Pavel Hobza

List of Publications by Year in descending order

546 papers	52,123 citations	1294 109 h-index	1792 211 g-index
576 all docs	576 docs citations	576 times ranked	28914 citing authors

#	Article	IF	Citations
1	Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications. Chemical Reviews, 2012, 112, 6156-6214.	23.0	3,531
2	Blue-Shifting Hydrogen Bonds. Chemical Reviews, 2000, 100, 4253-4264.	23.0	1,645
3	Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs. Physical Chemistry Chemical Physics, 2006, 8, 1985-1993.	1.3	1,635
4	Noncovalent Interactions:Â A Challenge for Experiment and Theory. Chemical Reviews, 2000, 100, 143-168.	23.0	1,572
5	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	0.9	1,449
6	Structure, Energetics, and Dynamics of the Nucleic Acid Base Pairs:â€‰ Nonempirical Ab Initio Calculations. Chemical Reviews, 1999, 99, 3247-3276.	23.0	984
7	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. Journal of Chemical Physics, 2001, 114, 5149-5155.	1.2	978
8	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	0.9	856
9	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. Journal of Chemical Theory and Computation, 2011, 7, 2427-2438.	2.3	821
10	Stabilization and Structure Calculations for Noncovalent Interactions in Extended Molecular Systems Based on Wave Function and Density Functional Theories. Chemical Reviews, 2010, 110, 5023-5063.	23.0	697
11	Density functional theory augmented with an empirical dispersion term. Interaction energies and geometries of 80 noncovalent complexes compared withab initioquantum mechanics calculations. Journal of Computational Chemistry, 2007, 28, 555-569.	1.5	620
12	Understanding of Assembly Phenomena by Aromaticâ”Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	1.1	617
13	Potential Energy Surface for the Benzene Dimer. Results ofab InitioCCSD(T) Calculations Show Two Nearly Isoenergetic Structures:Â T-Shaped and Parallel-Displaced. The Journal of Physical Chemistry, 1996, 100, 18790-18794.	2.9	573
14	Computer Modeling of Halogen Bonds and Other Ïƒ-Hole Interactions. Chemical Reviews, 2016, 116, 5155-5187.	23.0	537
15	Intermolecular interactions between medium-sized systems. Nonempirical and empirical calculations of interaction energies. Successes and failures. Chemical Reviews, 1988, 88, 871-897.	23.0	506
16	Density functional theory and molecular clusters. Journal of Computational Chemistry, 1995, 16, 1315-1325.	1.5	503
17	Accurate Interaction Energies of Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of the American Chemical Society, 2004, 126, 10142-10151.	6.6	444
18	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. Journal of Chemical Theory and Computation, 2012, 8, 141-151.	2.3	429

#	Article	IF	Citations
19	Potential Energy Surface of the Benzene Dimer: Ab Initio Theoretical Study. Journal of the American Chemical Society, 1994, 116, 3500-3506.	6.6	416
20	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. Biopolymers, 2001, 61, 3-31.	1.2	408
21	Nature of Nucleic Acidâ^'Base Stacking: Nonempirical ab Initio and Empirical Potential Characterization of 10 Stacked Base Dimers. Comparison of Stacked and H-Bonded Base Pairs. The Journal of Physical Chemistry, 1996, 100, 5590-5596.	2.9	404
22	Investigations into the Nature of Halogen Bonding Including Symmetry Adapted Perturbation Theory Analyses. Journal of Chemical Theory and Computation, 2008, 4, 232-242.	2.3	403
23	Structures and Energies of Hydrogen-Bonded DNA Base Pairs. A Nonempirical Study with Inclusion of Electron Correlation. The Journal of Physical Chemistry, 1996, 100, 1965-1974.	2.9	400
24	Non-covalent interactions in biomacromolecules. Physical Chemistry Chemical Physics, 2007, 9, 5291.	1.3	391
25	First local minimum of the formic acid dimer exhibits simultaneously red-shifted Oâ€"Hâ‹¯O and improper blue-shifted Câ€"Hâ‹¯O hydrogen bonds. Physical Chemistry Chemical Physics, 2004, 6, 37-41.	1.3	384
26	Toward True DNA Base-Stacking Energies:â€‰ MP2, CCSD(T), and Complete Basis Set Calculations. Journal of the American Chemical Society, 2002, 124, 11802-11808.	6.6	376
27	Describing Noncovalent Interactions beyond the Common Approximations: How Accurate Is the â€œGold Standard,â€•CCSD(T) at the Complete Basis Set Limit?. Journal of Chemical Theory and Computation, 2013, 9, 2151-2155.	2.3	365
28	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21453-21458.	3.3	362
29	True Stabilization Energies for the Optimal Planar Hydrogen-Bonded and Stacked Structures of GuanineÂ·Â·Â·Cytosine, AdenineÂ·Â·Â·Thymine, and Their 9- and 1-Methyl Derivatives:â€‰ Complete Basis Set Calculations at the MP2 and CCSD(T) Levels and Comparison with Experiment. Journal of the American Chemical Society, 2003, 125, 15608-15613.	6.6	353
30	Gas-Phase Spectroscopy of Biomolecular Building Blocks. Annual Review of Physical Chemistry, 2007, 58, 585-612.	4.8	352
31	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. Chemical Reviews, 2016, 116, 5038-5071.	23.0	346
32	Structure and Properties of Benzene-Containing Molecular Clusters: Nonempirical ab Initio Calculations and Experiments. Chemical Reviews, 1994, 94, 1767-1785.	23.0	345
33	Anti-Hydrogen Bond in the Benzene Dimer and Other Carbon Proton Donor Complexes. Journal of Physical Chemistry A, 1998, 102, 2501-2504.	1.1	340
34	Nature and magnitude of aromatic stacking of nucleic acid bases. Physical Chemistry Chemical Physics, 2008, 10, 2595.	1.3	317
35	Semiempirical Quantum Chemical PM6 Method Augmented by Dispersion and H-Bonding Correction Terms Reliably Describes Various Types of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2009, 5, 1749-1760.	2.3	312
36	The Nature of Improper, Blue-Shifting Hydrogen Bonding Verified Experimentally. Journal of the American Chemical Society, 2001, 123, 12290-12293.	6.6	306

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37	BrÂ·Â·Â·O Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone. Journal of Chemical Theory and Computation, 2009, 5, 155-163.	2.3	303
38	Intercalators. 1. Nature of Stacking Interactions between Intercalators (Ethidium, Daunomycin,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 71 Functional Theory, and Empirical Potential Study. Journal of the American Chemical Society, 2002, 124, 3366-3376.	6.6	293
39	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3364-3374.	2.3	275
40	Anti-hydrogen bond between chloroform and fluorobenzene. Chemical Physics Letters, 1999, 299, 180-186.	1.2	266
41	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4285-4292.	2.3	264
42	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), andab initio Hartree-Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree-Fock results. , 1997, 18, 1136-1150.		251
43	Photochemical selectivity in guanine-cytosine base-pair structures. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 20-23.	3.3	249
44	A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2010, 6, 344-352.	2.3	249
45	Nonplanar geometries of DNA bases. Ab initio second-order Moeller-Plesset study. The Journal of Physical Chemistry, 1994, 98, 3161-3164.	2.9	242
46	On the convergence of the (Î”ECCSD(T)â^'Î”EMP2) term for complexes with multiple H-bonds. Chemical Physics Letters, 2002, 365, 89-94.	1.2	235
47	Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2008, 4, 1829-1834.	2.3	232
48	Scaled MP3 Nonâ€€Covalent Interaction Energies Agree Closely with Accurate CCSD(T) Benchmark Data. ChemPhysChem, 2009, 10, 282-289.	1.0	232
49	Blue shifts vs red shifts in Ïƒ-hole bonding. Journal of Molecular Modeling, 2008, 14, 699-704.	0.8	231
50	Comparative Study of Selected Wave Function and Density Functional Methods for Noncovalent Interaction Energy Calculations Using the Extended S22 Data Set. Journal of Chemical Theory and Computation, 2010, 6, 2365-2376.	2.3	227
51	Hydrogen Bond versus Anti-Hydrogen Bond:â€‰ A Comparative Analysis Based on the Electron Density Topology. Journal of Physical Chemistry A, 1999, 103, 6394-6401.	1.1	223
52	Hydrogen Bonding and Stacking of DNA Bases: A Review of Quantum-chemicalab initioStudies. Journal of Biomolecular Structure and Dynamics, 1996, 14, 117-135.	2.0	222
53	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+,) Tj ETQq1 1 0.784314 rgBT Interaction. Journal of Physical Chemistry B, 1997, 101, 9670-9677.	1.2	222
54	Noncovalent interactions in biochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 3-17.	6.2	222

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55	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li+, Na+, K+, Rb+, Cs+; Cu+, Ag+, Au+; Mg2+, Ca2+, Sr2+, Ba2+; Zn2+, Cd2+, and Hg2+). The Journal of Physical Chemistry, 1996, 100, 7250-7255.	2.9	214
56	Nature of Base Stacking: Reference Quantum-Chemical Stacking Energies in Ten Unique B-DNA Base-Pair Steps. Chemistry - A European Journal, 2006, 12, 2854-2865.	1.7	211
57	On the Importance and Origin of Aromatic Interactions in Chemistry and Biodisciplines. Accounts of Chemical Research, 2013, 46, 927-936.	7.6	206
58	Correlated ab Initio Study of Nucleic Acid Bases and Their Tautomers in the Gas Phase, in a Microhydrated Environment and in Aqueous Solution. Guanine:Â Surprising Stabilization of Rare Tautomers in Aqueous Solution. Journal of the American Chemical Society, 2003, 125, 7678-7688.	6.6	201
59	Extensions of the S66 Data Set: More Accurate Interaction Energies and Angular-Displaced Nonequilibrium Geometries. Journal of Chemical Theory and Computation, 2011, 7, 3466-3470.	2.3	201
60	DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. , 1996, 57, 959-970.		197
61	Base-base and deoxyribose-base stacking interactions in B-DNA and Z-DNA: a quantum-chemical study. Biophysical Journal, 1997, 73, 76-87.	0.2	196
62	Nonempirical calculations on all the 29 possible DNA base pairs. Journal of the American Chemical Society, 1987, 109, 1302-1307.	6.6	192
63	The fluoroformâ‹¯ethylene oxide complex exhibits a Câ€“Hâ‹¯O anti-hydrogen bond. Chemical Physics Letters, 1999, 303, 447-452.	1.2	190
64	H-Bonded and Stacked DNA Base Pairs: Cytosine Dimer. An Ab Initio Second-Order Moeller-Plesset Study. Journal of the American Chemical Society, 1995, 117, 792-798.	6.6	187
65	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution : Part 1. Cytosine. Physical Chemistry Chemical Physics, 2002, 4, 4192-4203.	1.3	187
66	Correlated ab Initio Study of Nucleic Acid Bases and Their Tautomers in the Gas Phase, in a Microhydrated Environment, and in Aqueous Solution. Part 3. Adenine. Journal of Physical Chemistry B, 2004, 108, 2087-2097.	1.2	184
67	The World of Non-Covalent Interactions: 2006. Collection of Czechoslovak Chemical Communications, 2006, 71, 443-531.	1.0	184
68	Calculations on Noncovalent Interactions and Databases of Benchmark Interaction Energies. Accounts of Chemical Research, 2012, 45, 663-672.	7.6	184
69	Improper, blue-shifting hydrogen bond. Theoretical Chemistry Accounts, 2002, 108, 325-334.	0.5	178
70	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, Xâ‹¯HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2010, 6, 66-80.	2.3	175
71	Interaction between the Guanineâ‹¯Cytosine Watsonâ‹¯Crick DNA Base Pair and Hydrated Group IIa (Mg2+,) Tj ETQq1 1 0.784314 rgB 102, 5951-5957.	1.1	171
72	Assessment of the MP2 Method, along with Several Basis Sets, for the Computation of Interaction Energies of Biologically Relevant Hydrogen Bonded and Dispersion Bound Complexes. Journal of Physical Chemistry A, 2007, 111, 8257-8263.	1.1	170

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73	Structure and IR Spectrum of Phenylalanyl-Glycyl-Glycine Tripetide in the Gas-Phase: IR/UV Experiments, Ab Initio Quantum Chemical Calculations, and Molecular Dynamic Simulations. Chemistry - A European Journal, 2005, 11, 6803-6817.	1.7	169
74	Electronic structures, vibrational spectra, and revised assignment of aniline and its radical cation: Theoretical study. Journal of Chemical Physics, 2003, 118, 10900-10911.	1.2	163
75	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. Part 4. Uracil and thymine. Physical Chemistry Chemical Physics, 2005, 7, 2006-2017.	1.3	155
76	MP2 and CCSD(T) study on hydrogen bonding, aromatic stacking and nonaromatic stacking. Chemical Physics Letters, 1997, 267, 263-270.	1.2	154
77	State-of-the-art correlated ab initio potential energy curves for heavy rare gas dimers: Ar2, Kr2, and Xe2. Journal of Chemical Physics, 2003, 119, 2102-2119.	1.2	154
78	Molecular Dynamics Simulations and Thermodynamics Analysis of DNAâ˜'Drug Complexes. Minor Groove Binding between 4â€˜,6-Diamidino-2-phenylindole and DNA Duplexes in Solution. Journal of the American Chemical Society, 2003, 125, 1759-1769.	6.6	150
79	Sequence-dependent elastic properties of DNA 1 1Edited by I. Tinoco. Journal of Molecular Biology, 2000, 299, 695-709.	2.0	149
80	Floppy structure of the benzene dimer: Ab initio calculation on the structure and dipole moment. Journal of Chemical Physics, 1990, 93, 5893-5897.	1.2	147
81	Base stacking in cytosine dimer. A comparison of correlatedab initio calculations with three empirical potential models and density functional theory calculations. Journal of Computational Chemistry, 1996, 17, 841-850.	1.5	147
82	The Effect of Metal Binding to the N7 Site of Purine Nucleotides on Their Structure, Energy, and Involvement in Base Pairing. Journal of Physical Chemistry B, 2000, 104, 7535-7544.	1.2	147
83	Benchmark database on isolated small peptides containing an aromatic side chain: comparison between wave function and density functional theory methods and empirical force field. Physical Chemistry Chemical Physics, 2008, 10, 2747.	1.3	146
84	Structure and vibrational dynamics of the benzene dimer. Journal of Chemical Physics, 1999, 111, 572-582.	1.2	144
85	Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270.	1.0	144
86	Proton Transfer in the Adenine-Thymine Base Pair. Journal of the American Chemical Society, 1994, 116, 1457-1460.	6.6	143
87	Acetic Acid Dimer in the Gas Phase, Nonpolar Solvent, Microhydrated Environment, and Dilute and Concentrated Acetic Acid:â€‰ Ab Initio Quantum Chemical and Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2003, 107, 3086-3092.	1.1	143
88	Unexpectedly Strong Energy Stabilization Inside the Hydrophobic Core of Small Protein Rubredoxin Mediated by Aromatic Residues:Â Correlated Ab Initio Quantum Chemical Calculations. Journal of the American Chemical Society, 2005, 127, 2615-2619.	6.6	142
89	The lithium bond reexamined. Chemical Reviews, 1990, 90, 1061-1076.	23.0	141
90	The X3LYP extended density functional accurately describes H-bonding but fails completely for stacking. Physical Chemistry Chemical Physics, 2005, 7, 1624-1626.	1.3	141

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91	Improper, Blue-Shifting Hydrogen Bond between Fluorobenzene and Fluoroform. Journal of Physical Chemistry A, 2001, 105, 5560-5566.	1.1	138
92	Bifurcated hydrogen bonds in DNA crystal structures. An ab initio quantum chemical study. Journal of the American Chemical Society, 1994, 116, 709-714.	6.6	137
93	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	1.0	134
94	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	2.9	132
95	The strength and directionality of a halogen bond are co-determined by the magnitude and size of the Ïƒ-hole. Physical Chemistry Chemical Physics, 2014, 16, 9987-9996.	1.3	131
96	The relative roles of electrostatics and dispersion in the stabilization of halogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 17742.	1.3	129
97	On Extension of the Current Biomolecular Empirical Force Field for the Description of Halogen Bonds. Journal of Chemical Theory and Computation, 2012, 8, 1325-1333.	2.3	127
98	Counterpoise-corrected potential energy surfaces of simple H-bonded systems. Theoretical Chemistry Accounts, 1998, 99, 372-377.	0.5	125
99	Câ‹¯HÂ·Â·Â·O Contacts in the AdenineÂ·Â·Â·Uracil Watsonâ‹¯Crick and UracilÂ·Â·Â·Uracil Nucleic Acid Base Pairs:â€‰ Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. Journal of Physical Chemistry B, 2000, 104, 6286-6292.	1.2	125
100	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	7.2	124
101	Stabilization Energies of the Hydrogen-Bonded and Stacked Structures of Nucleic Acid Base Pairs in the Crystal Geometries of CG, AT, and AC DNA Steps and in the NMR Geometry of the 5â€˜-d(GCGAAGC)-3â€˜ Hairpin:â€‰ Complete Basis Set Calculations at the MP2 and CCSD(T) Levels. Journal of Physical Chemistry A, 2005, 109, 1131-1136.	1.1	123
102	On geometries of stacked and H-bonded nucleic acid base pairs determined at various DFT, MP2, and CCSD(T) levels up to the CCSD(T)/complete basis set limit level. Journal of Chemical Physics, 2005, 122, 204322.	1.2	121
103	Hydrogen bonding, stacking and cation binding of DNA bases. Computational and Theoretical Chemistry, 2001, 573, 43-53.	1.5	116
104	A Reliable Docking/Scoring Scheme Based on the Semiempirical Quantum Mechanical PM6-DH2 Method Accurately Covering Dispersion and H-Bonding: HIV-1 Protease with 22 Ligands. Journal of Physical Chemistry B, 2010, 114, 12666-12678.	1.2	116
105	Introduction: Noncovalent Interactions. Chemical Reviews, 2016, 116, 4911-4912.	23.0	116
106	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlatedabinitioquantum chemical calculations and anharmonic analysis of the aniline inversion motion. Journal of Chemical Physics, 1996, 105, 11042-11050.	1.2	115
107	Origin of the Xâ‹¯Hal (Hal = Cl, Br) Bond-Length Change in the Halogen-Bonded Complexes. Journal of Physical Chemistry A, 2008, 112, 4114-4119.	1.1	115
108	On the performance of the semiempirical quantum mechanical PM6 and PM7 methods for noncovalent interactions. Chemical Physics Letters, 2013, 568-569, 161-166.	1.2	115

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109	Base Stacking and Hydrogen Bonding in Protonated Cytosine Dimer: The Role of Molecular ion-dipole and Induction Interactions. Journal of Biomolecular Structure and Dynamics, 1996, 13, 695-706.	2.0	114
110	A halogen-bonding correction for the semiempirical PM6 method. Chemical Physics Letters, 2011, 506, 286-289.	1.2	114
111	Thioguanine and Thiouracil:Â Hydrogen-Bonding and Stacking Properties. Journal of Physical Chemistry A, 1997, 101, 9489-9495.	1.1	113
112	Highly Accurate CCSD(T) and DFTâ€“SAPT Stabilization Energies of Hâ€Bonded and Stacked Structures of the Uracil Dimer. ChemPhysChem, 2008, 9, 1636-1644.	1.0	110
113	Uracil Dimer:â€‰ Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartreeâ^'Fock and Empirical Potential Studies. Journal of Physical Chemistry A, 1998, 102, 6921-6926.	1.1	108
114	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. Journal of Physical Chemistry A, 2012, 116, 4159-4169.	1.1	107
115	RI-MP2 calculations with extended basis setsÃ¢â‚¬â€a promising tool for study of H-bonded and stacked DNA base pairs. Physical Chemistry Chemical Physics, 2001, 3, 4578-4582.	1.3	106
116	Ab initio secondâ€•and fourthâ€•order Mo/llerâ€“Plesset study on structure, stabilization energy, and stretching vibration of benzeneâ‹…â‹…â‹…X (X=He,Ne,Ar,Kr,Xe) van der Waals molecules. Journal of Chemical Physics, 1992, 97, 335-340.	1.2	105
117	Interaction Energies of Hydrogen-Bonded Formamide Dimer, Formamidine Dimer, and Selected DNA Base Pairs Obtained with Large Basis Sets of Atomic Orbitals. Journal of Physical Chemistry A, 2000, 104, 4592-4597.	1.1	103
118	Interaction of the Adenineâ^'Thymine Watsonâ^'Crick and Adenineâ^'Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:Â Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. Journal of Physical Chemistry B, 1999, 103, 2528-2534.	1.2	102
119	Nonplanar DNA Base Pairs. Journal of Biomolecular Structure and Dynamics, 1996, 13, 827-833.	2.0	101
120	New structure for the most stable isomer of the benzene dimer: a quantum chemical study. The Journal of Physical Chemistry, 1993, 97, 3937-3938.	2.9	100
121	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. Journal of Chemical Theory and Computation, 2011, 7, 3743-3755.	2.3	100
122	Potential Energy and Free Energy Surfaces of All Ten Canonical and Methylated Nucleic Acid Base Pairs:Â Molecular Dynamics and Quantum Chemical ab Initio Studies. Journal of Physical Chemistry B, 2001, 105, 5804-5817.	1.2	99
123	Vibrational Spectroscopy of the GÂ·â€‰Â·â€‰Â·C Base Pair:â€‰ Experiment, Harmonic and Anharmonic Calculations, and the Nature of the Anharmonic Couplings. Journal of Physical Chemistry A, 2005, 109, 6974-6984.	1.1	98
124	Comparison of Intrinsic Stacking Energies of Ten Unique Dinucleotide Steps in A-RNA and B-DNA Duplexes. Can We Determine Correct Order of Stability by Quantum-Chemical Calculations?. Journal of Physical Chemistry B, 2010, 114, 1191-1203.	1.2	97
125	On Differences between Hydrogen Bonding and Improper Blue-Shifting Hydrogen Bonding. ChemPhysChem, 2005, 6, 609-617.	1.0	96
126	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B, 2001, 105, 6051-6060.	1.2	95

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127	Reliable theoretical treatment of molecular clusters: Counterpoise-corrected potential energy surface and anharmonic vibrational frequencies of the water dimer. Physical Chemistry Chemical Physics, 1999, 1, 3073-3078.	1.3	93
128	Hydration of Sulfo and Methyl Groups in Dimethyl Sulfoxide Is Accompanied by the Formation of Red-Shifted Hydrogen Bonds and Improper Blue-Shifted Hydrogen Bonds:Â An ab Initio Quantum Chemical Study. Journal of Physical Chemistry A, 2003, 107, 1032-1039.	1.1	93
129	Potential Energy Surface of the Cytosine Dimer:Â MP2 Complete Basis Set Limit Interaction Energies, CCSD(T) Correction Term, and Comparison with the AMBER Force Field. Journal of Physical Chemistry B, 2004, 108, 5466-5471.	1.2	91
130	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	89
131	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlatedab InitioQuantum Chemical and Empirical Potential Procedures. Journal of Chemical Theory and Computation, 2009, 5, 982-992.	2.3	89
132	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	2.3	88
133	Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods. Journal of Chemical Theory and Computation, 2015, 11, 3065-3079.	2.3	87
134	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
135	The H-index unambiguously discriminates between hydrogen bonding and improper blue-shifting hydrogen bonding. Physical Chemistry Chemical Physics, 2001, 3, 2555-2556.	1.3	84
136	Critical Effect of the N2 Amino Group on Structure, Dynamics, and Elasticity of DNA Polypurine Tracts. Biophysical Journal, 2002, 82, 2592-2609.	0.2	84
137	Reference MP2/CBS and CCSD(T) quantum-chemical calculations on stacked adenine dimers. Comparison with DFT-D, MP2.5, SCS(MI)-MP2, M06-2X, CBS(SCS-D) and force field descriptions. Physical Chemistry Chemical Physics, 2010, 12, 3522.	1.3	84
138	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255.	1.1	84
139	Strength and Character of Halogen Bonds in Proteinâ€“Ligand Complexes. Crystal Growth and Design, 2011, 11, 4272-4278.	1.4	84
140	Structure, energetics, and harmonic vibrational spectra of the adenine-thymine and adenine*-thymine* base pairs: gradient nonempirical and semiempirical study. The Journal of Physical Chemistry, 1993, 97, 1542-1557.	2.9	83
141	Benzene trimer and benzene tetramer: Structures and properties determined by the nonempirical model (NEMO) potential calibrated from the CCSD(T) benzene dimer energies. Journal of Chemical Physics, 1999, 110, 5758-5762.	1.2	82
142	On the Nature of Bonding in Lone PairÂ·Â·Ï€-Electron Complexes: CCSD(T)/Complete Basis Set Limit Calculations. Journal of Chemical Theory and Computation, 2009, 5, 1180-1185.	2.3	82
143	Double-Helical â†' Ladder Structural Transition in the B-DNA is Induced by a Loss of Dispersion Energy. Journal of the American Chemical Society, 2008, 130, 16055-16059.	6.6	81
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