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	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
2	Optimal Arrangements of Tetracene Molecule Pairs for Fast Singlet Fission. Bulletin of the Chemical Society of Japan, 2019, 92, 1960-1971.	3.2	13
3	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
4	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
5	Structure and photophysics of indigoids for singlet fission: Cibalackrot. Journal of Chemical Physics, 2019, 151, 184903.	3.0	40
6	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
7	Electron Transfer Mechanism of Substituted Benzimidazoles: Dimer Switching, Oscillations, and Search for Singlet Fission Properties. Journal of Physical Chemistry C, 2017, 121, 9963-9969.	3.1	5
8	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
9	Singlet Fission: Optimization of Chromophore Dimer Geometry. Advances in Quantum Chemistry, 2017, 75, 175-227.	0.8	34
10	Single-Step Formation of Pyrimido[4,5-d]pyridazines by a Pyrimidine-Tetrazine Tandem Reaction. Organic Letters, 2016, 18, 3594-3597.	4.6	12
11	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
12	Guidance for Mutual Disposition of Chromophores for Singlet Fission. Israel Journal of Chemistry, 2016, 56, 96-106.	2.3	40
13	Electronic Spectra of the Tetraphenylcyclobutadienecyclopentadienylnickel(II) Cation and Radical. Journal of Physical Chemistry A, 2016, 120, 3456-3462.	2.5	2
14	Singlet fission: Towards efficient solar cells. AIP Conference Proceedings, 2015, , .	0.4	2
15	Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission. Journal of the American Chemical Society, 2015, 137, 165-172.	13.7	87
16	Two Thin Film Polymorphs of the Singlet Fission Compound 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry C, 2014, 118, 12121-12132.	3.1	85
17	Tetraarylcyclobutadienecyclopentadienylcobalt Complexes: Synthesis, Electronic Spectra, Magnetic Circular Dichroism, Linear Dichroism, and TD DFT Calculations. Organometallics, 2014, 33, 3251-3264.	2.3	9
18	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

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19	The Loss of a Prominent Scientist: Detlef SchrÃ¶der. ChemPlusChem, 2013, 78, 887-889.	2.8	0
20	Search for a Small Chromophore with Efficient Singlet Fission: Biradicaloid Heterocycles. Journal of the American Chemical Society, 2012, 134, 14624-14631.	13.7	99
21	HCB11(CF3)nF11-nâ^': Inert Anions with High Anodic Oxidation Potentials. Journal of the American Chemical Society, 2011, 133, 4123-4131.	13.7	43
22	Toward Designed Singlet Fission: Electronic States and Photophysics of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry A, 2010, 114, 1457-1473.	2.5	98
23	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
24	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
25	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
26	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
27	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
28	Structures and Properties of Three Polymorphic Modifications based on Tetrahedral Building Blocks of Dichlorobis(pyridazine-N) Zinc(II). Crystal Growth and Design, 2007, 7, 2627-2634.	3.0	8
29	On the Convergence of the Physicochemical Properties of [n]Helicenes. Journal of Physical Chemistry C, 2007, 111, 14948-14955.	3.1	79
30	Aromatic Substitution with Hypercloso C(BCH3)11:Â A New Mechanism. Journal of the American Chemical Society, 2007, 129, 4172-4174.	13.7	18
31	CB11Me11Boronium Ylides:Â Carba-closo-dodecaboranes with a Naked Boron Vertex. Journal of the American Chemical Society, 2006, 128, 6089-6100.	13.7	37
32	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	2.1	134
33	Ab initio electronic structure of thymine anions. Physical Chemistry Chemical Physics, 2005, 7, 840.	2.8	35
34	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
35	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
36	Electronic Spectra of Conjugated Polyynes, Cumulenes and Related Systems: A Theoretical Study. Collection of Czechoslovak Chemical Communications, 2005, 70, 559-578.	1.0	3

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37	Novel Acyclic Nucleoside Phosphonate Analogues with Potent Anti-Hepatitis B Virus Activities. Antimicrobial Agents and Chemotherapy, 2005, 49, 1177-1180.	3.2	48
38	Electron Binding to Nucleic Acid Bases. Experimental and Theoretical Studies. A Review. Collection of Czechoslovak Chemical Communications, 2004, 69, 1395-1428.	1.0	43
39	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
40	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
41	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
42	1,2-Diphenylbenzene Dianion: Alkali-Metal Salts with Drastically Spread C6 Rings. Angewandte Chemie - International Edition, 2003, 42, 4385-4389.	13.8	23
43	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
44	Sexual Attraction in the Silkworm Moth. Chemistry and Biology, 2003, 10, 331-340.	6.0	48
45	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
46	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
47	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 ETQq1 1 0.784314 rgBT /Over	7.8	80
48	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
49	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
50	Trimorphism of 4,4â€²-Di(tert.-butyl)-biphenyl: structural, thermodynamic and kinetic aspects. Solid State Sciences, 2002, 4, 859-871.	3.2	26
51	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.	3.0	80
52	Improper, blue-shifting hydrogen bond. Theoretical Chemistry Accounts, 2002, 108, 325-334.	1.4	178
53	The Nature of Improper, Blue-Shifting Hydrogen Bonding Verified Experimentally. Journal of the American Chemical Society, 2001, 123, 12290-12293.	13.7	306
54	Improper, Blue-Shifting Hydrogen Bond between Fluorobenzene and Fluoroform. Journal of Physical Chemistry A, 2001, 105, 5560-5566.	2.5	138

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55	Enhanced Long-Range SiÂ·Â·Â·N Interactions in Organosilicon Cations. A Theoretical Study. Collection of Czechoslovak Chemical Communications, 2001, 66, 473-482.	1.0	4
56	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
57	Chlorofluoroacetic Acid as a Highly Versatile Derivatizing Agent: Assignment of Stereochemistry to Esters of Chiral Alcohols. Collection of Czechoslovak Chemical Communications, 2000, 65, 695-707.	1.0	7
58	Single crystals of an ionic anthracene aggregate with a triplet ground state. Nature, 2000, 404, 267-269.	27.8	63
59	Wechselwirkungen in MolekÃ¼lkristallen, 155 [1, 2]. KristallzÃ¼chtung und Strukturbestimmung des Radikalkation-Salzes [Tetrahydrotetrathiafulvaleniumâ—êŠ•] [AlCl4 âŠ–]/Interaction in Molecular Crystals, 155 [1,2]. Crystallization and Structure Determination of the Radicalcation Salt [Tetrahydrotetrathiafulvaleniumâ—êŠ•][AlCl4 âŠ–]. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2000, 55, 597-602.	0.7	3
60	Ab Initio calculations of [CoY6â^'nXn]2+ complexes. Journal of Chemical Physics, 2000, 112, 149-157.	3.0	22
61	Blue-Shifting Hydrogen Bonds. Chemical Reviews, 2000, 100, 4253-4264.	47.7	1,645
62	Crystal Structure ofn-Bu3Sn+CB11Me12-. Journal of the American Chemical Society, 2000, 122, 10253-10254.	13.7	85
63	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
64	The fluoroformâ‹¯ethylene oxide complex exhibits a Câ€“Hâ‹¯O anti-hydrogen bond. Chemical Physics Letters, 1999, 303, 447-452.	2.6	190
65	Anti-hydrogen bond between chloroform and fluorobenzene. Chemical Physics Letters, 1999, 299, 180-186.	2.6	266
66	Tellurocarbonyldifluorid und seine Derivate: (HeI)-Photoelektronen-Spektren und HF-, GF- sowie DFT-Berechnungen. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 1999, 625, 1726-1731.	1.2	6
67	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
68	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
69	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
70	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
71	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	1
72	Tetralithium Bis(ethylaluminum) Tetrakis(catecholate) Pentakis(dimethoxyethane): An Oxygen-Rich		

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73	Structural Distortions in Diiodine-Substituted Unsaturated Hydrocarbons. Chemistry - A European Journal, 1998, 4, 677-685.	3.3	31
74	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
75	Counterpoise-corrected potential energy surfaces of simple H-bonded systems. Theoretical Chemistry Accounts, 1998, 99, 372-377.	1.4	125
76	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
77	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
78	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
79	Bare Molecular Anions of Unsaturated Hydrocarbons: Density Functional Charge and Spin Distributions Based on Their Single Crystal Structures. Collection of Czechoslovak Chemical Communications, 1998, 63, 1245-1263.	1.0	3
80	Tris(tetramethylethylenediamine-sodium)-9,9-bianthrylâ€"The Salt of a Ï€ Hydrocarbon Radical Trianion with Three Na+â€"C Contacts to One Molecular Half. Angewandte Chemie - International Edition, 1998, 37, 502-504.	13.8	1
81	Counterpoise-Corrected Potential Energy Surfaces of Simple Hydrogen-Bonded Systems. Collection of Czechoslovak Chemical Communications, 1998, 63, 1343-1354.	1.0	4
82	Spin-Orbit Coupling in Biradicals. 3. Heavy Atom Effects in Carbenes. Collection of Czechoslovak Chemical Communications, 1998, 63, 1485-1497.	1.0	16
83	Regular polyhedral molecules. P₂₀ and its inclusion compounds. Canadian Journal of Chemistry, 1998, 76, 1274-1279.	1.1	0
84	Spin-orbit coupling in biradicals: Structural aspects. Pure and Applied Chemistry, 1997, 69, 785-790.	1.9	8
85	Synthesis of New Perfluorinated Telluracarbonyls and 1,3-Ditelluretanes. Phosphorus, Sulfur and Silicon and the Related Elements, 1997, 124, 413-417.	1.6	3
86	Spin-orbit coupling in organic biradicals: zero-field splitting in triplet tetramethyleneethane. Computational and Theoretical Chemistry, 1997, 398-399, 281-291.	1.5	9
87	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
88	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
89	Neues von einem â€žaltenâ€¦Liganden: das Tripeldeckerâ€‹onentripel Tris([18]Kroneâ€6)â€‹dinatriumbis(tetraphenylcyclopentadienid). Angewandte Chemie, 1997, 109, 650-651.	2.0	5
90	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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91	Interactions in Molecular Crystals, 118. The Sodium(benzoâ€15â€crownâ€5) Salt of 2, 6â€Di(tertâ€butyl)â€4â€methylphenol, a Sodium Phenolate with an Extremely Short Na⁺â€¦O^{â^'} Distance: Structure and Density Functional Calculations. Chemische Berichte, 1997, 130, 1533-1537.	0.2	4
92	1-(3,5-O-Alkylidene-2-deoxy-4-C-hydroxymethyl-Î±-L-threo-pentofuranosyl)uracils. Collection of Czechoslovak Chemical Communications, 1997, 62, 957-970.	1.0	5
93	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
94	Symmetrical Tris(4,6-diamino-5-methylene-2-pyrimidones): New Building Blocks for Self-Assembly of Hollow Spherical Supramolecules Locked by Hydrogen Bonds. Collection of Czechoslovak Chemical Communications, 1996, 61, 1464-1472.	1.0	4
95	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
96	Wechselwirkungen in MolekÃ¼lkristallen, 111. KristallzÃ¼chtung und Strukturbestimmung von Donator/Akzeptorâ€Komplexen aus 1,2,4,5â€Tetrakis(alkylthio)benzolen und Brom oder Iod. Liebigs Annalen, 1996, 1996, 2185-2194.	0.8	5
97	[{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
98	[{Na+(thf)2}4(rubrene4â^')]: Crystallization and Structure Determination of a Contact-Ion Quintuple for the Firstπ-Hydrocarbon Tetraanion. Angewandte Chemie International Edition in English, 1996, 35, 631-632.	4.4	50
99	Orthorhombisches und monoklines 2,3,7,8â€Tetramethoxythianthren: kleiner Strukturunterschied â€“ groÃŸe GitterÃnderung. Angewandte Chemie, 1995, 107, 120-122.	2.0	9
100	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
101	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
102	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
103	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
104	Crystallization and structure of hexameric aci-9-nitrofluorene-potassium containing a lipophilically wrapped polyion aggregate [KâŠ•6(O12)âŠ–6] 1,2. Tetrahedron Letters, 1995, 36, 7855-7858.	1.4	5
105	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
106	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
107	Single crystal structure of [(Me2N-C6H4)2C+â€“+C(C6H4-NMe2)2](I3â€“)2: a twisted tetraphenylethylene dication with a Câ€“C single bond. Journal of the Chemical Society Chemical Communications, 1995, , 1111-1112.	2.0	6
108	The structures of solvent-separated naphthalene and anthracene radical anions. Journal of the Chemical Society Chemical Communications, 1995, .	2.0	38

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109	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
110	Thianthrenâ€Radikalkationâ€Tetrachloroaluminat. Chemische Berichte, 1994, 127, 2043-2049.	0.2	49
111	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
112	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
113	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
114	EINKRISTALL-MOLEKÃœLSTRUKTUREN 55^{1,2} DITHIOLO-DITHIOL-DITHION C₄S₆ UND DITHIOLO-DITHIOL-DION C₄O₂S₄. Phosphorus, Sulfur and Silicon and the Related Elements, 1994, 91, 53-67.	1.6	7
115	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
116	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
117	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
118	aci-Nitrodiphenylmethane: A Hydrogen-Bonded Dimer. Angewandte Chemie International Edition in English, 1993, 32, 1758-1760.	4.4	16
119	Tetracyanhydrochinon und sein Dimorpholiniumâ€Salz, WasserstoffbrÃ¼cken Oâ€H â€¦N und O+ â€¦ Hâ€â‹¯N zu Stickstoffâ€Basen unterschiedlicher StÃ¤rke. Angewandte Chemie, 1993, 105, 410-413.	2.0	14
120	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
121	Monoklines und triklines Tetraisopropylâ€paraâ€phenylendiamin: Wie strukturbestimmend sind n_N/Ï€â€Wechselwirkungen?. Angewandte Chemie, 1993, 105, 1823-1826.	2.0	14
122	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
123	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
124	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
125	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
126	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

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127	Distorted Molecules: Perturbation Design, Preparation and Structures. Angewandte Chemie International Edition in English, 1992, 31, 550-581.	4.4	169
128	Diprotoniertes Tetra(2â€pyridyl)pyrazin und seine chemische Mimese mit unterschiedlichen WasserstoffbrÃ¼cken. Angewandte Chemie, 1992, 104, 348-350.	2.0	27
129	VerzerrteMolekÃ¼le: StÃ¶rungsdesign, Synthesen und Strukturen. Angewandte Chemie, 1992, 104, 564-595.	2.0	140
130	Interaction of Lysine-Alanine-Alanine tripeptide with a fragment of DNA: An empirical potential study. Journal of Computational Chemistry, 1991, 12, 9-16.	3.3	6
131	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
132	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
133	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
134	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
135	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
136	2,3,6,7â€Tetramethoxythianthrenâ€Dikation: Ein aromatisches Ï€â€System gibt seinen Geist auf. Angewandte Chemie, 1991, 103, 706-708.	2.0	24
137	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
138	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
139	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
140	Properties and reactivity of first and second row hydrides. Introductory remarks, isomerizations, and inversion barriers of the AH2, AH3, AH4 and related systems. Collection of Czechoslovak Chemical Communications, 1990, 55, 869-889.	1.0	6
141	An empirical potential for interactions of large molecules: Application to binding of dipeptides to DNA. International Journal of Quantum Chemistry, 1989, 36, 287-298.	2.0	7
142	MBPT And coupled-cluster activation barriers. The model SN2 reaction: Hâ¯+CH3F*lrhar2;CH4+Fâ¯. Chemical Physics Letters, 1989, 159, 155-158.	2.6	7
143	Mechanism of the antipodal effect with borane cages. Journal of the Chemical Society Chemical Communications, 1989, , 1859-1861.	2.0	33
144	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

#	Article	IF	Citations
145	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
146	Theoretical Studies of Reaction Mechanisms in Chemistry. Advances in Quantum Chemistry, 1988, 19, 247-288.	0.8	7
147	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
148	Ab initio study of the anharmonic properties of dipole moment functions of ammonia and the oxonium ion. Collection of Czechoslovak Chemical Communications, 1988, 53, 2175-2190.	1.0	3
149	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
150	Ion solvation by dipolar aprotic solvents. An ab initio study. Collection of Czechoslovak Chemical Communications, 1987, 52, 6-13.	1.0	2
151	Ion solvation in mixed solvents. An ab initio study. Collection of Czechoslovak Chemical Communications, 1987, 52, 14-21.	1.0	3
152	Thermochemistry of unstable enols: the O-(Cd)(H) group equivalent. Journal of Organic Chemistry, 1986, 51, 4066-4067.	3.2	65
153	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
154	(E)- and (Z)-1-Hydroxy-1,3-butadiene: new kinetically unstable C4H6O isomers. Journal of Organic Chemistry, 1986, 51, 4061-4065.	3.2	17
155	The effect of geometry optimization on the reaction barrier height: SCF and MP2 studies of the dissociation and isomerization reactions of formaldehyde. Computational and Theoretical Chemistry, 1986, 136, 239-245.	1.5	4
156	Synthesis of anomeric 5-cyclopropyl-2'-deoxyuridines and 1H NMR spectroscopic study of their conformation. Collection of Czechoslovak Chemical Communications, 1986, 51, 1764-1771.	1.0	6
157	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
158	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
159	Discriminative interactions between chiral molecules: internal discrimination in 1,2-difluorohydrazine. Canadian Journal of Chemistry, 1985, 63, 1639-1641.	1.1	2
160	Does fluoroformic acid exist?. Journal of the American Chemical Society, 1985, 107, 7243-7246.	13.7	25
161	Solvation of ions by dipolar aprotic solvents and water. A CNDO/2 study. Collection of Czechoslovak Chemical Communications, 1985, 50, 2493-2508.	1.0	1
162	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. Helvetica Chimica Acta, 1984, 67, 1-17.	1.6	67

#	Article	IF	Citations
163	Theoretical studies of reaction mechanism in chemistry. International Journal of Quantum Chemistry, 1984, 26, 607-619.	2.0	25
164	Piano-stool complexes of the CpML4 type. Organometallics, 1982, 1, 180-188.	2.3	155
165	NMR and quantum chemical study of empiric 2',3'-cyclic sulphites of nucleosides. Collection of Czechoslovak Chemical Communications, 1981, 46, 400-408.	1.0	3
166	Semiempirical and ab initio study of the nature of the C-S bond in sulfonium ylides. Collection of Czechoslovak Chemical Communications, 1981, 46, 883-891.	1.0	3
167	Quantum chemical calculation of the (S)-9-(2,3-dihydroxypropyl)adenine moleculea. Nucleic Acids Research, 1980, 8, 6233-6238.	14.5	2
168	Molecular geometries - Accuracy test of the PCILO method. Collection of Czechoslovak Chemical Communications, 1980, 45, 321-329.	1.0	5
169	An attempt to construct a hybrid intermolecular potential. Collection of Czechoslovak Chemical Communications, 1978, 43, 1356-1365.	1.0	3