Zdenek Havlas

List of Publications by Year
in descending order

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169	7,937	61984	54911
papers	citations	43 h-index	84 g-index

178	178	178	5893
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Blue-Shifting Hydrogen Bonds. Chemical Reviews, 2000, 100, 4253-4264.	47.7	1,645
2	The Nature of Improper, Blue-Shifting Hydrogen Bonding Verified Experimentally. Journal of the American Chemical Society, 2001, 123, 12290-12293.	13.7	306
3	Anti-hydrogen bond between chloroform and fluorobenzene. Chemical Physics Letters, 1999, 299, 180-186.	2.6	266
4	The fluoroformâ‹¯ethylene oxide complex exhibits a Câ€“Hâ‹¯O anti-hydrogen bond. Chemical Physics Letters, 1999, 303, 447-452.	2.6	190
5	Theoretical Studies of Metal Ion Selectivity. 1. DFT Calculations of Interaction Energies of Amino Acid Side Chains with Selected Transition Metal Ions (Co2+, Ni2+, Cu2+, Zn2+, Cd2+, and Hg2+). Journal of the American Chemical Society, 2000, 122, 10428-10439.	13.7	179
6	Improper, blue-shifting hydrogen bond. Theoretical Chemistry Accounts, 2002, 108, 325-334.	1.4	178
7	Distorted Molecules: Perturbation Design, Preparation and Structures. Angewandte Chemie International Edition in English, 1992, 31, 550-581.	4.4	169
8	Piano-stool complexes of the CpML4 type. Organometallics, 1982, 1, 180-188.	2.3	155
9	Verzerrte MolekÃ¼le: StÃ¶rungsdesign, Synthesen und Strukturen. Angewandte Chemie, 1992, 104, 564-595.	2.0	140
10	Improper, Blue-Shifting Hydrogen Bond between Fluorobenzene and Fluoroform. Journal of Physical Chemistry A, 2001, 105, 5560-5566.	2.5	138
11	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	2.1	134
12	Racemization Barriers of 1,1â€˜-Binaphthyl and 1,1â€˜-Binaphthalene-2,2â€˜-diol:Â A DFT Study. Journal of Organic Chemistry, 2003, 68, 5677-5680.	3.2	132
13	Counterpoise-corrected potential energy surfaces of simple H-bonded systems. Theoretical Chemistry Accounts, 1998, 99, 372-377.	1.4	125
14	Toward Designed Singlet Fission: Solution Photophysics of Two Indirectly Coupled Covalent Dimers of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry B, 2013, 117, 4680-4695.	2.6	117
15	An Experimental and Theoretical Study of Stereoselectivity of Furanâ^'Maleic Anhydride and Furanâ^'Maleimide Dielsâ^'Alder Reactions. Journal of Organic Chemistry, 2005, 70, 6295-6302.	3.2	107
16	Search for a Small Chromophore with Efficient Singlet Fission: Biradicaloid Heterocycles. Journal of the American Chemical Society, 2012, 134, 14624-14631.	13.7	99
17	Toward Designed Singlet Fission: Electronic States and Photophysics of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry A, 2010, 114, 1457-1473.	2.5	98
18	Study of the Nature of Improper Blue-Shifting Hydrogen Bonding and Standard Hydrogen Bonding in the X3CHâ‹…â‹…â‹…OH2 and XHâ‹…â‹…â‹…OH2 Complexes (X=F, Cl, Br, I): A Correlated Ab Initio Study. ChemPhysChem, 2002, 3, 511.	2.6	90

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19	Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission. Journal of the American Chemical Society, 2015, 137, 165-172.	13.7	87
20	Crystal Structure ofn-Bu3Sn+CB11Me12-. Journal of the American Chemical Society, 2000, 122, 10253-10254.	13.7	85
21	Two Thin Film Polymorphs of the Singlet Fission Compound 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry C, 2014, 118, 12121-12132.	3.1	85
22	Triisopropylamine: A Sterically Overcrowded Molecule with a Flattened NC3 Pyramid and aâ€œp-Typeâ€• Nitrogen Electron Pair. Angewandte Chemie International Edition in English, 1991, 30, 187-190.	4.4	83
23	On the Convergence of the Physicochemical Properties of [n]Helicenes. Journal of Physical Chemistry C, 2007, 111, 14948-14955.	3.1	79
24	Pentaisopropylcyclopentadienyl: singlet anion, doublet radical, and triplet cation of a carbocyclic .pi. system. Journal of the American Chemical Society, 1993, 115, 12003-12009.	13.7	73
25	The Sixteen CB11HnMe12-n-Anions with Fivefold Substitution Symmetry:Â Anodic Oxidation and Electronic Structure. Journal of the American Chemical Society, 2007, 129, 12960-12980.	13.7	68
26	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. Helvetica Chimica Acta, 1984, 67, 1-17.	1.6	67
27	Thermochemistry of unstable enols: the O-(Cd)(H) group equivalent. Journal of Organic Chemistry, 1986, 51, 4066-4067.	3.2	65
28	Solvent-Shared and Solvent-Separated Ion Multiples of Perylene Radical Anions and Dianions:Â An Exemplary Case of Alkali Metal Cation Solvation. Organometallics, 1998, 17, 4707-4715.	2.3	65
29	Single crystals of an ionic anthracene aggregate with a triplet ground state. Nature, 2000, 404, 267-269.	27.8	63
30	Diprotonated Tetra(2-pyridyl)pyrazine and its Chemical Mimesis due to Different Hydrogen Bridges. Angewandte Chemie International Edition in English, 1992, 31, 299-301.	4.4	62
31	Metal Cationâ^'Methyl Interactions in CB11Me12-Salts of Me3Ge+, Me3Sn+, and Me3Pb+. Journal of the American Chemical Society, 2004, 126, 12033-12046.	13.7	62
32	Ether-Solvated Sodium Ions in Salts Containingï€-Hydrocarbon Anions: Crystallization, Structures, and Semiempirical Solvation Energies. Angewandte Chemie International Edition in English, 1994, 33, 875-878.	4.4	60
33	Efficiency of a second-generation HIV-1 protease inhibitor studied by molecular dynamics and absolute binding free energy calculations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 279-293.	2.6	60
34	Theoretical Studies of Metal Ion Selectivity.â€ 2. DFT Calculations of Complexation Energies of Selected Transition Metal Ions (Co2+, Ni2+, Cu2+, Zn2+, Cd2+, and Hg2+) in Metal-Binding Sites of Metalloproteins. Journal of Physical Chemistry A, 2002, 106, 3855-3866.	2.5	59
35	Tetraphenylallylsodium Diethyl Ether: A Contact Ion Pair with an Intramolecular NaâŠ• Sandwich. Angewandte Chemie International Edition in English, 1990, 29, 1042-1044.	4.4	50
36	[{Na+(thf)2}4(rubrene4â^')]: Crystallization and Structure Determination of a Contact-Ion Quintuple for the Firstï€-Hydrocarbon Tetraanion. Angewandte Chemie International Edition in English, 1996, 35, 631-632.	4.4	50

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37	Structural Changes on Twofold Oxidation of Tetrakis(dimethylamino)-p-benzoquinone: A Sterically Overcrowded Electron-Richâ€œChairâ€•Compound Turns into aâ€œTwistâ€•Dicyanine Salt. Angewandte Chemie International Edition in English, 1991, 30, 1180-1183.	4.4	49
38	Thianthrenâ€Radikalkationâ€Tetrachloroaluminat. Chemische Berichte, 1994, 127, 2043-2049.	0.2	49
39	Sexual Attraction in the Silkworm Moth. Chemistry and Biology, 2003, 10, 331-340.	6.0	48
40	Novel Acyclic Nucleoside Phosphonate Analogues with Potent Anti-Hepatitis B Virus Activities. Antimicrobial Agents and Chemotherapy, 2005, 49, 1177-1180.	3.2	48
41	Etherâ€umhÃ¼llte Natriumâ€Ionen in Salzen mit Ï€â€Kohlenwasserstoffâ€Anionen: Kristallisation, Strukturen und semiempirische Solvatationsenergien,. Angewandte Chemie, 1994, 106, 931-934.	2.0	45
42	Tetrakis(dimethylamino)ethene: An Extremely Electron-Rich Molecule with Unusual Structure both in the Crystal and in the Gas Phase. Angewandte Chemie International Edition in English, 1991, 30, 1678-1681.	4.4	44
43	Electron Binding to Nucleic Acid Bases. Experimental and Theoretical Studies. A Review. Collection of Czechoslovak Chemical Communications, 2004, 69, 1395-1428.	1.0	43
44	HCB11(CF3)nF11-nâˆ': Inert Anions with High Anodic Oxidation Potentials. Journal of the American Chemical Society, 2011, 133, 4123-4131.	13.7	43
45	Tetraphenylbutadiene disodium dimethoxyethane: solvent-shared and solvent-separated ion triples within a single crystal. Journal of the American Chemical Society, 1992, 114, 6907-6908.	13.7	42
46	Competing Na+ Solvation: Ether-Shared and Ether-Separated Triple Ions of Perylene Dianion. Journal of the American Chemical Society, 1995, 117, 3869-3870.	13.7	40
47	Ab Initio Calculations of Monosubstituted (CH3OH, CH3SH, NH3) Hydrated Ions of Zn2+and Ni2+. Journal of Physical Chemistry A, 1999, 103, 1634-1639.	2.5	40
48	Theoretical Studies of Metal Ion Selectivity. 3. A Theoretical Design of the Most Specific Combinations of Functional Groups Representing Amino Acid Side Chains for the Selected Metal Ions (Co2+, Ni2+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	40
49	Guidance for Mutual Disposition of Chromophores for Singlet Fission. Israel Journal of Chemistry, 2016, 56, 96-106.	2.3	40
50	Structure and photophysics of indigoids for singlet fission: Cibalackrot. Journal of Chemical Physics, 2019, 151, 184903.	3.0	40
51	Spinâ€Orbit Coupling in Biradicals. 2. Ab Initio Methodology and Application to 1,1-Biradicals:â€‰ Carbene and Silylene. Journal of Physical Chemistry A, 1998, 102, 5681-5692.	2.5	39
52	Using DFT methods for the prediction of the structure and energetics of metal-binding sites in metalloproteins. International Journal of Quantum Chemistry, 2003, 91, 504-510.	2.0	39
53	2,3,6,7-Tetramethoxythianthrene Dication: Anâ€œAromaticâ€Ï€ Systemâ€œGives Up the Ghostâ€• Angewandte Chemie International Edition in English, 1991, 30, 714-716.	4.4	38
54	The Triplet Biradical Tris(3,5-di-tert-butyl-4-oxophenylene)methane: Crystal Structure, and Spin and Charge Distribution. Angewandte Chemie International Edition in English, 1993, 32, 416-418.	4.4	38

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55	The structures of solvent-separated naphthalene and anthracene radical anions. Journal of the Chemical Society Chemical Communications, 1995, .	2.0	38
56	Singlet Fission Rate: Optimized Packing of a Molecular Pair. Ethylene as a Model. Journal of the American Chemical Society, 2019, 141, 17729-17743.	13.7	38
57	CB11Me11Boronium Ylides:Â Carba-closo-dodecaboranes with a Naked Boron Vertex. Journal of the American Chemical Society, 2006, 128, 6089-6100.	13.7	37
58	Ab initio electronic structure of thymine anions. Physical Chemistry Chemical Physics, 2005, 7, 840.	2.8	35
59	Excitation Localization/Delocalization Isomerism in a Strongly Coupled Covalent Dimer of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry A, 2016, 120, 3473-3483.	2.5	34
60	Singlet Fission: Optimization of Chromophore Dimer Geometry. Advances in Quantum Chemistry, 2017, 75, 175-227.	0.8	34
61	Mechanism of the antipodal effect with borane cages. Journal of the Chemical Society Chemical Communications, 1989, , 1859-1861.	2.0	33
62	Structural Distortions in Diiodine-Substituted Unsaturated Hydrocarbons. Chemistry - A European Journal, 1998, 4, 677-685.	3.3	31
63	Interactions in crystals. LXXXIII. The structures of 1,2,4,5-tetrakis(trimethylsilyl)benzene and of its solvent-separated radical anion salt [NaâŠ•(H3COCH2CHn2OCH3)3] [((H3C)3Si)4H2C6Â·âŠ–]. Journal of Organometallic Chemistry, 1995, 499, 63-71.	1.8	30
64	The CH â‹¯ O hydrogen bond adduct of two trinitromethanes to dioxane. Journal of the Chemical Society Chemical Communications, 1993, , 1792-1793.	2.0	28
65	The Li+-Initiated Twofold Dehydrogenation and Câ^'C Bond Formation of Hexaphenylbenzene to the Dilithium Salt of the 9,10-Diphenyltetrabenz[a,c,h,j]anthracene Dianion. Angewandte Chemie - International Edition, 1999, 38, 2240-2243.	13.8	28
66	Diprotoniertes Tetra(2â€pyridyl)pyrazin und seine chemische Mimese mit unterschiedlichen WasserstoffbrÃ¼cken. Angewandte Chemie, 1992, 104, 348-350.	2.0	27
67	Single-Crystal Structure of the Solvent-Separated Radical Ion Pair [9,10-diphenylanthracene.âŠ–][NaâŠ•(THF)6] and its implication for cation solvation. Helvetica Chimica Acta, 1994, 77, 41-50.	1.6	27
68	The Lipophilically Wrapped Polyion Aggregate{H120C144O24(OP)2Nâ^'Na6+}, a Hexameric Sodium Tetraphenyl Imidodiphosphate Containing an[Na6O12] Core in a Hydrocarbon Ellipsoid. Angewandte Chemie International Edition in English, 1995, 34, 1355-1357.	4.4	26
69	Trimorphism of 4,4â€²-Di(tert.-butyl)-biphenyl: structural, thermodynamic and kinetic aspects. Solid State Sciences, 2002, 4, 859-871.	3.2	26
70	Theoretical studies of reaction mechanism in chemistry. International Journal of Quantum Chemistry, 1984, 26, 607-619.	2.0	25
71	Does fluoroformic acid exist?. Journal of the American Chemical Society, 1985, 107, 7243-7246.	13.7	25
72	The Two-Electron Reduction of 1,1â€²-Diphenylethene by Lithium or Sodium to Different 1,1,4,4-Tetraphenylbutane-1,4-diide Salts via Cï£¿C Bond Formationâ€"A Monomeric Dilithium Contact Ion Triple and a Polymer String ofâ€œHydrocarbon Oysters Containing Solvated Sodium Pearlsâ€• Angewandte Chemie International Edition in English, 1991, 30, 1183-1186.	4.4	25

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73	Tris(tetramethylethylenediamine-sodium)-9,9-bianthrylâ€”The Salt of a Ï€ Hydrocarbon Radical Trianion with Three Na+-CÏ€ Contacts to One Molecular Half. Angewandte Chemie - International Edition, 1998, 37, 502-504.	13.8	25
74	Molecular Packing and Singlet Fission: The Parent and Three Fluorinated 1,3-Diphenylisobenzofurans. Journal of Physical Chemistry Letters, 2019, 10, 1947-1953.	4.6	25
75	Sulfenic acids in the gas phase. Preparation, ionization energies and heats of formation of methane-, ethene-, and benzenesulfenic acid. Collection of Czechoslovak Chemical Communications, 1988, 53, 2140-2158.	1.0	24
76	2,3,6,7â€Tetramethoxythianthrenâ€Dikation: Ein aromatisches Ï€â€System gibt seinen Geist auf. Angewandte Chemie, 1991, 103, 706-708.	2.0	24
77	[{Na⁺(thf)₂}₄(Rubren^{4â^’})]: Kristallisation und Strukturbestimmung eines Kontaktionenâ€Quintupels des ersten Ï€â€Kohlenwasserstoffâ€Tetraanions. Angewandte Chemie, 1996, 108, 720-722.	2.0	24
78	Higher Metalâ^’Ligand Coordination in the Catalytic Site of Cobalt-SubstitutedThermoanaerobacter brockiiAlcohol Dehydrogenase Lowers the Barrier for Enzyme Catalysisâ€. Biochemistry, 2004, 43, 7151-7161.	2.5	24
79	1,2-Diphenylbenzene Dianion: Alkali-Metal Salts with Drastically Spread C6 Rings. Angewandte Chemie - International Edition, 2003, 42, 4385-4389.	13.8	23
80	Ab Initio calculations of [CoY6â^’nXn]2+ complexes. Journal of Chemical Physics, 2000, 112, 149-157.	3.0	22
81	Spin-Orbit Coupling in Biradicals. 4. Zero-Field Splitting in Triplet Nitrenes, Phosphinidenes, and Arsinidenes. Collection of Czechoslovak Chemical Communications, 2003, 68, 2335-2343.	1.0	22
82	On the electronic structure of a dianion, a radical anion, and a neutral biradical (HB)11CCCC(BH)11 carborane dimer. Computational and Theoretical Chemistry, 2009, 912, 13-20.	1.5	22
83	Crystallization and Structure of {(H52C44O4-3)[Li+6(NH3)2](3-O4C44H52)}, an Edge-Shared Li+6 Double Tetrahedron between Calix[4]arenetrianion Half-Shells: Another Self-Organized and Lipophilically-Wrapped Polyion Aggregate. Journal of the American Chemical Society, 1995, 117, 9367-9368.	13.7	21
84	Ab initio calculation of zero-field splitting and spin-orbit coupling in ground and excited triplets of m-xylylene. Journal of the Chemical Society Perkin Transactions II, 1999, , 2299-2303.	0.9	21
85	An MS-CASPT2 Calculation of the Excited Electronic States of an Axial Difluoroborondipyrromethene (BODIPY) Dimer. Journal of Chemical Theory and Computation, 2018, 14, 4291-4297.	5.3	21
86	On the formation of C2H8+ in the reaction CH4+ + CH4 â† CH3 + CH5+: A theoretical study. Chemical Physics Letters, 1985, 121, 330-333.	2.6	20
87	Evaluation of the rate constant for the SN2 reaction fluoromethane + hydride .fwdarw. methane + fluoride in the gas phase. Journal of the American Chemical Society, 1988, 110, 8355-8359.	13.7	20
88	Monoclinic and Triclinic Tetraisopropyl-p-phenylenediamine: To what Extent do nN/Ï€ Interactions Determine Structures?. Angewandte Chemie International Edition in English, 1993, 32, 1755-1758.	4.4	20
89	Structurally recognizable electron density transfer in the donorâ€“acceptor complex {1,2,4,5-tetra(thioethyl) benzeneâ‹¯bromine2}â^ž. Chemical Communications, 1996, , 1529-1530.	4.1	20
90	News from an Old Ligand: The Triple-Decker Ion Triple, Tris([18]Crown-6)-disodium Bis(tetraphenycyclopentadienide). Angewandte Chemie International Edition in English, 1997, 36, 638-639.	4.4	20

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91	Structural, kinetic and thermodynamic aspects of the conformational dimorphism of diethyl 3,6-dibromo-2,5-dihydroxyterephthalate. Acta Crystallographica Section B: Structural Science, 1996, 52, 697-706.	1.8	19
92	StrukturÃnderungen bei Zweifachâ€Oxidation von Tetrakis(dimethylamino)â€pâ€benzochinon: Aus einer sterisch Ã¼berfÃ¼llten, elektronenreichen Sesselâ€Verbindung wird ein twistâ€Dicyaninâ€Salz. Angewandte Chemie, 1991, 103, 1194-1197.	2.0	18
93	Tetracyanohydroquinone and its Dimorpholinium Salt: Hydrogen Bonds Oï£¿Hâ€¦ N or OâŠ– Hï£¿âŠ•N to Nitrogen Bases of Different Strengths. Angewandte Chemie International Edition in English, 1993, 32, 411-414.	4.4	18
94	Aromatic Substitution with Hypercloso C(BCH3)11:Â A New Mechanism. Journal of the American Chemical Society, 2007, 129, 4172-4174.	13.7	18
95	(E)- and (Z)-1-Hydroxy-1,3-butadiene: new kinetically unstable C4H6O isomers. Journal of Organic Chemistry, 1986, 51, 4061-4065.	3.2	17
96	MNDO Calculations as a valuable tool for structure evaluation of contact ion pairs. International Journal of Quantum Chemistry, 1992, 44, 449-467.	2.0	17
97	Das Triplettâ€Diradikal Tris(3,5â€diâ€tertâ€butylâ€4â€oxoâ€phenylen)methan: Struktur im Kristall sowie Spinâ€• und Ladugsverteilung. Angewandte Chemie, 1993, 105, 416-418.	2.0	17
98	aci-Nitrodiphenylmethane: A Hydrogen-Bonded Dimer. Angewandte Chemie International Edition in English, 1993, 32, 1758-1760.	4.4	16
99	Molecular Design of Specific Metalâ€Binding Peptide Sequences from Protein Fragments: Theory and Experiment. Chemistry - A European Journal, 2008, 14, 7836-7846.	3.3	16
100	exo-Substituent effects in halogenated icosahedral (B12H122â€“) and octahedral (B6H62â€“) closo-borane skeletons: chemical reactivity studied by experimental and quantum chemical methods. Collection of Czechoslovak Chemical Communications, 2009, 74, 1-27.	1.0	16
101	Spin-Orbit Coupling in Biradicals. 3. Heavy Atom Effects in Carbenes. Collection of Czechoslovak Chemical Communications, 1998, 63, 1485-1497.	1.0	16
102	Die Zweielektronenâ€Reduktion von 1,1â€²â€Diphenylethen mit Lithium oder Natrium unter CCâ€VerknÃ¼pfung zu verschiedenartigen 1,1,4,4â€Tetraphenylbutanâ€•1,4â€diidâ€Salzen â€•einem monomeren Dilithiumâ€Kontaktionentripel und einer Polymerkette aus â€žKohlenwasserstoffâ€Austern mit solvatisierten Natriumâ€Perlenâ€¡ Angewandte Chemie, 1991, 103, 1197-1200.	2.0	15
103	Elektronentransfer und Ionenpaar-Bildung, 34 [1 - 3] Einkristallstruktur des Solvens-separierten Radikalionenpaares [9,9â€²-BianthryleÂ·âŠ–][NaâŠ•(DME)3] / Electron Transfer and Ion Pair Formation, 34 [1-3] Single Crystal Structure of the Solvent-Separated Ion Pair [9,9â€²-BianthryleÂ·âŠ–][NaâŠ•(DME)3]. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1994, 49, 1339-1347.	0.7	15
104	Spinâ€“orbit coupling in biradicals. 5. Zero-field splitting in triplet dimethylnitrenium, dimethylphosphenium and dimethylarsenium cations. Molecular Physics, 2005, 103, 407-411.	1.7	15
105	Ab initio quantum chemical study of the SN2 reaction, CH3F+Hâ¯ â† CH4+Fâ¯, in the gas phase. Chemical Physics, 1988, 127, 53-63.	1.9	14
106	Tetracyanhydrochinon und sein Dimorpholiniumâ€Salz, WasserstoffbrÃ¼cken Oâ€H â€¦N und O+ â€¦ Hâ€â¯N zu Stickstoffâ€Basen unterschiedlicher StÃrke. Angewandte Chemie, 1993, 105, 410-413.	2.0	14
107	Monoklines und triklines Tetraisopropylâ€paraâ€phenylendiamin: Wie strukturbestimmend sind n_N/Ï€â€Wechselwirkungen?. Angewandte Chemie, 1993, 105, 1823-1826.	2.0	14
108	Wechselwirkungen in Kristallen. 106. Mitteilung. Die Klaviatur der Na?-Koordinationszahlen in ihren Carbazolanion-Salzen. Helvetica Chimica Acta, 1997, 80, 606-620.	1.6	14

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109	Preparation, Structure, and Density Functional Calculation of the Solvent-Separated Ion Pair [(H5C2)Al(OC6H5)3-Â·Â·Â·Li+Â·Â·Â·-(H5C6O)3Al(C4H9)]-[Li+(DME)3]â€. Inorganic Chemistry, 1998, 37, 5046-5049.	4.0	14
110	Prediction of an Inverse Heavy-Atom Effect in Hâ^'Câ^'CH2Br:Â Bromine Substituent as a Ï€ Acceptor. Journal of the American Chemical Society, 2002, 124, 5606-5607.	13.7	14
111	Optimal Arrangements of Tetracene Molecule Pairs for Fast Singlet Fission. Bulletin of the Chemical Society of Japan, 2019, 92, 1960-1971.	3.2	13
112	Orthorhombic and Monoclinic 2,3,7,8-Tetramethoxythianthrene: Small Structural Differenceâ€"Large Lattice Change. Angewandte Chemie International Edition in English, 1995, 34, 76-78.	4.4	12
113	Single-Step Formation of Pyrimido[4,5-d]pyridazines by a Pyrimidine-Tetrazine Tandem Reaction. Organic Letters, 2016, 18, 3594-3597.	4.6	12
114	Electronic States of 2,3-Diamino-1,4-naphthoquinone and Its N-Alkylated Derivatives. Journal of Physical Chemistry C, 2020, 124, 60-69.	3.1	12
115	The mass spectra of organic compounds. 8thCommunication. 1-Buten-3-yn-2-ol. A new kinetically unstable C4H4O isomer. Helvetica Chimica Acta, 1986, 69, 683-691.	1.6	11
116	Investigation of the acid-base and electromigration properties of 5â€azacytosine derivatives using capillary electrophoresis and density functional theory calculations. Journal of Chromatography A, 2017, 1479, 185-193.	3.7	11
117	Orthorhombisches und monoklines 2,3,7,8â€Tetramethoxythianthren: kleiner Strukturunterschied â€" groÃŸe GitterÃnderung. Angewandte Chemie, 1995, 107, 120-122.	2.0	9
118	Spin-orbit coupling in organic biradicals: zero-field splitting in triplet tetramethyleneethane. Computational and Theoretical Chemistry, 1997, 398-399, 281-291.	1.5	9
119	Interactions between allosteric modulators and 4-DAMP and other antagonists at muscarinic receptors: potential significance of the distance between the N and carboxyl C atoms in the molecules of antagonists. Neurochemical Research, 2001, 26, 383-394.	3.3	9
120	Substituent Effect on exo Stereoselectivity in the 1,3-Dipolar Cycloaddition Reaction of Tulipalin A with Nitrile Ylides. Journal of Organic Chemistry, 2008, 73, 3032-3039.	3.2	9
121	Tetraarylcyclobutadienecyclopentadienylcobalt Complexes: Synthesis, Electronic Spectra, Magnetic Circular Dichroism, Linear Dichroism, and TD DFT Calculations. Organometallics, 2014, 33, 3251-3264.	2.3	9
122	A theoretical study on acetylene dimer, acetylene-s-tetrazine and acetylene-benzene associates. Collection of Czechoslovak Chemical Communications, 1988, 53, 2495-2502.	1.0	9
123	Energy barriers to the Dielsâ€"Alder cycloadditions and cycloreversions of cation-radicals in the gas phase. Journal of the Chemical Society Perkin Transactions II, 1986, , 1011-1014.	0.9	8
124	Elektronentransfer und Ionenpaar-Bildung. 40. Mitteilung. Einkristall-Struktur von Bis(Natrium-1,1â€²-Biphenyl-2-thiolat-Diglyme): Ein Zwischenprodukt der reduktiven RingÃ¶ffnung von Dibenzothiophen. Helvetica Chimica Acta, 1995, 78, 866-878.	1.6	8
125	Spin-orbit coupling in biradicals: Structural aspects. Pure and Applied Chemistry, 1997, 69, 785-790.	1.9	8
126	Carbazole deprotonation by sodium metal mirror in various ethers: Structures with Na+-coordination numbers 3 and 4 to 7. Journal of Organometallic Chemistry, 1997, 548, 115-120.	1.8	8

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127	Are 1,4-Dihydropyrazines Antiaromatic? Ab initio Study of 1,4-Dihydropyrazines and Their Tetrahydro Derivatives. Collection of Czechoslovak Chemical Communications, 1999, 64, 633-648.	1.0	8
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