Pavel Hobza

List of Publications by Citations

531 papers	46,812 citations	105 h-index	201 g-index
576 ext. papers	49,438 ext. citations	6.5 avg, IF	7.81 L-index

#	Paper	IF	Citations
531	Functionalization of graphene: covalent and non-covalent approaches, derivatives and applications. *Chemical Reviews*, **2012**, 112, 6156-214	68.1	3041
530	Blue-Shifting Hydrogen Bonds. *Chemical Reviews*, **2000**, 100, 4253-4264	68.1	1505
529	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, 1985-93	3.6	1499
528	Noncovalent interactions: a challenge for experiment and theory. *Chemical Reviews*, **2000**, 100, 143-68	68.1	1403
527	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
526	Structure, energetics, and dynamics of the nucleic Acid base pairs: nonempirical ab initio calculations. *Chemical Reviews*, **1999**, 99, 3247-76	68.1	932
525	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. *Journal of Chemical Physics*, **2001**, 114, 5149-5155	3.9	925
524	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
523	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. *Journal of Chemical Theory and Computation*, **2011**, 7, 2427-2438	6.4	686
522	Stabilization and structure calculations for noncovalent interactions in extended molecular systems based on wave function and density functional theories. *Chemical Reviews*, **2010**, 110, 5023-63	68.1	666
521	Density functional theory augmented with an empirical dispersion term. Interaction energies and geometries of 80 noncovalent complexes compared with ab initio quantum mechanics calculations. *Journal of Computational Chemistry*, **2007**, 28, 555-69	3.5	592
520	Understanding of assembly phenomena by aromatic-aromatic interactions: benzene dimer and the substituted systems. *Journal of Physical Chemistry A*, **2007**, 111, 3446-57	2.8	584
519	Potential Energy Surface for the Benzene Dimer. Results of ab Initio CCSD(T) Calculations Show Two Nearly Isoenergetic Structures: T-Shaped and Parallel-Displaced. *The Journal of Physical Chemistry*, **1996**, 100, 18790-18794		546
518	Density functional theory and molecular clusters. *Journal of Computational Chemistry*, **1995**, 16, 1315-1325	3.5	473
517	Intermolecular interactions between medium-sized systems. Nonempirical and empirical calculations of interaction energies. Successes and failures. *Chemical Reviews*, **1988**, 88, 871-897	68.1	473
516	Computer Modeling of Halogen Bonds and Other σ-Hole Interactions. *Chemical Reviews*, **2016**, 116, 5155-87	68.1	444
515	Accurate interaction energies of hydrogen-bonded nucleic acid base pairs. *Journal of the American Chemical Society*, **2004**, 126, 10142-51	16.4	413

514	Investigations into the Nature of Halogen Bonding Including Symmetry Adapted Perturbation Theory Analyses. *Journal of Chemical Theory and Computation*, **2008**, 4, 232-42	6.4	386
513	Potential Energy Surface of the Benzene Dimer: Ab Initio Theoretical Study. *Journal of the American Chemical Society*, **1994**, 116, 3500-3506	16.4	380
512	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		378
511	Nature of Nucleic AcidBase 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		376
510	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. *Biopolymers*, **2001**, 61, 3-31	2.2	374
509	Toward true DNA base-stacking energies: MP2, CCSD(T), and complete basis set calculations. *Journal of the American Chemical Society*, **2002**, 124, 11802-8	16.4	348
508	First local minimum of the formic acid dimer exhibits simultaneously red-shifted OH?O and improper blue-shifted CH?O hydrogen bonds. *Physical Chemistry Chemical Physics*, **2004**, 6, 37-41	3.6	341
507	Non-covalent interactions in biomacromolecules. *Physical Chemistry Chemical Physics*, **2007**, 9, 5291-303	3.6	339
506	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. *Journal of Chemical Theory and Computation*, **2012**, 8, 141-51	6.4	336
505	True stabilization energies for the optimal planar hydrogen-bonded and stacked structures of guanine...cytosine, adenine...thymine, and their 9- and 1-methyl derivatives: complete basis set calculations at the MP2 and CCSD(T) levels and comparison with experiment. *Journal of the American Chemical Society*, **2003**, 125, 15608-13	16.4	335
504	Gas-phase spectroscopy of biomolecular building blocks. *Annual Review of Physical Chemistry*, **2007**, 58, 585-612	15.7	328
503	Structure and Properties of Benzene-Containing Molecular Clusters: Nonempirical ab Initio Calculations and Experiments. *Chemical Reviews*, **1994**, 94, 1767-1785	68.1	326
502	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21453-8	11.5	323
501	Anti-Hydrogen Bond in the Benzene Dimer and Other Carbon Proton Donor Complexes. *Journal of Physical Chemistry A*, **1998**, 102, 2501-2504	2.8	319
500	Describing Noncovalent Interactions beyond the Common Approximations: How Accurate Is the "Gold Standard," CCSD(T) at the Complete Basis Set Limit?. *Journal of Chemical Theory and Computation*, **2013**, 9, 2151-5	6.4	305
499	Nature and magnitude of aromatic stacking of nucleic acid bases. *Physical Chemistry Chemical Physics*, **2008**, 10, 2595-610	3.6	300
498	BrO Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone. *Journal of Chemical Theory and Computation*, **2009**, 5, 155-63	6.4	291
497	The nature of improper, blue-shifting hydrogen bonding verified experimentally. *Journal of the American Chemical Society*, **2001**, 123, 12290-3	16.4	281

496	Intercalators. 1. Nature of stacking interactions between intercalators (ethidium, daunomycin, ellipticine, and 4',6-diaminide-2-phenylindole) and DNA base pairs. Ab initio quantum chemical, density functional theory, and empirical potential study. *Journal of the American Chemical Society*, **2002**, 124, 3366-76	16.4	275
495	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, 1749-60	6.4	270
494	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. *Chemical Reviews*, **2016**, 116, 5038-71	68.1	267
493	Anti-hydrogen bond between chloroform and fluorobenzene. *Chemical Physics Letters*, **1999**, 299, 180-186	2.5	255
492	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartree–Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree–Fock results **1997**, 18, 1136-1150		239
491	Photochemical selectivity in guanine-cytosine base-pair structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 20-3	11.5	233
490	Nonplanar geometries of DNA bases. Ab initio second-order Moeller-Plesset study. *The Journal of Physical Chemistry*, **1994**, 98, 3161-3164		227
489	The accuracy of quantum chemical methods for large noncovalent complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3364-3374	6.4	223
488	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 4285-92	6.4	223
487	On the convergence of the (–CCSD(T)–MP2) term for complexes with multiple H-bonds. *Chemical Physics Letters*, **2002**, 365, 89-94	2.5	223
486	A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. *Journal of Chemical Theory and Computation*, **2010**, 6, 344-52	6.4	222
485	Blue shifts vs red shifts in sigma-hole bonding. *Journal of Molecular Modeling*, **2008**, 14, 699-704	2	221
484	Scaled MP3 non-covalent interaction energies agree closely with accurate CCSD(T) benchmark data. *ChemPhysChem*, **2009**, 10, 282-9	3.2	218
483	Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations. *Journal of Chemical Theory and Computation*, **2008**, 4, 1829-34	6.4	215
482	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+, Cd2+, and Hg2+): Nonempirical ab Initio Calculations on Structures, Energies, and Nonadditivity of the Interaction. *Journal of Physical Chemistry B*, **1997**, 101, 9670-9677	3.4	208
481	Hydrogen Bond versus Anti-Hydrogen Bond: A Comparative Analysis Based on the Electron Density Topology. *Journal of Physical Chemistry A*, **1999**, 103, 6394-6401	2.8	206
480	Nature of base stacking: reference quantum-chemical stacking energies in ten unique B-DNA base-pair steps. *Chemistry - A European Journal*, **2006**, 12, 2854-65	4.8	204
479	Hydrogen bonding and stacking of DNA bases: a review of quantum-chemical ab initio studies. *Journal of Biomolecular Structure and Dynamics*, **1996**, 14, 117-35	3.6	202

478	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		196
477	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, 2365-76	6.4	194
476	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. guanine: surprising stabilization of rare tautomers in aqueous solution. *Journal of the American Chemical Society*, **2003**, 125, 7678-88	16.4	192
475	Base-base and deoxyribose-base stacking interactions in B-DNA and Z-DNA: a quantum-chemical study. *Biophysical Journal*, **1997**, 73, 76-87	2.9	185
474	Noncovalent interactions in biochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 3-17	7.9	184
473	The fluoroform?ethylene oxide complex exhibits a CH?O anti-hydrogen bond. *Chemical Physics Letters*, **1999**, 303, 447-452	2.5	179
472	DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations **1996**, 57, 959-970		179
471	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	16.4	177
470	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	3.4	175
469	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. *Physical Chemistry Chemical Physics*, **2002**, 4, 4192-4203	3.6	175
468	On the importance and origin of aromatic interactions in chemistry and biodisciplines. *Accounts of Chemical Research*, **2013**, 46, 927-36	24.3	171
467	Nonempirical calculations on all the 29 possible DNA base pairs. *Journal of the American Chemical Society*, **1987**, 109, 1302-1307	16.4	171
466	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	6.4	169
465	Improper, blue-shifting hydrogen bond. *Theoretical Chemistry Accounts*, **2002**, 108, 325-334	1.9	167
464	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, X-H/π) of WFT and DFT Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 66-80	6.4	166
463	Interaction between the Guanine–Cytosine Watson–Crick DNA Base Pair and Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and Group IIb (Zn2+, Cd2+, Hg2+) Metal Cations. *Journal of Physical Chemistry A*, **1998**, 102, 5951-5957	2.8	166
462	The World of Non-Covalent Interactions: 2006. *Collection of Czechoslovak Chemical Communications* , **2006**, 71, 443-531		161
461	Calculations on noncovalent interactions and databases of benchmark interaction energies. *Accounts of Chemical Research*, **2012**, 45, 663-72	24.3	160

460	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, 8257-63	2.8	160
459	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, 6803-17	4.8	155
458	MP2 and CCSD(T) study on hydrogen bonding, aromatic stacking and nonaromatic stacking. *Chemical Physics Letters*, **1997**, 267, 263-270	2.5	149
457	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	3.9	145
456	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, 2006-17	3.6	143
455	Electronic structures, vibrational spectra, and revised assignment of aniline and its radical cation: Theoretical study. *Journal of Chemical Physics*, **2003**, 118, 10900-10911	3.9	143
454	Structure and vibrational dynamics of the benzene dimer. *Journal of Chemical Physics*, **1999**, 111, 572-582	3.9	140
453	Floppy structure of the benzene dimer: Ab initio calculation on the structure and dipole moment. *Journal of Chemical Physics*, **1990**, 93, 5893-5897	3.9	139
452	Molecular dynamics simulations and thermodynamics analysis of DNA-drug complexes. Minor groove binding between 4',6-diamidino-2-phenylindole and DNA duplexes in solution. *Journal of the American Chemical Society*, **2003**, 125, 1759-69	16.4	136
451	The X3LYP extended density functional accurately describes H-bonding but fails completely for stacking. *Physical Chemistry Chemical Physics*, **2005**, 7, 1624-6	3.6	135
450	Unexpectedly strong energy stabilization inside the hydrophobic core of small protein rubredoxin mediated by aromatic residues: correlated ab initio quantum chemical calculations. *Journal of the American Chemical Society*, **2005**, 127, 2615-9	16.4	134
449	Base stacking in cytosine dimer. A comparison of correlated ab initio calculations with three empirical potential models and density functional theory calculations. *Journal of Computational Chemistry*, **1996**, 17, 841-850	3.5	134
448	Sequence-dependent elastic properties of DNA. *Journal of Molecular Biology*, **2000**, 299, 695-709	6.5	132
447	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, 2747-57	3.6	131
446	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	3.4	131
445	Improper, Blue-Shifting Hydrogen Bond between Fluorobenzene and Fluoroform *Journal of Physical Chemistry A*, **2001**, 105, 5560-5566	2.8	130
444	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		129
443	Acetic Acid Dimer in the Gas Phase, Nonpolar Solvent, Microhydrated Environment, and Dilute and Concentrated Acetic Acid: Ab Initio Quantum Chemical and Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2003**, 107, 3086-3092	2.8	129

442	Proton Transfer in the Adenine-Thymine Base Pair. *Journal of the American Chemical Society*, **1994**, 116, 1457-1460	16.4	129
441	Bifurcated hydrogen bonds in DNA crystal structures. An ab initio quantum chemical study. *Journal of the American Chemical Society*, **1994**, 116, 709-714	16.4	128
440	The lithium bond reexamined. *Chemical Reviews*, **1990**, 90, 1061-1076	68.1	126
439	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 5'-d(GCGAAGC)-3' hairpin: Complete basis set calculations at the MP2 and CCSD(T) levels. *Journal of Physical Chemistry A*, **2005**, 109, 1131-6	2.8	120
438	Design of HIV protease inhibitors based on inorganic polyhedral metallacarboranes. *Journal of Medicinal Chemistry*, **2009**, 52, 7132-41	8.3	119
437	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	3.9	119
436	Interaction of carboranes with biomolecules: formation of dihydrogen bonds. *ChemPhysChem*, **2006**, 7, 1100-5	3.2	118
435	C□H□□O Contacts in the Adenine□□Uracil Watson□Crick and Uracil□□Uracil Nucleic Acid Base Pairs: Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. *Journal of Physical Chemistry B*, **2000**, 104, 6286-6292	3.4	118
434	On Extension of the Current Biomolecular Empirical Force Field for the Description of Halogen Bonds. *Journal of Chemical Theory and Computation*, **2012**, 8, 1325-33	6.4	115
433	Counterpoise-corrected potential energy surfaces of simple H-bonded systems. *Theoretical Chemistry Accounts*, **1998**, 99, 372-377	1.9	114
432	The relative roles of electrostatics and dispersion in the stabilization of halogen bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 17742-51	3.6	113
431	Origin of the X-Hal (Hal = Cl, Br) bond-length change in the halogen-bonded complexes. *Journal of Physical Chemistry A*, **2008**, 112, 4114-9	2.8	110
430	The strength and directionality of a halogen bond are co-determined by the magnitude and size of the □hole. *Physical Chemistry Chemical Physics*, **2014**, 16, 9987-96	3.6	109
429	Thioguanine and Thiouracil: Hydrogen-Bonding and Stacking Properties. *Journal of Physical Chemistry A*, **1997**, 101, 9489-9495	2.8	109
428	Highly accurate CCSD(T) and DFT-SAPT stabilization energies of H-bonded and stacked structures of the uracil dimer. *ChemPhysChem*, **2008**, 9, 1636-44	3.2	108
427	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	3.6	107
426	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlated ab initio quantum chemical calculations and anharmonic analysis of the aniline inversion motion. *Journal of Chemical Physics*, **1996**, 105, 11042-11050	3.9	104
425	The dominant role of chalcogen bonding in the crystal packing of 2D/3D aromatics. *Angewandte Chemie - International Edition*, **2014**, 53, 10139-42	16.4	103

424	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, 12666-78	3.4	103
423	RI-MP2 calculations with extended basis sets□ promising tool for study of H-bonded and stacked DNA base pairs. *Physical Chemistry Chemical Physics*, **2001**, 3, 4578-4582	3.6	103
422	Assessment of the performance of MP2 and MP2 variants for the treatment of noncovalent interactions. *Journal of Physical Chemistry A*, **2012**, 116, 4159-69	2.8	101
421	Ab initio second- and fourth-order Mo/ller□Plesset study on structure, stabilization energy, and stretching vibration of benzene???X (X=He,Ne,Ar,Kr,Xe) van der Waals molecules. *Journal of Chemical Physics*, **1992**, 97, 335-340	3.9	101
420	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartree□Fock and Empirical Potential Studies. *Journal of Physical Chemistry A*, **1998**, 102, 6921-6926	2.8	100
419	A halogen-bonding correction for the semiempirical PM6 method. *Chemical Physics Letters*, **2011**, 506, 286-289	2.5	99
418	Hydrogen bonding, stacking and cation binding of DNA bases. *Computational and Theoretical Chemistry*, **2001**, 573, 43-53		98
417	Interaction of the Adenine□Thymine Watson□Crick and Adenine□Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:□Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. *Journal of Physical Chemistry B*, **1999**, 103, 2528-2534	3.4	98
416	Nonplanar DNA base pairs. *Journal of Biomolecular Structure and Dynamics*, **1996**, 13, 827-33	3.6	95
415	New structure for the most stable isomer of the benzene dimer: a quantum chemical study. *The Journal of Physical Chemistry*, **1993**, 97, 3937-3938		93
414	Potential Energy and Free Energy Surfaces of All Ten Canonical and Methylated Nucleic Acid Base Pairs: Molecular Dynamics and Quantum Chemical ab Initio Studies. *Journal of Physical Chemistry B*, **2001**, 105, 5804-5817	3.4	92
413	On differences between hydrogen bonding and improper blue-shifting hydrogen bonding. *ChemPhysChem*, **2005**, 6, 609-17	3.2	91
412	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	2.8	91
411	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	6.4	90
410	Vibrational spectroscopy of the G...C base pair: experiment, harmonic and anharmonic calculations, and the nature of the anharmonic couplings. *Journal of Physical Chemistry A*, **2005**, 109, 6974-84	2.8	90
409	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	3.4	89
408	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, 1191-203	3.4	87
407	Potential Energy Surface of the Cytosine Dimer:□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	3.4	86

406	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	3.6	86
405	On the performance of the semiempirical quantum mechanical PM6 and PM7 methods for noncovalent interactions. *Chemical Physics Letters*, **2013**, 568-569, 161-166	2.5	85
404	Study of the nature of improper blue-shifting hydrogen bonding and standard hydrogen bonding in the X3CH...OH2 and XH...OH2 complexes (X = F, Cl, Br, I): A correlated Ab initio study. *ChemPhysChem*, **2002**, 3, 511-8	3.2	83
403	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: An ab Initio Quantum Chemical Study. *Journal of Physical Chemistry A*, **2003**, 107, 1032-1039	2.8	83
402	Introduction: Noncovalent Interactions. *Chemical Reviews*, **2016**, 116, 4911-2	68.1	83
401	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. *Journal of Chemical Theory and Computation*, **2013**, 9, 4287-92	6.4	80
400	On the Nature of Bonding in Lone Pair Electron Complexes: CCSD(T)/Complete Basis Set Limit Calculations. *Journal of Chemical Theory and Computation*, **2009**, 5, 1180-5	6.4	79
399	Hydration and stability of nucleic acid bases and base pairs. *Physical Chemistry Chemical Physics*, **2007**, 9, 903-17	3.6	79
398	The H-index unambiguously discriminates between hydrogen bonding and improper blue-shifting hydrogen bonding. *Physical Chemistry Chemical Physics*, **2001**, 3, 2555-2556	3.6	79
397	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		79
396	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, 3522-34	3.6	78
395	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlated ab Initio Quantum Chemical and Empirical Potential Procedures. *Journal of Chemical Theory and Computation*, **2009**, 5, 982-92	6.4	78
394	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	3.9	78
393	Nonadiabatic dynamics of uracil: population split among different decay mechanisms. *Journal of Physical Chemistry A*, **2011**, 115, 5247-55	2.8	77
392	Strength and Character of Halogen Bonds in Protein Ligand Complexes. *Crystal Growth and Design*, **2011**, 11, 4272-4278	3.5	76
391	Na+, Mg2+, and Zn2+ binding to all tautomers of adenine, cytosine, and thymine and the eight most stable keto/enol tautomers of guanine: a correlated ab initio quantum chemical study. *Journal of Physical Chemistry B*, **2006**, 110, 14515-23	3.4	76
390	Modulation of aldose reductase inhibition by halogen bond tuning. *ACS Chemical Biology*, **2013**, 8, 2484-92	4.9	75
389	Semiempirical quantum mechanical method PM6-DH2X describes the geometry and energetics of CK2-inhibitor complexes involving halogen bonds well, while the empirical potential fails. *Journal of Physical Chemistry B*, **2011**, 115, 8581-9	3.4	75

388	Molecular Interactions of Nucleic Acid Bases. A Review of Quantum-Chemical Studies. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 2231-2282		75
387	Ab initio calculations on the structure, stabilization, and dipole moment of benzene???Ar complex. *Journal of Chemical Physics*, **1991**, 95, 391-394	3.9	74
386	Significant structural deformation of nucleic acid bases in stacked base pairs: an ab initio study beyond Hartree□ock. *Chemical Physics Letters*, **1998**, 288, 7-14	2.5	73
385	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. *ChemPlusChem*, **2013**, 78, 921-931	2.8	70
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