Ernest Davidson

List of Publications by Year in Descending Order

399 papers	32,044 citations	78 h-index	167 g-index
462 ext. papers	33,366 ext. citations	6 avg, IF	7.01 L-index

#	Paper	IF	Citations
399	Atomic isotropic hyperfine properties for first row elements (B-F) revisited.. *Journal of Chemical Physics*, **2022**, 156, 034304	3.9	2
398	A viewpoint on population analyses. *International Journal of Quantum Chemistry*, **2022**, 122,	2.1	1
397	Complete-active-space extended Koopmans theorem method. *Journal of Chemical Physics*, **2021**, 155, 051102	3.9	3
396	The Right Answer for the Right Reason: My Personal Goal for Quantum Chemistry. *Annual Review of Physical Chemistry*, **2019**, 70, 1-20	15.7	6
395	A theoretical study of the adiabatic and vertical ionization potentials of water. *Journal of Chemical Physics*, **2018**, 148, 234308	3.9	4
394	Nature of ground and electronic excited states of higher acenes. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E5098-107	11.5	113
393	The benzene radical anion: A computationally demanding prototype for aromatic anions. *Journal of Chemical Physics*, **2015**, 142, 204304	3.9	18
392	Singlet-triplet energy gaps for diradicals from particle-particle random phase approximation. *Journal of Physical Chemistry A*, **2015**, 119, 4923-32	2.8	27
391	Approximate singly excited states from a two-component Hartree-Fock reference. *Journal of Chemical Physics*, **2015**, 143, 144106	3.9	10
390	Canonical form of the Hartree-Fock orbitals in open-shell systems. *Journal of Chemical Physics*, **2014** , 140, 014102	3.9	15
389	A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. *Journal of Chemical Physics*, **2014**, 141, 104302	3.9	27
388	Linear inequalities for density matrices: IV Factorizations. *Computational and Theoretical Chemistry*, **2013**, 1003, 28-31	2	3
387	Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. *Journal of Chemical Physics*, **2010**, 133, 164107	3.9	12
386	Koopmans theorem in the restricted open-shell Hartree Fock method. II. The second canonical set for orbitals and orbital energies. *Journal of Chemical Physics*, **2010**, 132, 184110	3.9	16
385	Comment on Combined open shell Hartree Fock theory of atomic-molecular and nuclear systems [J. Math. Chem. 42 (2007) 177]. *Journal of Mathematical Chemistry*, **2009**, 45, 859-866	2.1	2
384	Qualitatively significant effects of electron correlation. *International Journal of Quantum Chemistry*, **2009**, 20, 65-68	2.1	
383	SCF methods for excited states. *International Journal of Quantum Chemistry*, **2009**, 10, 21-31	2.1	62

382	Theoretical and spectroscopic investigations of the bonding and reactivity of (RO)3M[triple bond]N molecules, where M = Cr, Mo, and W. *Inorganic Chemistry*, **2009**, 48, 828-37	5.1	8
381	Koopmans' theorem in the restricted open-shell Hartree-Fock method. 1. A variational approach. *Journal of Physical Chemistry A*, **2009**, 113, 12386-95	2.8	35
380	Size extensivity of the direct optimized effective potential method. *Journal of Chemical Physics*, **2008**, 128, 114702	3.9	5
379	Large ground-state entropy changes for hydrogen atom transfer reactions of iron complexes. *Journal of the American Chemical Society*, **2007**, 129, 5153-66	16.4	116
378	Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions. *Reviews in Computational Chemistry*, **2007**, 1-43		22
377	The effective local potential method: implementation for molecules and relation to approximate optimized effective potential techniques. *Journal of Chemical Physics*, **2007**, 126, 084107	3.9	34
376	Self-consistent effective local potentials. *Journal of Chemical Physics*, **2007**, 127, 084113	3.9	20
375	Understanding Electron Correlation: Recent Progress in Molecular Synchrotron Photoelectron Spectroscopy. *Advances in Chemical Physics*, **2007**, 215-266		18
374	Linear Inequalities for Diagonal Elements of Density Matrices. *Advances in Chemical Physics*, **2007**, 443-483		19
373	Analysis of wave functions for open-shell molecules. *Physical Chemistry Chemical Physics*, **2007**, 9, 1881-946		45
372	Effective local potentials for orbital-dependent density functionals. *Journal of Chemical Physics*, **2006**, 125, 081104	3.9	79
371	High-density limit of the Perdew-Burke-Ernzerhof generalized gradient approximation and related density functionals. *Physical Review A*, **2006**, 74,	2.6	35
370	Ab initio diradical/zwitterionic polarizabilities and hyperpolarizabilities in twisted double bonds. *Journal of Physical Chemistry A*, **2006**, 110, 7189-96	2.8	30
369	Optimized effective potentials yielding Hartree-Fock energies and densities. *Journal of Chemical Physics*, **2006**, 124, 141103	3.9	162
368	Necessary conditions for the N-representability of pair distribution functions. *International Journal of Quantum Chemistry*, **2006**, 106, 1487-1498	2.1	46
367	Löwdin population analysis with and without rotational invariance. *International Journal of Quantum Chemistry*, **2006**, 106, 2065-2072	2.1	53
366	Stoichiometric oxidations of □bonds: Radical and possible non-radical pathways. *Journal of Molecular Catalysis A*, **2006**, 251, 24-33		26
365	Charge and Spin Distributions **2006**, 1001-1001		

364	Computational studies of the thermal fragmentation of P-arylphosphiranes: have arylphosphinidenes been generated by this method?. *Journal of the American Chemical Society*, **2005**, 127, 9886-94	16.4	19
363	Ligand-assisted reduction of osmium tetroxide with molecular hydrogen via a [3+2] mechanism. *Journal of the American Chemical Society*, **2005**, 127, 3423-32	16.4	36
362	Spin polarization and annihilation for radicals and diradicals. *International Journal of Quantum Chemistry*, **2005**, 103, 1-9	2.1	44
361	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. *Physical Review A*, **2004**, 70,	2.6	30
360	Bonding in FHF□(HF)2, and FHF. *International Journal of Quantum Chemistry*, **2004**, 98, 317-324	2.1	21
359	Large spin differences in structurally related Fe6 molecular clusters and their magnetostructural explanation. *Inorganic Chemistry*, **2004**, 43, 5505-21	5.1	130
358	Polynuclear manganese complexes with the dicarboxylate ligand m-phenylenedipropionate: a hexanuclear mixed-valence (3Mn(III), 3Mn(IV)) complex. *Inorganic Chemistry*, **2004**, 43, 101-15	5.1	51
357	An investigation into the relative influence of alkoxide and thiolate ligands on the metal□arbon triple bond in X3M?CH compounds, where M=Cr, Mo and W and X=OH, SH, OCH3, SCH3, OCF3 and SCF3 from electronic structure calculations. *Polyhedron*, **2003**, 22, 145-152	2.7	3
356	Linear inequalities for density matrices: III. *International Journal of Quantum Chemistry*, **2003**, 91, 1-4	2.1	21
355	Semiempirical local spin: Theory and implementation of the ZILSH method for predicting Heisenberg exchange constants of polynuclear transition metal complexes. *International Journal of Quantum Chemistry*, **2003**, 92, 294-325	2.1	45
354	Population analyses that utilize projection operators. *International Journal of Quantum Chemistry*, **2003**, 93, 384-394	2.1	64
353	Single-molecule magnets: two-electron reduced version of a Mn12 complex and environmental influences on the magnetization relaxation of (PPh4)(2)[Mn(12)O(12)(O(2)CCHCl2)(16)(H2O)4]. *Journal of the American Chemical Society*, **2003**, 125, 3576-88	16.4	144
352	Methanolysis and phenolysis routes to Fe6, Fe8, and Fe1) complexes and their magnetic properties: a new type of Fe8 ferric wheel. *Inorganic Chemistry*, **2003**, 42, 7819-29	5.1	59
351	34S isotope effect on sulfate ester hydrolysis: mechanistic implications. *Journal of the American Chemical Society*, **2003**, 125, 13036-7	16.4	24
350	p-Benzyne derivatives that have exceptionally small singlet-triplet gaps and even a triplet ground state. *Journal of Organic Chemistry*, **2003**, 68, 3387-96	4.2	22
349	Non-Stern□olmer Quenching of S1pDFB Fluorescence by O2and the Charge Transfer Complex□ *Journal of Physical Chemistry A*, **2003**, 107, 3552-3558	2.8	6
348	A TDDFT description of the low-energy excited states of copper and zinc metalloenediynes. *Chemical Communications*, **2003**, 2876-7	5.8	4
347	Exactness of the general two-body cluster expansion in many-body quantum theory. *Physical Review Letters*, **2003**, 91, 123001	7.4	21

346	New time-independent perturbation theory for the multireference problem. *International Journal of Quantum Chemistry*, **2002**, 86, 256-264	2.1	21
345	The effect of the basis set superposition error on the geometry optimization of the p-DFBN2 complex. *Chemical Physics Letters*, **2002**, 360, 99-103	2.5	13
344	Local spin II. *Molecular Physics*, **2002**, 100, 373-383	1.7	70
343	Local Spin III: Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzyne. *Journal of Physical Chemistry A*, **2002**, 106, 6890-6896	2.8	47
342	Tristhiolatomolybdenum nitrides, (RS)(3)Mo[triple bond]N where R = (i)Pr and (t)Bu, preparation, characterization and comparisons with related trialkoxymolybdenumnitrides. *Inorganic Chemistry*, **2002**, 41, 3437-43	5.1	11
341	Insights into the metathesis reaction involving M-M, C-C, and M-C triple bonds from computations employing density functional theory on model compounds M2(OH)6 and M2(SH)6, where M = Mo and W. *Journal of the American Chemical Society*, **2002**, 124, 15351-8	16.4	21
340	Model Molecular Magnets. *Journal of Physical Chemistry A*, **2002**, 106, 7456-7461	2.8	32
339	Comparison of CH and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. *Molecular Physics*, **2002**, 100, 533-540	1.7	21
338	Two new hexanuclear iron(III) complexes with S = 5 ground states. *Dalton Transactions RSC*, **2002**, 4005-4010		36
337	Insights into the Schrock 'chop-chop' reaction gained from density functional theory and preparation and structure of W2(mu-PhCCPh)(SC6H4-2-Me)6. *Chemical Communications*, **2002**, 2770-1	5.8	7
336	Model studies of hydrogen atom addition and abstraction processes involving ortho-, meta-, and para-benzynes. *Journal of the American Chemical Society*, **2001**, 123, 10691-8	16.4	31
335	Theoretical study of the photoelectron spectra of gaseous Cu3Cl3. *Molecular Physics*, **2001**, 99, 1329-1334	1.7	9
334	Use of the dicarboxylate ligand m-phenylenedipropionate for the synthesis of new Mn/O clusters. Synthesis, characterization and magnetic properties. *Polyhedron*, **2001**, 20, 1375-1380	2.7	18
333	Ab initio calculations on XFnq (X = I, Xe, Cs, and Ba; n=1, 2, 4, and 6; q=-1, 0, +1, and +2) molecules. *International Journal of Quantum Chemistry*, **2001**, 81, 238-245	2.1	1
332	A density functional method for degenerate spin-multiplet components. *Chemical Physics Letters*, **2001**, 340, 142-150	2.5	25
331	The Cope rearrangement in theoretical retrospect. *Computational and Theoretical Chemistry*, **2001**, 573, 81-89		52
330	Ab initio Compton maps of small molecules. *Molecular Physics*, **2001**, 99, 175-186	1.7	6
329	Local spin. *Journal of Chemical Physics*, **2001**, 115, 7382-7392	3.9	156

328	Structure of the exact wave function. II. Iterative configuration interaction method. *Journal of Chemical Physics*, **2001**, 115, 2000-2006	3.9	56
327	A comparison of the influences of alkoxide and thiolate ligands on the electronic structure and reactivity of molybdenum(3+) and tungsten(3+) complexes. preparation and structures of M(2)(O(T)Bu)(2)(S(t)Bu)(4), [Mo(S(t)Bu)(3)(NO)](2), and W(S(t)Bu)(3)(NO)(py). *Journal of the American Chemical Society*, **2001**, 123, 9652-64	16.4	30
326	Electronic, Structural, and Hyperfine Interaction Investigations on Rydberg Molecules: NH4, OH3, and FH2. *Journal of Physical Chemistry A*, **2001**, 105, 10915-10921	2.8	27
325	UDFT and MCSCF descriptions of the photochemical Bergman cyclization of enediynes. *Journal of the American Chemical Society*, **2001**, 123, 2650-7	16.4	55
324	Theoretical Study of the Electronic Spectrum and ESR of the CH2OH Radical. *Journal of Physical Chemistry A*, **2001**, 105, 4558-4562	2.8	12
323	Kinetic and potential energy of isoelectronic atomic ions from density functional theory compared with exact values. *Molecular Physics*, **2000**, 98, 1089-1097	1.7	11
322	Theoretical investigation of electronic structure and ESR hyperfine parameters for the CuH+ molecule. *International Journal of Quantum Chemistry*, **2000**, 77, 291-300	2.1	28
321	Electron distributions in radicals. *International Journal of Quantum Chemistry*, **2000**, 77, 316-323	2.1	19
320	Charge densities for singlet and triplet electron pairs. *International Journal of Quantum Chemistry*, **2000**, 77, 651-660	2.1	26
319	Enhanced second-order treatment of electron pair correlation. *International Journal of Quantum Chemistry*, **2000**, 78, 226-236	2.1	18
318	Distribution of effectively unpaired electrons. *Chemical Physics Letters*, **2000**, 330, 161-168	2.5	171
317	A third isolated oxidation state for the Mn12 family of single-molecule magnets. *Chemical Communications*, **2000**, 2417-2418	5.8	86
316	Dimolybdenum bis((S,S,S)-triisopropanolaminate(3-)): a blue compound with an unusual Mo-Mo triple bond. *Inorganic Chemistry*, **2000**, 39, 3544-50	5.1	8
315	Facile and Reversible Cleavage of C Bonds. Contrasting Thermodynamic Selectivity for RuCF2H vs FOsCFH. *Journal of the American Chemical Society*, **2000**, 122, 8916-8931	16.4	88
314	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. *New Journal of Chemistry*, **2000**, 24, 9-26	3.6	73
313	Diradical Character of the Cope Rearrangement Transition State. *Journal of the American Chemical Society*, **2000**, 122, 186-187	16.4	111
312	Fate of CH2CHE (E = H, OMe) in the Presence of Unsaturated Ru(X)(H)L2q+(X = Cl,q= 0; X = CO,q= 1):Highly Sensitive to X and E. *Organometallics*, **2000**, 19, 2291-2298	3.8	15
311	Transition Regions in the Cope Rearrangement of 1,5-Hexadiene and Its Cyano Derivatives. *Journal of the American Chemical Society*, **2000**, 122, 7377-7385	16.4	73

310	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. *Journal of the American Chemical Society*, **2000**, 122, 1210-1214	16.4	161
309	Charge densities for singlet and triplet electron pairs **2000**, 77, 651		1
308	MULTI-REFERENCE PERTURBATION THEORY. *Recent Advances in Computational*, **1999**, 31-63		12
307	Electron spin resonance studies of 45Sc17O, 89Y17O, and 139La17O in rare gas matrices: Comparison with ab initio electronic structure and nuclear hyperfine calculations. *Journal of Chemical Physics*, **1999**, 110, 5658-5669	3.9	36
306	Orbital momentum profiles and binding energy spectra for the complete valence shell of propane. *Journal of Chemical Physics*, **1999**, 111, 9526-9535	3.9	27
305	Electron spin resonance and theoretical studies of the 14N????14N and 15N????15N spin-pair radicals in neon matrices: The effects of mixing among the 1□+, 3□+, 5□+, and 7□+ electronic states. *Journal of Chemical Physics*, **1999**, 111, 3145-3154	3.9	16
304	Reassignment of the AlSi□photoelectron spectrum by ab initio configuration interaction calculations. *Molecular Physics*, **1999**, 96, 735-740	1.7	3
303	Density functional theory calculations for F□*Chemical Physics Letters*, **1999**, 300, 44-52	2.5	38
302	Scaled quantum mechanical study of vibrational force field for p-difluorobenzene and p-fluorotoluene. *International Journal of Quantum Chemistry*, **1999**, 72, 249-260	2.1	8
301	Thermal Rearrangements of Norcaradiene. *Journal of the American Chemical Society*, **1999**, 121, 6928-6935	16.4	51
300	Electronic Structure and Low-Lying Electronic States of Al3O and Al3O-: Photoelectron Spectrum of Al3O-. *Journal of Physical Chemistry A*, **1999**, 103, 2867-2872	2.8	27
299	Theoretical Interpretation of the Photoelectron Spectra of Al3O2- and Al3O3-. *Journal of Physical Chemistry A*, **1999**, 103, 8985-8993	2.8	33
298	[2.2.2]propellane rearrangements. *Chemical Physics Letters*, **1998**, 284, 301-307	2.5	18
297	Zero point corrections to vertical excitation energies. *Chemical Physics Letters*, **1998**, 285, 155-159	2.5	60
296	The reduced model space method in multireference second-order perturbation theory. *Chemical Physics Letters*, **1998**, 296, 435-444	2.5	28
295	How robust is present-day DFT?. *International Journal of Quantum Chemistry*, **1998**, 69, 241-245	2.1	68
294	Does Unrestricted M□ller□Plesset Perturbation Theory for Low Spin Converge When the System Has a Triplet Ground State?. *Journal of Physical Chemistry A*, **1998**, 102, 4742-4746	2.8	23
293	Carbene Complexes from Olefins, Using RuHCl(PiPr3)2. Influence of the Olefin Substituent. *Journal of the American Chemical Society*, **1998**, 120, 9388-9389	16.4	37

292	Theoretical and electron spin resonance studies of the H?H, H?D, and D?D spin-pair radicals in rare gas matrices: A case of extreme singlet□triplet mixing. *Journal of Chemical Physics*, **1998**, 109, 1409-1424	3.9	37
291	Ground-state energies of isoelectronic atomic series from density-functional theory: Exploring the accuracy of density functionals. *Physical Review A*, **1998**, 58, 1902-1909	2.6	24
290	Density functional calculations for Mgn+ clusters. *Journal of Chemical Physics*, **1997**, 106, 2331-2341	3.9	22
289	Electron momentum spectroscopy of H2 and D2: Ionization to ground and excited final states. *Physical Review A*, **1997**, 56, 1393-1402	2.6	25
288	Correlation states of propene. *Journal of Chemical Physics*, **1997**, 107, 4295-4306	3.9	12
287	Electron spin resonance matrix isolation studies of 27Al16,17O, 69,71Ga16,17O and 115In16,17O: Observed hyperfine interactions compared with ab initio theoretical results. *Journal of Chemical Physics*, **1997**, 107, 7011-7019	3.9	33
286	Calculational Evidence for Lack of Intermediates in the Thermal Unimolecular Vinylcyclopropane to Cyclopentene 1,3-Sigmatropic Shift. *Journal of the American Chemical Society*, **1997**, 119, 10543-10544	16.4	54
285	Could 2.2.2-Propellatriene Exist?. *Journal of the American Chemical Society*, **1997**, 119, 1449-1449	16.4	6
284	The ground state of ethylene. *Computational and Theoretical Chemistry*, **1997**, 400, 169-176		5
283	Evaluation of a characteristic atomic radius by an ab initio method. *International Journal of Quantum Chemistry*, **1997**, 62, 47-53	2.1	58
282	Evaluation of a characteristic atomic radius by an ab initio method **1997**, 62, 47		1
281	The Spatial Extent of the V State of Ethylene and Its Relation to Dynamic Correlation in the Cope Rearrangement. *The Journal of Physical Chemistry*, **1996**, 100, 6161-6166		53
280	The Importance of Including Dynamic Electron Correlation in ab Initio Calculations. *Accounts of Chemical Research*, **1996**, 29, 67-75	24.3	221
279	Electron momentum spectroscopy experiments and calculations for the production of excited states of He+ and. *Canadian Journal of Physics*, **1996**, 74, 748-756	1.1	18
278	Electron spin resonance matrix isolation and ab initio theoretical investigations of 69,71GaH2, 69,71GaD2, H69,71GaCH3, and D69,71GaCD3. *Journal of Chemical Physics*, **1996**, 105, 6607-6615	3.9	34
277	Ab initio Calculations on Excited Molecular Ions of Ethylene and Acetylene. *Australian Journal of Physics*, **1996**, 49, 247		7
276	Comment on □omment on Dunning's correlation-consistent basis sets□*Chemical Physics Letters*, **1996**, 260, 514-518	2.5	325
275	Refinement of the Asymptotic Z Expansion for the Ground-State Correlation Energies of Atomic Ions. *The Journal of Physical Chemistry*, **1996**, 100, 6167-6172		105

274	An electron spin resonance investigation of vanadium dioxide (51V16O2 and 51V17O2) and 51V17O in neon matrices with preliminary assignments for VO3 and V+2: Comparison with ab initio theoretical calculations. *Journal of Chemical Physics*, **1996**, 105, 10237-10250	3.9	56
273	One-electron properties of molecules calculated using second-order multireference perturbation theory. *International Journal of Quantum Chemistry*, **1995**, 53, 149-160	2.1	11
272	On electron correlation in NaCl2. *International Journal of Quantum Chemistry*, **1995**, 54, 299-304	2.1	16
271	Study of correlation states of acetylene by synchrotron photoelectron spectroscopy. *Journal of Chemical Physics*, **1995**, 103, 10537-10547	3.9	24
270	ESR observation of the H???H, H???D, and D???D spin-pair radicals in rare gas matrices. *Journal of Chemical Physics*, **1995**, 103, 5275-5278	3.9	11
269	Theoretical study of the adsorption of carbon monoxide on a NaCl (100) surface. *Surface Science*, **1995**, 322, 342-360	1.8	19
268	N2 activation by iron-sulfur complexes. *Theoretica Chimica Acta*, **1995**, 92, 315-326		14
267	The Cope Rearrangement Revisited with Multireference Perturbation Theory. *Journal of the American Chemical Society*, **1995**, 117, 774-778	16.4	97
266	Theory and Mechanism of the Allylidenecyclopropane-to-Methylenecyclopentene Thermal Isomerization. *Journal of the American Chemical Society*, **1995**, 117, 8495-8501	16.4	28
265	Correlation states of ethylene. *Journal of Chemical Physics*, **1995**, 102, 6385-6399	3.9	40
264	Reply to comment on A possible definition of basis set superposition error *Chemical Physics Letters*, **1995**, 241, 146-148	2.5	11
263	N-representability of the electron pair density. *Chemical Physics Letters*, **1995**, 246, 209-213	2.5	63
262	High-resolution zero kinetic energy photoelectron spectra of para-n-propylaniline. *Journal of Chemical Physics*, **1994**, 100, 5411-5421	3.9	19
261	Electron spin resonance investigation of small magnesium cluster cation radicals, Mg+N, in neon and argon matrices at 4 K: Comparison with ab initio calculations. *Journal of Chemical Physics*, **1994**, 100, 7867-7874	3.9	21
260	A possible definition of basis set superposition error. *Chemical Physics Letters*, **1994**, 217, 48-54	2.5	98
259	Considerations in constructing a multireference second-order perturbation theory. *Journal of Chemical Physics*, **1994**, 100, 3672-3682	3.9	164
258	Configuration Interaction Wave Functions. *NATO ASI Series Series B: Physics*, **1994**, 105-131		3
257	Ground-state correlation energies for atomic ions with 3 to 18 electrons. *Physical Review A*, **1993**, 47, 3649-3670	2.6	457

256	Some Perspectives on Quantum Calculations. *Israel Journal of Chemistry*, **1993**, 33, 243-252	3.4	8
255	The transition metal-carbonyl bond. *Accounts of Chemical Research*, **1993**, 26, 628-635	24.3	104
254	The water dimer: correlation energy calculations. *The Journal of Physical Chemistry*, **1993**, 97, 6373-6383		81
253	Binding energy of chromium hexacarbonyl. 2. Revisited with correlation effects. *The Journal of Physical Chemistry*, **1993**, 97, 4397-4403		19
252	Vibrations of S1 (1B2u) p-difluorobenzene-d4 S1-S0 fluorescence spectroscopy and ab initio calculations. *The Journal of Physical Chemistry*, **1993**, 97, 5506-5518		21
251	Alkali-metal dihalide molecules: electronic spectrum. *The Journal of Physical Chemistry*, **1993**, 97, 5882-5885		4
250	Electron correlation contribution to the hydrogen bond in hydrogen fluoride dimer. *The Journal of Physical Chemistry*, **1993**, 97, 6367-6372		51
249	Zero kinetic energy photoelectron spectra of jet-cooled aniline. *Journal of Chemical Physics*, **1993**, 99, 3224-3233	3.9	93
248	Comparison of ab initio and multipole determinations of the electrostatic interaction of acetamide dimers. *Computational and Theoretical Chemistry*, **1993**, 282, 19-31		8
247	Alkali-metal dihalide molecules. *The Journal of Physical Chemistry*, **1992**, 96, 3683-3688		10
246	A theoretical study of the x-ray photoelectron ionization energies of related carbonyl compounds: formaldehyde, acetaldehyde, and acetone. *The Journal of Physical Chemistry*, **1992**, 96, 10682-10687		17
245	A theoretical investigation of some low-lying electronic states of imidazole. *Journal of Chemical Physics*, **1992**, 97, 1881-1891	3.9	34
244	Energetics and electronic structure of chromium hexacarbonyl. *The Journal of Physical Chemistry*, **1992**, 96, 2129-2141		27
243	Stereomutation of cyclopropane revisited. An ab initio investigation of the potential surface and calculation of secondary isotope effects. *Journal of the American Chemical Society*, **1992**, 114, 2085-2093	16.4	58
242	Momentum distributions, spin distributions, and bonding in methylamine and its radical cation. *Journal of the American Chemical Society*, **1992**, 114, 6496-6504	16.4	20
241	Calculations on model systems using quasi-degenerate variational perturbation theory with an average pair correction. *International Journal of Quantum Chemistry*, **1992**, 42, 273-285	2.1	19
240	Different forms of perturbation theory for the calculation of the correlation energy. *International Journal of Quantum Chemistry*, **1992**, 43, 755-768	2.1	69
239	A test of the Hirshfeld definition of atomic charges and moments. *Theoretica Chimica Acta*, **1992**, 83, 319-330		249

238	Improved algorithms for the lowest few eigenvalues and associated eigenvectors of large matrices. *Journal of Computational Physics*, **1992**, 103, 382-389	4.1	110
237	Theoretical calculation of the photoelectron spectrum of ethylene. *Chemical Physics Letters*, **1992**, 190, 231-235	2.5	21
236	Harmonic mode scrambling in p-difluorobenzene. *Chemical Physics Letters*, **1992**, 197, 123-130	2.5	5
235	Perturbation theory for open shell systems. *Chemical Physics Letters*, **1991**, 187, 451-454	2.5	124
234	Potential surface symmetry and vibronic wave functions for methane cation. *Journal of Chemical Physics*, **1991**, 95, 6551-6561	3.9	21
233	Dependence of p-n-propylaniline ionization potential on molecular conformation: comparison of experiment with theory. *Journal of the American Chemical Society*, **1991**, 113, 3202-3203	16.4	12
232	Ground-state correlation energies for two- to ten-electron atomic ions. *Physical Review A*, **1991**, 44, 7071-7083	2.6	337
231	The Cope rearrangement revisited. *Journal of the American Chemical Society*, **1991**, 113, 9756-9759	16.4	70
230	Theoretical Approaches to ESR Spectroscopy **1991**, 429-455		7
229	MELD: A Many Electron Description **1991**, 381-433		4
228	Theoretical study of excitation energies of methaniminium cation, propeniminium cation, and propenimine. *The Journal of Physical Chemistry*, **1990**, 94, 3944-3951		15
227	The correlation potential for two-electron atomic ions. *International Journal of Quantum Chemistry*, **1990**, 37, 811-819	2.1	27
226	The estimation of electron affinities fromab initio 1s orbital energies. *Theoretica Chimica Acta*, **1990** , 78, 25-30		3
225	Configuration interaction calculations on the propane radical cation, C3H +8. *Theoretica Chimica Acta*, **1990**, 77, 111-122		18
224	Corollary to density-functional theory. *Physical Review A*, **1990**, 42, 2539-2541	2.6	5
223	Ab initio study on the excitation energies of the protonated Schiff base of 11-cis-retinal. *The Journal of Physical Chemistry*, **1990**, 94, 7013-7020		31
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219	Analysis of the bond energy of ScCO. *Journal of Chemical Physics*, **1989**, 90, 5541-5554	3.9	12
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