	16
115	Spin-projected coupled-cluster theory with single and double excitations. Theoretical Chemistry Accounts, 2000, 105, 132-144.	1.4	16
116	A variationally stable quasi-relativistic method: low-order approximation to the normalized elimination of the small component using an effective potential. Theoretical Chemistry Accounts, 2002, 108, 168-178.	1.4	16
117	The microwave spectrum, ab initio analysis, and structure of the fluorobenzeneâ€“hydrogen chloride complex. Journal of Chemical Physics, 2003, 118, 9278-9290.	3.0	16
118	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
119	Cyclopropyl Homoconjugationâ€”Experimental Facts and Interpretations. , 0, , 411-468.		12
120	Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. Journal of Computational Chemistry, 2018, 39, 293-306.	3.3	11
121	Correlation of the Vibrational Spectra of Isotopomers:â€‰ Theory and Application. Journal of Physical Chemistry A, 2003, 107, 10272-10279.	2.5	10
122	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
123	Cyclopropyl Homoconjugation, Homoaromaticity and Homoantiaromaticityâ€”Theoretical Aspects and Analysis. , 0, , 339-410.		9
124	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
125	On the role of single excitations in quasi-degenerate perturbation theory. Theoretical Chemistry Accounts, 1997, 96, 71-74.	1.4	3
126	A new way of analyzing vibrational spectra. I. Derivation of adiabatic internal modes. International Journal of Quantum Chemistry, 1998, 67, 1-9.	2.0	3

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127	Preface: 25th Austin Symposium on Molecular Structure and Dynamics. Journal of Physical Chemistry A, 2015, 119, 1443-1445.	2.5	1
128	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	1
129	p-Benzyne. Angewandte Chemie - International Edition, 1998, 37, 955-958.	13.8	1
130	Atmospheric Formation of OH Radicals and H2O2 from Alkene Ozonolysis under Humid Conditions. , 0, .		1