Jan M L Martin

List of Publications by Citations

307 papers	24,002 citations	82 h-index	144 g-index
319 ext. papers	25,926 ext. citations	4.5 avg, IF	7.41 L-index

#	Paper	IF	Citations
307	Development of density functionals for thermochemical kinetics. *Journal of Chemical Physics*, **2004**, 121, 3405-16	3.9	1213
306	Correlation consistent valence basis sets for use with the Stuttgart–Dresden–Bonn relativistic effective core potentials: The atoms Ga–Kr and In–Xe. *Journal of Chemical Physics*, **2001**, 114, 3408-3420	3.9	1139
305	Towards standard methods for benchmark quality ab initio thermochemistry—W1 and W2 theory. *Journal of Chemical Physics*, **1999**, 111, 1843-1856	3.9	852
304	Ab initio total atomization energies of small molecules—towards the basis set limit. *Chemical Physics Letters*, **1996**, 259, 669-678	2.5	620
303	Highly accurate first-principles benchmark data sets for the parametrization and validation of density functional and other approximate methods. Derivation of a robust, generally applicable, double-hybrid functional for thermochemistry and thermochemical kinetics. *Journal of Physical Chemistry A*, **2008**, 112, 12868-86	2.8	578
302	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. *Journal of Chemical Physics*, **2006**, 125, 144108	3.9	561
301	W3 theory: robust computational thermochemistry in the kJ/mol accuracy range. *Journal of Chemical Physics*, **2004**, 120, 4129-41	3.9	401
300	Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities. *Journal of Chemical Physics*, **2001**, 114, 6014-6029	3.9	400
299	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 1525-39	6.4	389
298	Halogen Bonds: Benchmarks and Theoretical Analysis. *Journal of Chemical Theory and Computation*, **2013**, 9, 1918-31	6.4	357
297	The anharmonic force field of ethylene, C2H4, by means of accurate ab initio calculations. *Journal of Chemical Physics*, **1995**, 103, 2589-2602	3.9	338
296	Comment on: "Estimating the Hartree–Fock limit from finite basis set calculations" [Jensen F (2005) Theor Chem Acc 113:267]. *Theoretical Chemistry Accounts*, **2006**, 115, 330-333	1.9	318
295	Frequency and zero-point vibrational energy scale factors for double-hybrid density functionals (and other selected methods): can anharmonic force fields be avoided?. *Journal of Physical Chemistry A*, **2015**, 119, 1701-14	2.8	315
294	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. *Physical Chemistry Chemical Physics*, **2011**, 13, 20104-7	3.6	304
293	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. *Chemical Physics Letters*, **2011**, 510, 165-178	2.5	285
292	"Turning Over" Definitions in Catalytic Cycles. *ACS Catalysis*, **2012**, 2, 2787-2794	13.1	282
291	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. *Journal of Physical and Chemical Reference Data*, **2005**, 34, 573-656	4.3	275

290	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction *Journal of Physical Chemistry C*, **2010**, 114, 20801-20808	3.8	261
289	An accurate ab initio quartic force field and vibrational frequencies for CH4 and isotopomers. *Journal of Chemical Physics*, **1995**, 102, 254-261	3.9	201
288	Spin-component-scaled double hybrids: An extensive search for the best fifth-rung functionals blending DFT and perturbation theory. *Journal of Computational Chemistry*, **2013**, 34, 2327-44	3.5	200
287	Basis set convergence for geometry and harmonic frequencies. Are h functions enough?. *Chemical Physics Letters*, **1994**, 225, 473-479	2.5	197
286	Double-hybrid functionals for thermochemical kinetics. *Journal of Physical Chemistry A*, **2008**, 112, 3-8	2.8	194
285	Benchmark study of DFT functionals for late-transition-metal reactions. *Journal of Physical Chemistry A*, **2006**, 110, 709-16	2.8	193
284	Benchmark ab Initio Energy Profiles for the Gas-Phase SN2 Reactions Y- + CH3X -hCH3Y + X- (X,Y = F,Cl,Br). Validation of Hybrid DFT Methods. *Journal of Physical Chemistry A*, **2001**, 105, 895-904	2.8	185
283	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2687-93	6.4	184
282	Explicitly correlated Wn theory: W1-F12 and W2-F12. *Journal of Chemical Physics*, **2012**, 136, 124114	3.9	176
281	Evidence for a terminal Pt(iv)-oxo complex exhibiting diverse reactivity. *Nature*, **2008**, 455, 1093-1096	50.4	176
280	Structure and vibrational spectra of carbon clusters Cn (n = 2 10, 12, 14, 16, 18) using density functional theory including exact exchange contributions. *Chemical Physics Letters*, **1995**, 242, 570-579	2.5	174
279	Basis set convergence in second-row compounds. The importance of core polarization functions. *Chemical Physics Letters*, **1998**, 282, 16-24	2.5	173
278	On the performance of density functional methods for describing atomic populations, dipole moments and infrared intensities. *Chemical Physics Letters*, **1996**, 250, 393-401	2.5	170
277	The atomization energy and proton affinity of NH3. An ab initio calibration study. *Chemical Physics Letters*, **1996**, 258, 136-143	2.5	169
276	Basis set convergence study of the atomization energy, geometry, and anharmonic force field of SO2: The importance of inner polarization functions. *Journal of Chemical Physics*, **1998**, 108, 2791-2800	3.9	161
275	The role of the basis set: Assessing density functional theory. *Journal of Chemical Physics*, **2003**, 119, 3005-3014	3.9	159
274	Basis set convergence and performance of density functional theory including exact exchange contributions for geometries and harmonic frequencies. *Molecular Physics*, **1995**, 86, 1437-1450	1.7	156
273	Formation of 2 CH Agostic Rhodium Arene Complexes and Their Relevance to Electrophilic Bond Activation. *Journal of the American Chemical Society*, **1998**, 120, 12539-12544	16.4	153

272	Computational study of a new heck reaction mechanism catalyzed by palladium(II/IV) species. *Chemistry - A European Journal*, **2001**, 7, 1703-11	4.8	149
271	Vibrational Spectra of the Azabenzenes Revisited:Anharmonic Force Fields *Journal of Physical Chemistry A*, **2004**, 108, 3085-3096	2.8	145
270	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. *Journal of Chemical Physics*, **2003**, 119, 5965-5980	3.9	145
269	Structure and Vibrations of Small Carbon Clusters from Coupled-Cluster Calculations. *The Journal of Physical Chemistry*, **1996**, 100, 6047-6056		145
268	Structure and Vibrational Spectrum of Some Polycyclic Aromatic Compounds Studied by Density Functional Theory. 1. Naphthalene, Azulene, Phenanthrene, and Anthracene *The Journal of Physical Chemistry*, **1996**, 100, 15358-15367		141
267	The geometry, vibrational frequencies, and total atomization energy of ethylene. A calibration study. *Chemical Physics Letters*, **1996**, 248, 336-344	2.5	141
266	Calculation of molecular electrostatic potentials and Fukui functions using density functional methods. *Chemical Physics Letters*, **1996**, 256, 400-408	2.5	136
265	Performance of ab initio and density functional methods for conformational equilibria of C(n)H(2n+2) alkane isomers (n = 4-8). *Journal of Physical Chemistry A*, **2009**, 113, 11974-83	2.8	134
264	A computational foray into the formation and reactivity of metallabenzenes. *Journal of the American Chemical Society*, **2004**, 126, 11699-710	16.4	131
263	Benchmark quality total atomization energies of small polyatomic molecules. *Journal of Chemical Physics*, **1997**, 106, 8620-8623	3.9	129
262	Gd3+ complexes as potential spin labels for high field pulsed EPR distance measurements. *Journal of the American Chemical Society*, **2007**, 129, 14138-9	16.4	129
261	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. *Journal of Physical Chemistry A*, **2019**, 123, 5129-5143	2.8	128
260	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 20905-25	3.6	127
259	Basis set convergence of post-CCSD contributions to molecular atomization energies. *Journal of Chemical Physics*, **2007**, 127, 064104	3.9	127
258	On the performance of correlation consistent basis sets for the calculation of total atomization energies, geometries, and harmonic frequencies. *Journal of Chemical Physics*, **1994**, 100, 8186-8193	3.9	124
257	Photochemical reduction of carbon dioxide catalyzed by a ruthenium-substituted polyoxometalate. *Chemistry - A European Journal*, **2010**, 16, 1356-64	4.8	123
256	On the effect of core correlation on the geometry and harmonic frequencies of small polyatomic molecules. *Chemical Physics Letters*, **1995**, 242, 343-350	2.5	123
255	The mechanism of aluminum-catalyzed Meerwein-Schmidt-Ponndorf-Verley reduction of carbonyls to alcohols. *Journal of the American Chemical Society*, **2004**, 126, 14796-803	16.4	120

254	An accurate ab initio quartic force field for ammonia. *Journal of Chemical Physics*, **1992**, 97, 8361-8371	3.9	118
253	A purely ab initio spectroscopic quality quartic force field for acetylene. *Journal of Chemical Physics*, **1998**, 108, 676-691	3.9	115
252	An Accurate ab Initio Quartic Force Field for Formaldehyde and Its Isotopomers. *Journal of Molecular Spectroscopy*, **1993**, 160, 105-116	1.3	112
251	Ab initio study of boron, nitrogen, and boron–nitrogen clusters. I. Isomers and thermochemistry of B3, B2N, BN2, and N3. *Journal of Chemical Physics*, **1989**, 90, 6469-6485	3.9	112
250	Chirality-induced spin polarization places symmetry constraints on biomolecular interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2474-2478	11.5	110
249	Benchmark thermochemistry of the C(n)H(2n+2) alkane isomers (n = 2-8) and performance of DFT and composite ab initio methods for dispersion-driven isomeric equilibria. *Journal of Physical Chemistry A*, **2009**, 113, 8434-47	2.8	110
248	On the integration accuracy in molecular density functional theory calculations using Gaussian basis sets. *Computer Physics Communications*, **2001**, 133, 189-201	4.2	110
247	Comparison of steric and electronic requirements for C-C and C-H bond activation. Chelating vs nonchelating case. *Journal of the American Chemical Society*, **2001**, 123, 9064-77	16.4	108
246	What Makes for a Bad Catalytic Cycle? A Theoretical Study on the Suzuki–Miyaura Reaction within the Energetic Span Model. *ACS Catalysis*, **2011**, 1, 246-253	13.1	106
245	The Silabenzenes: Structure, Properties, and Aromaticity. *Organometallics*, **2000**, 19, 1477-1487	3.8	105
244	Aromatic vs aliphatic C-H bond activation by rhodium(I) as a function of agostic interactions: catalytic H/D exchange between olefins and methanol or water. *Journal of the American Chemical Society*, **2003**, 125, 11041-50	16.4	104
243	Metallacarbenes from diazoalkanes: an experimental and computational study of the reaction mechanism. *Journal of the American Chemical Society*, **2003**, 125, 6532-46	16.4	102
242	The rate-determining step is dead. Long live the rate-determining state!. *ChemPhysChem*, **2011**, 12, 1413-8	3.2	99
241	Alkali and alkaline earth metal compounds: core–valence basis sets and importance of subvalence correlation. *Molecular Physics*, **2003**, 101, 1345-1361	1.7	99
240	ortho C–H Activation of Haloarenes and Anisole by an Electron-Rich Iridium(I) Complex: Mechanism and Origin of Regio- and Chemoselectivity. An Experimental and Theoretical Study. *Organometallics*, **2006**, 25, 3190-3210	3.8	98
239	On the performance of large Gaussian basis sets for the computation of total atomization energies. *Journal of Chemical Physics*, **1992**, 97, 5012-5018	3.9	93
238	Charge Transport in Conjugated Aromatic Molecular Junctions: Molecular Conjugation and Molecule–Electrode Coupling. *Journal of Physical Chemistry C*, **2007**, 111, 14893-14902	3.8	89
237	Active site electronic structure and dynamics during metalloenzyme catalysis. *Nature Structural Biology*, **2003**, 10, 98-103		89

236	Electron affinities of the first- and second-row atoms: Benchmark ab initio and density-functional calculations. *Physical Review A*, **1999**, 60, 1034-1045	2.6	89
235	Ab initio study of the infrared spectra of linear Cn clusters (n=6). *Journal of Chemical Physics*, **1990**, 93, 8850-8861	3.9	89
234	A simple DFT-based diagnostic for nondynamical correlation. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	88
233	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. *Journal of Computational Chemistry*, **2017**, 38, 2063-2075	3.5	85
232	Basis set limit coupled cluster study of h-bonded systems and assessment of more approximate methods. *Journal of Physical Chemistry A*, **2007**, 111, 11122-33	2.8	85
231	Structure and Vibrational Spectra of the Azabenzenes. A Density Functional Study Including Exact Exchange Contributions. *The Journal of Physical Chemistry*, **1996**, 100, 6973-6983		85
230	Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 3791-9	6.4	84
229	Accurate ab initio quartic force field for trans-HNNH and treatment of resonance polyads. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1997**, 53, 1039-1050	4.4	84
228	A Thiourea Tether in the Second Coordination Sphere as a Binding Site for CO and a Proton Donor Promotes the Electrochemical Reduction of CO to CO Catalyzed by a Rhenium Bipyridine-Type Complex. *Journal of the American Chemical Society*, **2018**, 140, 12451-12456	16.4	83
227	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. *Chemical Physics Letters*, **1997**, 275, 414-422	2.5	82
226	Heats of formation of beryllium, boron, aluminum, and silicon re-examined by means of W4 theory. *Journal of Physical Chemistry A*, **2007**, 111, 5936-44	2.8	82
225	Co-Crystallization of Sym-Triiodo-Trifluorobenzene with Bipyridyl Donors: Consistent Formation of Two Instead of Anticipated Three N Halogen Bonds. *Crystal Growth and Design*, **2007**, 7, 386-392	3.5	81
224	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. *Journal of Physical Chemistry A*, **2013**, 117, 2269-77	2.8	77
223	Selective C vs C H Bond Activation by Rhodium(I) PCP Pincer Complexes. A Computational Study. *Journal of the American Chemical Society*, **2000**, 122, 7095-7104	16.4	77
222	Ab initio multireference study of the BN molecule. *Journal of Chemical Physics*, **1992**, 97, 6549-6556	3.9	76
221	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 444-54	6.4	75
220	The ground-state spectroscopic constants of Be2 revisited. *Chemical Physics Letters*, **1999**, 303, 399-407	2.5	75
219	On the structure and vibrational frequencies of C20. *Chemical Physics Letters*, **1996**, 248, 345-352	2.5	73

218	Reactions of pulsed laser produced boron and nitrogen atoms in a condensing argon stream. *Journal of Chemical Physics*, **1993**, 98, 922-931	3.9	72
217	Post-CCSD(T) ab initio thermochemistry of halogen oxides and related hydrides XOX, XOOX, HOX, XOn, and HXOn (X = F, Cl), and evaluation of DFT methods for these systems. *Journal of Physical Chemistry A*, **2009**, 113, 4802-16	2.8	71
216	A critical comparison of MINDO/3, MNDO, AM1, and PM3 for a model problem: Carbon clusters C2-C10. An ad hoc reparametrization of MNDO well suited for the accurate prediction of their spectroscopic constants. *Journal of Computational Chemistry*, **1991**, 12, 52-70	3.5	71
215	Empirical Double-Hybrid Density Functional Theory: A 'third Way' in Between WFT and DFT. *Israel Journal of Chemistry*, **2020**, 60, 787-804	3.4	71
214	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides: Surprisingly Demanding Targets for High-Level ab Initio Procedures. *Journal of Physical Chemistry A*, **2003**, 107, 5617-5630	2.8	70
213	Accurate ab initio quartic force fields for the N2O and CO2 molecules. *Chemical Physics Letters*, **1993**, 205, 535-542	2.5	70
212	Spectroscopic quality ab initio potential curves for CH, NH, OH and HF. A convergence study. *Chemical Physics Letters*, **1998**, 292, 411-420	2.5	69
211	Structure and relative energetics of C2n+1 (n = 2–7) carbon clusters using coupled cluster and hybrid density functional methods. *Chemical Physics Letters*, **1996**, 252, 9-18	2.5	69
210	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. *Journal of Chemical Physics*, **2016**, 144, 214101	3.9	69
209	Ab Initio Geometry Determinations of Proteins. 1. Crambin. *Journal of Physical Chemistry A*, **1998**, 102, 2246-2251	2.8	66
208	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. *Journal of Chemical Theory and Computation*, **2017**, 13, 3136-3152	6.4	65
207	Metallabenzene versus Cp complex formation: a DFT investigation. *Journal of the American Chemical Society*, **2003**, 125, 13020-1	16.4	65
206	Pulsed laser evaporated boron atom reactions with acetylene. Infrared spectra and quantum chemical structure and frequency calculations for several novel organoborane BC2H2 and HBC2 molecules. *The Journal of Physical Chemistry*, **1993**, 97, 5839-5847		65
205	Borane-lewis base complexes as homolytic hydrogen atom donors. *Chemistry - A European Journal*, **2010**, 16, 6861-5	4.8	64
204	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. *International Journal of Quantum Chemistry*, **2005**, 104, 830-845	2.1	64
203	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	63
202	Selective sp3 C-H activation of ketones at the beta position by Ir(I). Origin of regioselectivity and water effect. *Journal of the American Chemical Society*, **2006**, 128, 12400-1	16.4	63
201	Ab initio study of the structure, infrared spectra, and heat of formation of C4. *Journal of Chemical Physics*, **1991**, 94, 3753-3761	3.9	63

200	Directing aryl-I versus Aryl-Br bond activation by nickel via a ring walking process. *Inorganic Chemistry*, **2008**, 47, 5114-21	5.1	60
199	The unexpected role of CO in C--H oxidative addition by a cationic rhodium(I) complex. *Angewandte Chemie - International Edition*, **2007**, 46, 1901-4	16.4	60
198	First principles computation of thermochemical properties beyond the harmonic approximation. I. Method and application to the water molecule and its isotopomers. *Journal of Chemical Physics*, **1992**, 96, 7633-7645	3.9	60
197	TpPtMe(H)(2): why is there H/D scrambling of the methyl group but not methane loss?. *Journal of the American Chemical Society*, **2002**, 124, 7041-54	16.4	59
196	Anharmonic force field and vibrational frequencies of tetrafluoromethane (CF4) and tetrafluorosilane (SiF4). *Journal of Chemical Physics*, **2000**, 112, 1353-1366	3.9	59
195	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. *Physical Chemistry Chemical Physics*, **2013**, 15, 7028-31	3.6	57
194	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Born□Oppenheimer corrections for a □simple□ organic molecule. *Computational and Theoretical Chemistry*, **2007**, 811, 345-353		57
193	Definitive heat of formation of methylenimine, CH2?NH, and of methylenimmonium ion, CH2NH2+, by means of W2 theory. *Journal of Computational Chemistry*, **2001**, 22, 1297-1305	3.5	57
192	Ab initio study of the spectroscopy and thermochemistry of the C2N and CN2 molecules. *Chemical Physics Letters*, **1994**, 226, 475-483	2.5	57
191	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. *Journal of Chemical Physics*, **2010**, 133, 144102	3.9	56
190	Accurate ab initio quartic force fields for borane and BeH2. *Chemical Physics Letters*, **1992**, 200, 502-510	2.5	56
189	Economical post-CCSD(T) computational thermochemistry protocol and applications to some aromatic compounds. *Journal of Physical Chemistry A*, **2009**, 113, 7610-20	2.8	55
188	Platinum stilbazoles: ring-walking coupled with aryl-halide bond activation. *Journal of the American Chemical Society*, **2005**, 127, 9322-3	16.4	54
187	Infrared Spectra of Boron-Ammonia Reaction Products in Solid Argon. *The Journal of Physical Chemistry*, **1995**, 99, 13839-13849		54
186	Accurate ab initio quartic force fields for the ions HCO+ and HOC+. *Journal of Chemical Physics*, **1993**, 99, 286-292	3.9	53
185	Potential energy surface of B4 and total atomization energies of B2, B3, and B4. *Chemical Physics Letters*, **1992**, 189, 529-536	2.5	53
184	Anharmonic force fields and thermodynamic functions using density functional theory. *Molecular Physics*, **2005**, 103, 863-876	1.7	52
183	Heat of atomization of sulfur trioxide, SO3: a benchmark for computational thermochemistry. *Chemical Physics Letters*, **1999**, 310, 271-276	2.5	52

182	What can we learn about dispersion from the conformer surface of n-pentane?. *Journal of Physical Chemistry A*, **2013**, 117, 3118-32	2.8	51
181	Cycloaddition reactions of metalloaromatic complexes of iridium and rhodium: a mechanistic DFT investigation. *Journal of the American Chemical Society*, **2003**, 125, 11702-9	16.4	51
180	Note on the vibrational spectrum of C4 and C5. *Journal of Chemical Physics*, **1989**, 90, 3403-3405	3.9	50
179	Accurate ab initio quartic force field and vibrational frequencies of the NH4+ ion and its deuterated forms. *Chemical Physics Letters*, **1996**, 258, 129-135	2.5	48
178	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. *Journal of Computational Chemistry*, **2016**, 37, 49-58	3.5	47
177	Explicitly correlated benchmark calculations on C8H8 isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. *Molecular Physics*, **2012**, 110, 2477-2491	1.7	47
176	DFT study of the structure and reactivity of the terminal Pt(IV)-oxo complex bearing no electron-withdrawing ligands. *Journal of the American Chemical Society*, **2010**, 132, 14886-900	16.4	46
175	sp3 C□H and sp2 C□H agostic ruthenium complexes: a combined experimental and theoretical study. *Inorganica Chimica Acta*, **2004**, 357, 1854-1864	2.7	46
174	Conformational equilibria in butane-1,4-diol: a benchmark of a prototypical system with strong intramolecular H-bonds. *Journal of Physical Chemistry A*, **2014**, 118, 293-303	2.8	45
173	Effect of CO on the oxidative addition of arene C-H bonds by cationic rhodium complexes. *Chemistry - A European Journal*, **2010**, 16, 328-53	4.8	45
172	Discovery of the First Metallaquinone. *Journal of the American Chemical Society*, **2000**, 122, 8797-8798	16.4	45
171	The structure, stability, and infrared spectrum of B2N, B2N+, B2N□BO, B2O and B2N2.. *Chemical Physics Letters*, **1992**, 193, 243-250	2.5	45
170	Benchmark ab initio calculations of the total atomization energies of the first-row hydrides AHn (A = Li?F). *Chemical Physics Letters*, **1997**, 273, 98-106	2.5	44
169	Pi-accepting-pincer rhodium complexes: an unusual coordination mode of PCP-type systems. *Chemistry - A European Journal*, **2005**, 11, 2319-26	4.8	44
168	Thermochemical analysis of core correlation and scalar relativistic effects on molecular atomization energies. *Journal of Chemical Physics*, **2000**, 113, 1348-1358	3.9	44
167	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. *Molecular Physics*, **2015**, 113, 1551-1558	1.7	43
166	NLO properties of metallabenzene-based chromophores: a time-dependent density functional study. *Journal of Physical Chemistry A*, **2005**, 109, 5454-62	2.8	43
165	Structure and vibrations of BnNn (n = 3□10). *Chemical Physics Letters*, **1996**, 248, 95-101	2.5	43

164	Structure and infrared spectroscopy of the C11 molecule. *Chemical Physics Letters*, **1991**, 187, 367-374	2.5	43
163	Electron Transfer Oxidation of Benzene and Aerobic Oxidation to Phenol. *ACS Catalysis*, **2016**, 6, 6403-6407	11.1	41
162	Chapter 3 Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches. *Annual Reports in Computational Chemistry*, **2005**, 1, 31-43	1.8	41
161	On the structure and vibrational frequencies of C24. *Chemical Physics Letters*, **1996**, 255, 7-14	2.5	41
160	Heats of formation of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. Probing the limits of W1 and W2 theory. *Computational and Theoretical Chemistry*, **2006**, 771, 19-26		40
159	The lowest singlet-triplet excitation energy of BN: A converged coupled cluster perspective. *Journal of Chemical Physics*, **2006**, 125, 144313	3.9	39
158	Pulsed laser evaporation of boron/carbon pellets: Infrared spectra and quantum chemical structures and frequencies for BC2. *Journal of Chemical Physics*, **1993**, 99, 12-17	3.9	39
157	Polyoxometalate-catalyzed insertion of oxygen from O(2) into tin-alkyl bonds. *Journal of the American Chemical Society*, **2013**, 135, 19304-10	16.4	38
156	Energetics of Acetylene Loss from C14H10+ Cations: A Density Functional Calculation. *Journal of Physical Chemistry A*, **1997**, 101, 219-226	2.8	38
155	Accurate ab initio total atomization energies of the Cn clusters (n=2–10). *Journal of Chemical Physics*, **1995**, 102, 8270-8273	3.9	38
154	The total atomization energy and heat of formation of HCN(g). *Chemical Physics Letters*, **1996**, 259, 679-682	2.5	38
153	Is there evidence for detection of cyclic C4 in IR spectra? An accurate ab initio computed quartic force field. *Journal of Chemical Physics*, **1996**, 104, 4657-4663	3.9	38
152	Ab initio study of the molecules BC and B2C. *Journal of Chemical Physics*, **1994**, 100, 9002-9006	3.9	38
151	Atomization energies of the carbon clusters C n (n = 2–10) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. *Molecular Physics*, **2009**, 107, 977-990	1.7	37
150	Fully ab initio atomization energy of benzene via Weizmann-2 theory. *Journal of Chemical Physics*, **2001**, 115, 2051-2054	3.9	37
149	The vibrational spectra of corannulene and coronene. A density functional study. *Chemical Physics Letters*, **1996**, 262, 97-104	2.5	37
148	Combined bond-polarization basis sets for accurate determination of dissociation energies. *Theoretica Chimica Acta*, **1989**, 76, 195-209		37
147	Anharmonic Force Fields and Accurate Thermochemistry of H2SiO, cis-HSiOH, and trans-HSiOH. *Journal of Physical Chemistry A*, **1998**, 102, 1394-1404	2.8	36

146	Tuning of Au/n-GaAs Diodes with Highly Conjugated Molecules. *Journal of Physical Chemistry B*, **2001**, 105, 12011-12018	3.4	36
145	Structures of Furanosides: Density Functional Calculations and High-Resolution X-ray and Neutron Diffraction Crystal Structures. *Journal of Physical Chemistry A*, **1999**, 103, 744-753	2.8	36
144	Accurate ab-Initio Quartic Force Fields for the Sulfur Compounds H2S, CS2, OCS, and CS. *Journal of Molecular Spectroscopy*, **1995**, 169, 445-457	1.3	36
143	Structures and thermochemistry of B3N3 and B4N4. *Chemical Physics Letters*, **1995**, 232, 289-294	2.5	36
142	Novel azine reactivity: facile N-N bond cleavage, C-H activation, and N-N coupling mediated by RhI. *Angewandte Chemie - International Edition*, **2003**, 42, 1949-52	16.4	35
141	Benchmark ab initio thermochemistry of the isomers of diimide, N2H2, using accurate computed structures and anharmonic force fields. *Molecular Physics*, **1999**, 96, 681-692	1.7	35
140	C28: the smallest stable fullerene?. *Chemical Physics Letters*, **1996**, 255, 1-6	2.5	35
139	The mechanism of the reaction CH+N2-ĦCN+N. *Chemical Physics Letters*, **1993**, 209, 143-150	2.5	35
138	The aug-cc-pVnZ-F12 basis set family: Correlation consistent basis sets for explicitly correlated benchmark calculations on anions and noncovalent complexes. *Journal of Chemical Physics*, **2017**, 147, 134106	3.9	34
137	Assessment of CCSD(T)-F12 Approximations and Basis Sets for Harmonic Vibrational Frequencies. *Journal of Chemical Theory and Computation*, **2014**, 10, 2085-90	6.4	34
136	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	33
135	Ab Initio Calibration Study of the Heat of Formation, Geometry, and Anharmonic Force Field of Fluoroacetylene. *Journal of Physical Chemistry A*, **1998**, 102, 2483-2492	2.8	33
134	Revised Heat of Formation for Gaseous Boron: Basis Set Limit ab Initio Binding Energies of BF3 and BF. *Journal of Physical Chemistry A*, **1998**, 102, 2995-2998	2.8	33
133	Accurate ab Initio Quartic Force Fields, Vibrational Frequencies, and Heats of Formation for FCN, FNC, ClCN, and ClNC. *The Journal of Physical Chemistry*, **1995**, 99, 15858-15863		33
132	Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted pyridines in the gas phase by means of MINDO/3, MNDO, and AM1. *Journal of Computational Chemistry*, **1989**, 10, 449-467	3.5	33
131	What Are the Ground State Structures of C20 and C24? An Explicitly Correlated Ab Initio Approach. *Journal of Physical Chemistry A*, **2016**, 120, 153-60	2.8	32
130	What makes for a good catalytic cycle? A theoretical study of the SPhos ligand in the Suzuki-Miyaura reaction. *Chemical Communications*, **2011**, 47, 4935-7	5.8	32
129	Ab initio study of the X2Π and A2□states of the SiN radical. *Chemical Physics Letters*, **1996**, 252, 398-404	2.5	32

128	Exclusive C Activation in the Rhodium(I) PCN Pincer Complex. A Computational Study. *Organometallics*, **2001**, 20, 1783-1791	3.8	31
127	A fully ab initio quartic force field of spectroscopic quality for SO3. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1999**, 55, 709-718	4.4	31
126	Boron Heat of Formation Revisited:Relativistic Effects on the BF3Atomization Energy. *Journal of Physical Chemistry A*, **1999**, 103, 7715-7718	2.8	31
125	Accurate ab initio predictions of the dissociation energy and heat of formation of first-row hydrides. *Chemical Physics Letters*, **1989**, 163, 387-391	2.5	31
124	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. *Australian Journal of Chemistry*, **2018**, 71, 238	1.2	30
123	Exclusive C Oxidative Addition in a Rhodium Thiophosphoryl Pincer Complex and Computational Evidence for an B-C H Agostic Intermediate. *Organometallics*, **2012**, 31, 505-512	3.8	30
122	Mechanistic aspects of acetone addition to metalloaromatic complexes of iridium: a DFT investigation. *Chemical Communications*, **2003**, 132-3	5.8	30
121	Anharmonic force field, structure, and thermochemistry of CF2 and CCl2. *Physical Chemistry Chemical Physics*, **2002**, 4, 3282-3288	3.6	30
120	A Definitive Heat of Vaporization of Silicon through Benchmark ab Initio Calculations on SiF4. *Journal of Physical Chemistry A*, **1999**, 103, 4427-4431	2.8	30
119	The dissociation energy of N3. *Journal of Chemical Physics*, **1990**, 93, 4485-4487	3.9	30
118	Thermodynamic Properties of C1and C2Bromo Compounds and Radicals. A Relativistic ab Initio Study. *Journal of Physical Chemistry A*, **2004**, 108, 7752-7761	2.8	29
117	Accurate ab initio anharmonic force field and heat of formation for silane. *Molecular Physics*, **1999**, 97, 945-953	1.7	29
116	Boron atom reactions with acetylene. Ab initio calculated and observed isotopic infrared spectra of the borirene radical BC2H2. A fingerprint match. *Journal of the American Chemical Society*, **1993**, 115, 2510-2511	16.4	29
115	Accurate ab initio spectroscopic and thermodynamic properties for the SiC molecule. *Journal of Chemical Physics*, **1990**, 92, 6655-6667	3.9	29
114	Benchmark ab initio potential curves for the light diatomic hydrides. Unusually large nonadiabatic effects in BeH and BH. *Chemical Physics Letters*, **1998**, 283, 283-293	2.5	28
113	On the geometrical structure of the C+3 cationAn ab initio study. *Journal of Chemical Physics*, **1990**, 93, 5037-5045	3.9	28
112	Density-Functional Theory Concepts and Techniques for Studying Molecular Charge Distributions and Related Properties. *Theoretical and Computational Chemistry*, **1996**, 773-809		27
111	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. *Journal of Chemical Physics*, **2018**, 149, 154109	3.9	27

110	Very accurate ab initio binding energies: a comparison between empirical corrections and extrapolation methods. *Computational and Theoretical Chemistry*, **1997**, 398-399, 135-144		26
109	The protonation of N2O reexamined: A case study on the reliability of various electron correlation methods for minima and transition states. *Journal of Chemical Physics*, **1993**, 98, 7951-7957	3.9	26
108	Ab Initio Study of the Isoelectronic Molecules BCN, BNC, and C3 Including Anharmonicity. *The Journal of Physical Chemistry*, **1994**, 98, 6105-6109		26
107	On the heat of formation of C5 and higher carbon clusters. *Journal of Chemical Physics*, **1991**, 95, 9420-9421	3.9	26
106	Combined bond-polarization basis sets for accurate determination of dissociation energies. II. Basis set superposition error as a function of the parent basis set. *Journal of Computational Chemistry*, **1989**, 10, 875-886	3.5	26
105	Halogen-Bonded Supramolecular Assemblies Based on Phenylethynyl Pyridine Derivatives: Driving Crystal Packing through Systematic Chemical Modifications. *Crystal Growth and Design*, **2008**, 8, 3066-3072	3.5	25
104	An accurate quartic force field, fundamental frequencies, and binding energy for the high energy density material TdN4. *Chemical Physics Letters*, **2002**, 357, 319-325	2.5	25
103	Combined bond polarization function basis sets for accurate ab initio calculation of the dissociation energies of AHn molecules (A=LI to F). *Journal of Computational Chemistry*, **1989**, 10, 152-162	3.5	25
102	Coupling between the convergence behavior of basis set and electron correlation: a quantitative study. *Theoretical Chemistry Accounts*, **1997**, 97, 227-231	1.9	24
101	The X40□10 Halogen Bonding Benchmark Revisited: Surprising Importance of (n-1)d Subvalence Correlation. *Journal of Physical Chemistry A*, **2018**, 122, 2184-2197	2.8	23
100	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. *Journal of Chemical Physics*, **2011**, 135, 144119	3.9	23
99	Arene Hapticity in (C6H6)Cr(CO)n (n = 1□3) Complexes: A DFT Study of Singlet and Triplet Energy Surfaces. *Organometallics*, **2004**, 23, 2315-2325	3.8	23
98	The structure, energetics, and harmonic vibrations of B3N and BN3. *Molecular Physics*, **1994**, 82, 155-164	1.7	23
97	The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. *ChemPhysChem*, **2020**, 21, 688-696	3.2	23
96	W1 and W2 Theories, and Their Variants: Thermochemistry in the kJ/mol Accuracy Range **2001**, 31-65		23
95	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: Hückel-Möbius Interconversions in Expanded Porphyrins. *Journal of Chemical Theory and Computation*, **2020**, 16, 3641-3653	6.4	22
94	A fully ab initio potential curve of near-spectroscopic quality for OH- ion: importance of connected quadruple excitations and scalar relativistic effects. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2001**, 57, 875-85	4.4	22
93	Accurate ab Initio Quartic Force Fields and Thermochemistry of FNO and ClNO. *The Journal of Physical Chemistry*, **1994**, 98, 11394-11400		22

92	On the vibrational spectrum of C9, C11 and C13. *Chemical Physics Letters*, **1995**, 240, 521-525	2.5	22
91	The eight-valence-electron systems re-examined: convergence of the coupled-cluster series and performance of quasiperturbative methods for quadruple excitations. *Molecular Physics*, **2014**, 112, 785-793	1.7	21
90	Mechanism of the Methylene Transfer Reaction. C□ Activation and Reductive Elimination in One System. A DFT Study. *Organometallics*, **2004**, 23, 2336-2342	3.8	21
89	The structure and energetics of B3N2, B2N3, and BN4. *Molecular Physics*, **1995**, 85, 527-537	1.7	21
88	Ab initio study of the carbon (C3+) cation using multireference methods. *The Journal of Physical Chemistry*, **1991**, 95, 6530-6534		21
87	The structure, energetics and harmonic vibrations of B3N. *Chemical Physics Letters*, **1993**, 201, 54-58	2.5	21
86	The impact of quantum chemical methods on the interpretation of molecular spectra of carbon clusters. *Journal of Molecular Structure*, **1993**, 294, 21-24	3.4	21
85	Tautomerization and Dissociation of Dimethyl Phosphonate Ions(CH3O)2P(H)=O□:Theory and Experiment in Concert. *Zeitschrift Fur Physikalische Chemie*, **2001**, 215,	3.1	20
84	The Anharmonic Force Field of Thioformaldehyde, H2CS, by ab Initio Methods. *Journal of Molecular Spectroscopy*, **1994**, 168, 363-373	1.3	20
83	Ab initio study of the proton affinity of a number of ortho-substituted pyridines. *Journal of Computational Chemistry*, **1989**, 10, 346-357	3.5	20
82	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. *Journal of Chemical Theory and Computation*, **2020**, 16, 4238-4255	6.4	19
81	Structure and Vibrations of the C2P and CNP Radicals and Their Cations Using Density Functional and Coupled Cluster Theories. *Journal of Physical Chemistry A*, **1997**, 101, 8319-8326	2.8	19
80	Catalytic reduction of acetone by [(bpy)Rh]+: a theoretical mechanistic investigation and insight into cooperativity effects in this system. *Journal of the American Chemical Society*, **2003**, 125, 11430-41	16.4	19
79	The heats of formation of the haloacetylenes XCCY [X, Y = H, F, Cl]: basis set limit ab initio results and thermochemical analysis. *Molecular Physics*, **2002**, 100, 453-464	1.7	19
78	Ab initio study of the spectroscopy, kinetics, and thermochemistry of the BN2 molecule. *Chemical Physics Letters*, **1994**, 222, 517-523	2.5	19
77	Concerning the heats of formation of the [C, H3, N]+ radical cations. *Chemical Physics Letters*, **1994**, 221, 149-155	2.5	18
76	On the effect of centrifugal stretching on the rotational partition function of an asymmetric top. *Journal of Chemical Physics*, **1991**, 95, 8374-8389	3.9	18
75	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. *Journal of Chemical Theory and Computation*, **2021**, 17, 1368-1379	6.4	18

74	Ab Initio Study of the Electronic Spectrum of the SiN Radical. *Journal of Molecular Spectroscopy*, **1998**, 188, 27-36	1.3	17
73	Calibration Study of Atomization Energies of Small Polyatomics. *ACS Symposium Series*, **1998**, 212-236	0.4	17
72	First principles computation of thermochemical properties beyond the harmonic approximation. II. Application to the amino radical NH2. *Journal of Chemical Physics*, **1992**, 97, 3530-3536	3.9	17
71	On size-consistency corrections for limited configuration-interaction calculations. *Chemical Physics Letters*, **1990**, 172, 346-353	2.5	17
70	CO-Induced Methyl Migration in a Rhodium Thiophosphoryl Pincer Complex and Its Comparison with Phosphine-Based Complexes: The Divergent Effects of S and P Donor Ligands. *Organometallics* , **2013**, 32, 7163-7180	3.8	16
69	Can DFT methods correctly and efficiently predict the coordination number of copper(I) complexes? A case study. *Journal of Computational Chemistry*, **2010**, 31, 75-83	3.5	16
68	Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted phenolate ions in the gas phase by means of MINDO/3, MNDO, and AM1. *Journal of Computational Chemistry*, **1990**, 11, 269-290	3.5	16
67	O(3P) + CO2 collisions at hyperthermal energies: dynamics of nonreactive scattering, oxygen isotope exchange, and oxygen-atom abstraction. *Journal of Physical Chemistry A*, **2012**, 116, 64-84	2.8	15
66	Insertion of Amines and Alcohols into Proton-Bound Dimers. A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 2597-2606	2.8	15
65	Fundamental vibrational frequencies and dominant resonances in methylamine isotopologues by ab initio and density functional theory methods. *Journal of Computational Chemistry*, **2008**, 29, 1268-76	3.5	15
64	Structures and thermochemistry of calcium-containing molecules. *Journal of Physical Chemistry A*, **2005**, 109, 9156-68	2.8	15
63	Comment on A theoretical study of the dissociation energy of BH using quadratic configuration interaction *Journal of Chemical Physics*, **1989**, 91, 4425-4426	3.9	15
62	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with DSD as a Special Case. *Journal of Physical Chemistry A*, **2021**, 125, 4614-4627	2.8	15
61	W4 thermochemistry of P2 and P4. Is the CODATA heat of formation of the phosphorus atom correct?. *Molecular Physics*, **2007**, 105, 2499-2505	1.7	14
60	Ab initio spectroscopy and thermochemistry of the BN molecule. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 21, 47-55		14
59	The impact of larger clusters formation C5, C6, C7, C8, C9, and C10 on the rates of carbon sublimation at elevated temperatures. *Journal of Nuclear Materials*, **1998**, 258-263, 782-786	3.3	13
58	Polarizability of small carbon cluster anions from first principles. *Journal of Physical Chemistry A*, **2007**, 111, 2028-32	2.8	13
57	Proton walk in the aqueous platinum complex [TpPtMeCO] via a sticky sigma-methane ligand. *Chemistry - A European Journal*, **2007**, 13, 2812-23	4.8	13

56	Anharmonic force fields of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. An extreme case of inner polarization. *Journal of Molecular Structure*, **2006**, 780-781, 310-316	3.4	13
55	Modeling Proton-Bound Methanol, Ammonia, and Amine Complexes of 12-Crown-4-Ether and Dimethoxyethane (Glyme) Using Density Functional Theory. *Journal of Physical Chemistry A*, **1998**, 102, 6357-6365	2.8	13
54	A coordination controlled aryl-halide oxidative addition to platinum. *Chemistry - A European Journal* , **2009**, 15, 10025-8	4.8	12
53	Comment on "Revised electron affinity of SF6 from kinetic data" [J. Chem. Phys. 136, 121102 (2012)]. *Journal of Chemical Physics*, **2012**, 136, 197101	3.9	12
52	Density Functional Study of the Complexation Reaction of Sn(CH3)3X (X = F, Cl, Br and I) with Halide Anions. *European Journal of Inorganic Chemistry*, **2003**, 2003, 3803-3810	2.3	12
51	Structures of Furanosides: A Study of the Conformational Space of Methyl -d-Lyxofuranoside by Density Functional Methods. *Journal of Physical Chemistry A*, **2000**, 104, 5291-5297	2.8	12
50	On the validity of Pople's infinite-order Mller-Plesset extrapolation and an alternative formula within MBP/CC theories. *Chemical Physics Letters*, **1989**, 157, 217-223	2.5	12
49	Prediction of electronic couplings for molecular charge transfer using optimally tuned range-separated hybrid functionals. *Molecular Physics*, **2018**, 116, 2497-2505	1.7	12
48	Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Core-Valence Correlation, and F12 Alternatives. *Journal of Chemical Theory and Computation*, **2020**, 16, 7507-7524	6.4	11
47	Performance of Electronic Structure Methods for the Description of Hkel-Mbius Interconversions in Extended Systems. *Journal of Physical Chemistry A*, **2020**, 124, 2380-2397	2.8	11
46	Probing the basis set limit for thermochemical contributions of inner-shell correlation: balance of core-core and core-valence contributions** In memory of Dieter Cremer (19442017)View all notes. *Molecular Physics*, **2019**, 117, 1078-1087	1.7	11
45	Comment on "Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0" [J. Chem. Phys. 136, 174103 (2012)]. *Journal of Chemical Physics*, **2015**, 143, 187101; discussion 187102	3.9	11
44	Modeling stabilization of Si?O bonds by Pd/Pt complexes using density functional theory. *Chemical Physics Letters*, **1998**, 288, 356-362	2.5	11
43	The impact of weak C-H...Rh interactions on the structure and reactivity of trans-[Rh(CO)2(phosphine)2]+: an experimental and theoretical examination. *Chemistry - A European Journal*, **2008**, 14, 8183-94	4.8	11
42	Energetics of the naphthalene/azulene monocation isomerization: density functional and coupled cluster calculations *Journal of the Chemical Society Perkin Transactions II*, **1999**, 2383-2387		11
41	On the relative stabilities of the linear and triangular forms of B3N. *Chemical Physics*, **1993**, 178, 77-82	2.3	11
40	New ruthenium nitrosyl pincer complexes bearing an O2 ligand. Mono-oxygen transfer. *Inorganic Chemistry*, **2015**, 54, 2253-63	5.1	10
39	Is there a satisfactory description of the molecular structure of Roesky ketone?. *Chemical Physics Letters*, **2005**, 413, 440-444	2.5	10

38	Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections. *Journal of Physical Chemistry A*, **2021**, 125, 4628-4638	2.8	10
37	Why Does the Tetrakis(trimethylphosphine)iridium(III) Hydridochloride Cation Adopt the Sterically and Electronically Unfavorable Cis Geometry?. *Organometallics*, **2000**, 19, 4608-4612	3.8	9
36	Unusually large effects of single excitations on the geometry of radical species and limiting spin-projection invariance of some correlated methods. *Chemical Physics Letters*, **1990**, 166, 295-302	2.5	9
35	Coupled cluster benchmark of new density functionals and of domain pair natural orbital methods: Mechanisms of hydroarylation and oxidative coupling catalyzed by Ru(II) chloride carbonyls **2019**,		9
34	A simple □ange extender□ For basis set extrapolation methods for MP2 and coupled cluster correlation energies **2018**,		9
33	Designing low-ionization potential analogs of tetrakis-dimethylamino-ethylene using density functional calculations. *Chemical Physics Letters*, **1997**, 279, 389-395	2.5	8
32	Rozen's epoxidation reagent, CH3CN.HOF: a theoretical study of its structure, vibrational spectroscopy, and reaction mechanism. *Journal of Physical Chemistry A*, **2006**, 110, 8275-81	2.8	8
31	Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark **2019**,		8
30	Molecular dynamics simulations of the interaction of Mouse and Torpedo acetylcholinesterase with covalent inhibitors explain their differential reactivity: Implications for drug design. *Chemico-Biological Interactions*, **2019**, 310, 108715	5	7
29	A DFT study on the mechanism of a novel, regioselective, intramolecular N-pi rearrangement of cis and trans-eta1-N-Cp*Rh-hydroxytamoxifen complexes to their eta6 derivatives; potential breast cancer pharmaceuticals, and fluorescent probes. *Dalton Transactions*, **2009**, 4334-43	4.3	7
28	Time-dependent mass spectra and breakdown graphs. 20. Bromoanthracene. Heat of formation of the anthracenyl ion. *International Journal of Mass Spectrometry and Ion Processes*, **1997**, 160, 39-48		7
27	Ab Initio Thermochemistry Beyond Chemical Accuracy for First-and Second-Row Compounds **1999**, 373-415		7
26	The kinetics and mechanism of oxidation of reduced phosphovanadomolybdates by molecular oxygen: theory and experiment in concert. *Physical Chemistry Chemical Physics*, **2018**, 20, 7579-7587	3.6	6
25	Benzyl Cation Stabilized by Metal Complexation. Relative Stability of Coordinated Methylene Arenium, □Benzylic, and □Benzylic Structures. *Organometallics*, **2013**, 32, 4813-4819	3.8	6
24	Surprising performance for vibrational frequencies of the distinguishable clusters with singles and doubles (DCSD) and MP2.5 approximations **2017**,		6
23	Can Si?O bonds be stabilized by Rh/Ir complexes?. *Chemical Physics Letters*, **1998**, 290, 535-542	2.5	6
22	Coupled Cluster Benchmark of New DFT and Local Correlation Methods: Mechanisms of Hydroarylation and Oxidative Coupling Catalyzed by Ru(II, III) Chloride Carbonyls. *Journal of Physical Chemistry A*, **2021**, 125, 8987-8999	2.8	6
21	Equilibrium gas-phase structures of sodium fluoride, bromide, and iodide monomers and dimers. *Journal of Physical Chemistry A*, **2014**, 118, 1927-35	2.8	5

20	The rotational partition function of the symmetric top and the effect of K doubling thereon. *Chemical Physics Letters*, **1991**, 187, 375-386	2.5	5
19	Some cost-effective approximations to CCSD and QCISD. *Chemical Physics Letters*, **1990**, 172, 354-360	2.5	5
18	The MOBH35 Metal-Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	5
17	A simple model for scalar relativistic corrections to molecular total atomisation energies. *Molecular Physics*, **2019**, 117, 2225-2232	1.7	4
16	Benchmark ab initio thermochemistry of the isomers of diimide, N2H2, using accurate computed structures and anharmonic force fields		4
15	Electron Correlation: Nature's Weird and Wonderful Chemical Glue. *Israel Journal of Chemistry*, **2022**, 62,	3.4	4
14	The Protonation Site of Aniline Revisited: A 'Torture Test' for Electron Correlation Methods. *ACS Symposium Series*, **2007**, 183-192	0.4	3
13	Matrix Infrared Spectrum and ab Initio Calculations on the PNP Radical. *The Journal of Physical Chemistry*, **1994**, 98, 10706-10709		3
12	Prototypical □d□imers re-examined by means of high-level CCSDT(Q) composite ab initio methods. *Journal of Chemical Physics*, **2021**, 154, 124117	3.9	3
11	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark.. *Journal of Physical Chemistry Letters*, **2022**, 3499-3506	6.4	3
10	MP2-F12 basis set convergence for the S66 noncovalent interactions benchmark: Transferability of the complementary auxiliary basis set (CABS) **2017**,		2
9	Boron atom reactions with acetylene. Ab initio calculated and observed isotopic infrared spectra of the borirene radical BC2H2. A fingerprint match. *AIP Conference Proceedings*, **1993**,	0	2
8	Benchmark Studies on Small Molecules		2
7	Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. *Journal of Physical Chemistry Letters*, **2021**, 12, 9368-9376	6.4	2
6	Pure and Hybrid SCAN, rSCAN, and rSCAN: Which One Is Preferred in KS- and HF-DFT Calculations, and How Does D4 Dispersion Correction Affect This Ranking?. *Molecules*, **2021**, 27,	4.8	2
5	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. *Highlights in Theoretical Chemistry*, **2015**, 233-246		1
4	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part 1.. *ChemInform*, **2005**, 36, no		1
3	Heavy-Atom Tunneling in the Covalent/Dative Bond Complexation of Cyclo[18]carbon-Piperidine.. *Journal of Physical Chemistry B*, **2022**, 126, 1799-1804	3.4	1

2 Why computed entropies of quasi-linear species are sometimes random?. *Computational and Theoretical Chemistry*, **1993**, 280, 83-87

1 A simple DFT-based diagnostic for nondynamical correlation. *Highlights in Theoretical Chemistry*, **2014**, 251-259