T Daniel Crawford

List of Publications by Year
in descending order

150 papers	8,514 citations	71061 41 h-index	46771 89 g-index
154 all docs	154 docs citations	154 times ranked	6035 citing authors

#	Article	IF	Citations
1	The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry C, 2022, 126, 1-2.	1.5	0
2	A Venue for Advances in Experimental and Theoretical Methods in Physical Chemistry. Journal of Physical Chemistry A, 2022, 126, 177-179.	1.1	0
3	The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry A, 2022, 126, 1-2.	1.1	0
4	The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry B, 2022, 126, 1-2.	1.2	0
5	50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2022, 126, 6093-6095.	1.5	0
6	50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry B, 2022, 126, 2609-2611.	1.2	0
7	50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry A, 2022, 126, 2149-2151.	1.1	0
8	The <scp>MolSSI</scp> QCA<scp>rchive</scp> project: An openâ€source platform to compute, organize, and share quantum chemistry data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1491.	6.2	42
9	The MolSSI Driver Interface Project: A framework for standardized, on-the-fly interoperability between computational molecular sciences codes. Computer Physics Communications, 2021, 261, 107688.	3.0	11
10	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry A, 2021, 125, 1-2.	1.1	0
11	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry A, 2021, 125, 2019-2020.	1.1	0
12	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry B, 2021, 125, 2465-2466.	1.2	3
13	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry C, 2021, 125, 5425-5426.	1.5	0
14	Structure Elucidation and Confirmation of Phloroglucinols from the Roots of Garcinia dauphinensis by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. Journal of Natural Products, 2021, 84, 1163-1174.	1.5	2
15	Modeling Complex Solvent Effects on the Optical Rotation of Chiral Molecules: A Combined Molecular Dynamics and Density Functional Theory Study. Journal of Physical Chemistry A, 2021, 125, 3095-3108.	1.1	13
16	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry B, 2021, 125, 1-2.	1.2	0
17	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2021, 125, 1-2.	1.5	1
18	PNO++: Perturbed Pair Natural Orbitals for Coupled Cluster Linear Response Theory. Journal of Chemical Theory and Computation, 2021, 17, 290-301.	2.3	7

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19	Theory and implementation of a novel stochastic approach to coupled cluster. Journal of Chemical Physics, 2020, 153, 144117.	1.2	3
20	Machine-Learning Coupled Cluster Properties through a Density Tensor Representation. Journal of Physical Chemistry A, 2020, 124, 4861-4871.	1.1	21
21	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
22	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry A. Journal of Physical Chemistry A, 2020, 124, 5059-5060.	1.1	3
23	Building capacity for undergraduate education and training in computational molecular science: A collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. International Journal of Quantum Chemistry, 2020, 120, e26359.	1.0	9
24	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
25	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
26	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	1.5	1
27	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2
28	Tensor representations and symmetry in many-electron wave functions. Annual Reports in Computational Chemistry, 2019, 15, 79-101.	0.9	1
29	Basis Set Superposition Errors in the Many-Body Expansion of Molecular Properties. Journal of Physical Chemistry A, 2019, 123, 4500-4511.	1.1	11
30	Diagrammatic Coupled Cluster Monte Carlo. Journal of Physical Chemistry Letters, 2019, 10, 925-935.	2.1	14
31	Reducedâ€scaling coupled cluster response theory: Challenges and opportunities. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1406.	6.2	26
32	Phloroglucinols from the Roots of Garcinia dauphinensis and Their Antiproliferative and Antiplasmodial Activities. Journal of Natural Products, 2019, 82, 431-439.	1.5	16
33	Frontiers of Coupled Cluster Chiroptical Response Theory. , 2018, , 49-68.		3
34	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
35	Calculating Optical Rotatory Dispersion Spectra in Solution Using a Smooth Dielectric Model. Journal of Physical Chemistry A, 2018, 122, 8557-8564.	1.1	6
36	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106

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37	Performance of Property-Optimized Basis Sets for Optical Rotation with Coupled Cluster Theory. Journal of Physical Chemistry A, 2018, 122, 5962-5969.	1.1	15
38	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	2.3	961
39	Antiplasmodial Sesquiterpenoid Lactones from Trichospira verticillata: Structure Elucidation by Spectroscopic Methods and Comparison of Experimental and Calculated ECD Data. Journal of Natural Products, 2017, 80, 1639-1647.	1.5	23
40	Frozen Virtual Natural Orbitals for Coupled-Cluster Linear-Response Theory. Journal of Physical Chemistry A, 2017, 121, 708-716.	1.1	40
41	Electronically Excited States in Solution via a Smooth Dielectric Model Combined with Equation-of-Motion Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2017, 13, 5572-5581.	2.3	10
42	â€œNew Physical Insightsâ€•in Theoretical and Computational Studies. Journal of Physical Chemistry A, 2017, 121, 4850-4850.	1.1	6
43	A Comparison of Three Approaches to the Reduced-Scaling Coupled Cluster Treatment of Non-Resonant Molecular Response Properties. Journal of Chemical Theory and Computation, 2016, 12, 209-222.	2.3	24
44	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	1.2	42
45	Frozen-Density Embedding Potentials and Chiroptical Properties. Journal of Chemical Theory and Computation, 2015, 11, 5305-5315.	2.3	16
46	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	1.1	81
47	Incremental evaluation of coupled cluster dipole polarizabilities. Physical Chemistry Chemical Physics, 2015, 17, 14284-14296.	1.3	13
48	Simulation of circularly polarized luminescence spectra using coupled cluster theory. Journal of Chemical Physics, 2015, 142, 154101.	1.2	26
49	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OFc-C₃H^{â€“}. Astrophysical Journal, 2014, 796, 139.	1.6	17
50	Computing optical rotation via an N-body approach. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	14
51	Large Solvation Effect in the Optical Rotatory Dispersion of Norbornenone. Angewandte Chemie - International Edition, 2014, 53, 1386-1389.	7.2	46
52	Fundamental Vibrational Frequencies and Spectroscopic Constants of cis- and trans-HOCS, HSCO, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry B, 2014, 118, 6498-6510.	1.2	16
53	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C₂H₃⁺, and Its Isotopologues. Journal of Physical Chemistry A, 2014, 118, 7034-7043.	1.1	75
54	Insights on the Origin of the Unusually Large Specific Rotation of (1S,4S)-Norbornenone. Journal of Physical Chemistry A, 2014, 118, 4863-4871.	1.1	31

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55	Dipole Surface and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939.	1.1	30
56	Vibrational Frequencies and Spectroscopic Constants for 1 ³Aâ€² HNC and 1 ³Aâ€² HOC⁺ from High-Accuracy Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 11339-11345.	1.1	10
57	The 1 ³Aâ€² HCN and 1 ³Aâ€² HCO⁺ Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 9324-9330.	1.1	23
58	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 1¹Aâ€²l-C₃H^{â€“}: A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. Astrophysical Journal, 2013, 772, 39.	1.6	63
59	THE POSSIBLE INTERSTELLAR ANION CH₂CN^{â€“}: SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. Astrophysical Journal, 2013, 762, 121.	1.6	38
60	The optical activity of carvone: A theoretical and experimental investigation. Journal of Chemical Physics, 2012, 136, 114512.	1.2	25
61	Properties of atoms under pressure: Bonded interactions of the atoms in three perovskites. Journal of Chemical Physics, 2012, 137, 164313.	1.2	12
62	Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS⁺, HSCO⁺, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry A, 2012, 116, 9582-9590.	1.1	70
63	Localized optimized orbitals, coupled cluster theory, and chiroptical response properties. Physical Chemistry Chemical Physics, 2012, 14, 7830.	1.3	26
64	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	6.2	838
65	The optimized orbital coupled cluster doubles method and optical rotation. Chemical Physics, 2012, 401, 125-129.	0.9	12
66	Quartic force field predictions of the fundamental vibrational frequencies and spectroscopic constants of the cations HOCO+ and DOCO+. Journal of Chemical Physics, 2012, 136, 234309.	1.2	105
67	Role of Long-Range Intermolecular Forces in the Formation of Inorganic Nanoparticle Clusters. Journal of Physical Chemistry A, 2011, 115, 12933-12940.	1.1	20
68	Singlet Excited States of Silicon-Containing Anions Relevant to Interstellar Chemistry. Journal of Physical Chemistry A, 2011, 115, 8119-8124.	1.1	28
69	Theoretical prediction of new dipole-bound singlet states for anions of interstellar interest. Journal of Chemical Physics, 2011, 134, 154304.	1.2	48
70	Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore. Journal of Chemical Physics, 2011, 134, 034310.	1.2	47
71	Basis Set Dependence of Coupled Cluster Optical Rotation Computations. Journal of Physical Chemistry A, 2011, 115, 10045-10051.	1.1	37
72	Coupledâ€Cluster Calculations of Vibrational Raman Optical Activity Spectra. ChemPhysChem, 2011, 12, 3442-3448.	1.0	34

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73	The trans-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301.	1.2	116
74	Vibrational frequencies and spectroscopic constants from quartic force fields for cis-HOCO: The radical and the anion. Journal of Chemical Physics, 2011, 135, 214303.	1.2	62
75	Electronically Excited States in Interstellar Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 195-214.	0.9	9
76	The life and science of Fritz Schaefer. Molecular Physics, 2010, 108, 2439-2445.	0.8	3
77	Reduced-Scaling Coupled-Cluster Theory for Response Properties of Large Molecules. Challenges and Advances in Computational Chemistry and Physics, 2010, , 37-55.	0.6	14
78	Introduction to proceedings of Molecular Quantum Mechanics 2010: from methylene to DNA and beyond. Molecular Physics, 2010, 108, 2437-2438.	0.8	0
79	A Coupled Cluster Benchmark Study of the Electronic Spectrum of the Allyl Radical^{â€}. Journal of Physical Chemistry A, 2010, 114, 8852-8857.	1.1	17
80	A benchmark study of the vertical electronic spectra of the linear chain radicals C2H and C4H. Journal of Chemical Physics, 2010, 132, 144303.	1.2	40
81	Symmetry breaking in the cyclic C3C2H radical. Physical Chemistry Chemical Physics, 2010, 12, 15459.	1.3	17
82	Optical activity in conformationally flexible molecules: a theoretical study of large-amplitude vibrational averaging in (R)-3-chloro-1-butene. Molecular Physics, 2009, 107, 1041-1057.	0.8	32
83	Gas phase optical rotation calculated from coupled cluster theory with zeroâ€point vibrational corrections from density functional theory. Chirality, 2009, 21, E68-75.	1.3	37
84	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. Journal of Chemical Physics, 2009, 130, 034310.	1.2	43
85	A special issue of Molecular Physics honoring Prof. Henry F. Schaefer III. Molecular Physics, 2009, 107, 711-711.	0.8	2
86	On the Performance of a Size-Extensive Variant of Equation-of-Motion Coupled Cluster Theory for Optical Rotation in Chiral Molecules. Progress in Theoretical Chemistry and Physics, 2009, , 225-239.	0.2	9
87	Lowâ€lying singlet excited states of isocyanogen. International Journal of Quantum Chemistry, 2008, 108, 1137-1140.	1.0	17
88	Comparison of Time-Dependent Density-Functional Theory and Coupled Cluster Theory for the Calculation of the Optical Rotations of Chiral Molecules. Journal of Physical Chemistry A, 2008, 112, 1339-1345.	1.1	98
89	Bornâ^'Oppenheimer Symmetry Breaking in the Cl̀f State of NO₂:â€‰ Importance of Static and Dynamic Correlation Effects. Journal of Physical Chemistry A, 2008, 112, 2669-2676.	1.1	4
90	Optical Rotatory Dispersion of 2,3-Hexadiene and 2,3-Pentadiene. Journal of Physical Chemistry A, 2008, 112, 2415-2422.	1.1	41

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91	Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12Â model. Journal of Chemical Physics, 2008, 128, 244113.	1.2	113
92	Experimental Bond Critical Point and Local Energy Density Properties Determined for Mnâ€'O, Feâ€'O, and Coâ€'O Bonded Interactions for Tephroite, Mn2SiO4, Fayalite, Fe2SiO4, and Co2SiO4 Olivine and Selected Organic Metal Complexes: Comparison with Properties Calculated for Non-Transition and Transition Metal Mâ€'O Bonded Interactions for Silicates and Oxides. Journal of Physical Chemistry A, 2008, 112, 8811-8823.	1.1	35
93	Local correlation domains for coupled cluster theory: optical rotation and magnetic-field perturbations. Physical Chemistry Chemical Physics, 2008, 10, 3345.	1.3	39
94	Room-Temperature and Near-Room-Temperature Molecule-Based Magnets. Inorganic Chemistry, 2008, 47, 5649-5655.	1.9	24
95	M₂@C₇₉N (M = Y, Tb): Isolation and Characterization of Stable Endohedral Metallofullerenes Exhibiting Mâ€'M Bonding Interactions inside Aza[80]fullerene Cages. Journal of the American Chemical Society, 2008, 130, 12992-12997.	6.6	155
96	The Current State of Ab Initio Calculations of Optical Rotation and Electronic Circular Dichroism Spectra. Journal of Physical Chemistry A, 2007, 111, 12057-12068.	1.1	251
97	The problematic case of (S)-methylthiirane: electronic circular dichroism spectra and optical rotatory dispersion. Molecular Physics, 2007, 105, 2607-2617.	0.8	33
98	Chiroptical Properties of (R)-3-Chloro-1-butene and (R)-2-Chlorobutane. Journal of Physical Chemistry A, 2007, 111, 11232-11241.	1.1	22
99	PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616.	1.5	258
100	An Introduction to Coupled Cluster Theory for Computational Chemists. Reviews in Computational Chemistry, 2007, , 33-136.	1.5	531
101	Protonated 2-Methyl-1,2-epoxypropane:Â A Challenging Problem for Density Functional Theory. Journal of Organic Chemistry, 2006, 71, 1592-1597.	1.7	35
102	Ab initio and analytic intermolecular potentials for Arâ€"CH3OH. Physical Chemistry Chemical Physics, 2006, 8, 4678-4684.	1.3	9
103	Ab Initio Optical Rotatory Dispersion and Electronic Circular Dichroism Spectra of (S)-2-Chloropropionitrile. Journal of Physical Chemistry A, 2006, 110, 7649-7654.	1.1	39
104	Ab Initio Determination of Optical Rotatory Dispersion in the Conformationally Flexible Molecule (R)-Epichlorohydrin. Journal of Physical Chemistry A, 2006, 110, 2290-2298.	1.1	36
105	Ab initio calculation of molecular chiroptical properties. Theoretical Chemistry Accounts, 2006, 115, 227-245.	0.5	362
106	Sources of error in electronic structure calculations on small chemical systems. Journal of Chemical Physics, 2006, 124, 054107.	1.2	183
107	The lowest Aâ€²2 excited state of the water-hydroxyl complex. Journal of Chemical Physics, 2006, 125, 204302.	1.2	29
108	A mapping of the electron localization function for earth materials. Physics and Chemistry of Minerals, 2005, 32, 208-221.	0.3	19

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109	The structures of m-benzyne and tetrafluoro-m-benzyne. Journal of Chemical Physics, 2005, 122, 174309.	1.2	48
110	Application of equation-of-motion coupled-cluster methods to low-lying singlet and triplet electronic states of HBO and BOH. Journal of Chemical Physics, 2005, 122, 234316.	1.2	7
111	Coupled cluster methods including triple excitations for excited states of radicals. Journal of Chemical Physics, 2005, 122, 054110.	1.2	64
112	Comparison of the Electron Localization Function and Deformation Electron Density Maps for Selected Earth Materials. Journal of Physical Chemistry A, 2005, 109, 10022-10027.	1.1	20
113	Ab Initio Calculation of Optical Rotation in (P)-(+)-[4]Triangulane. Journal of the American Chemical Society, 2005, 127, 1368-1369.	6.6	75
114	Local correlation in coupled cluster calculations of molecular response properties. Chemical Physics Letters, 2004, 400, 104-111.	1.2	77
115	Potential energy surface discontinuities in local correlation methods. Journal of Chemical Physics, 2004, 121, 691-696.	1.2	66
116	Coupled cluster calculations of optical rotatory dispersion of (S)-methyloxirane. Journal of Chemical Physics, 2004, 121, 3550-3557.	1.2	128
117	Real versus artifactual symmetry-breaking effects in Hartreeâ€“Fock, density-functional, and coupled-cluster methods. Journal of Chemical Physics, 2004, 120, 7298-7306.	1.2	68
118	A Family of Decamethylmetallocene Charge-Transfer Salt Magnets Using Methyl Tricyanoethylenecarboxylate (MTCE) as the Electron Acceptor. Journal of the American Chemical Society, 2004, 126, 16890-16895.	6.6	27
119	Hartreeâ^'Fock Orbital Instabilities and Symmetry-Breaking in ScO2:Â Is aCsEquilibrium Structure Viable?â€. Journal of Physical Chemistry A, 2004, 108, 3097-3102.	1.1	12
120	The aminoboranylideneâ€“iminoborane isomerization. Journal of Chemical Physics, 2003, 119, 10647-10652.	1.2	10
121	The electron cusp condition and the virial ratio as indicators of basis set quality. Journal of Chemical Physics, 2003, 118, 2491.	1.2	6
122	The Equilibrium Geometry, Harmonic Vibrational Frequencies, and Estimated ab Initio Limit for the Barrier to Planarity of the Ethylene Radical Cation. Journal of Physical Chemistry A, 2002, 106, 2671-2675.	1.1	18
123	Potential curves and spectroscopic properties for the ground state of ClO and for the ground and various excited states of ClOâ^. Journal of Chemical Physics, 2002, 117, 9703-9709.	1.2	9
124	A mapping of the electron localization function for the silica polymorphs: evidence for domains of electron pairs and sites of potential electrophilic attack. Physics and Chemistry of Minerals, 2002, 29, 307-318.	0.3	19
125	Locally correlated equation-of-motion coupled cluster theory for the excited states of large molecules. Chemical Physics Letters, 2002, 366, 611-622.	1.2	98
126	Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650.	1.2	161

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127	A new diagnostic for open-shell coupled-cluster theory. Chemical Physics Letters, 2000, 328, 431-436.	1.2	79
128	Some surprising failures of Brueckner coupled cluster theory. Journal of Chemical Physics, 2000, 112, 7873-7879.	1.2	54
129	Thermokinetic Proton Transfer and Ab Initio Studies of the [2H,S,O]+ System. The Proton Affinity of HSO. Journal of Physical Chemistry A, 2000, 104, 4636-4647.	1.1	14
130	Conformations of [10]Annulene:â€‰ More Bad News for Density Functional Theory and Second-Order Perturbation Theory. Journal of the American Chemical Society, 1999, 121, 10788-10793.	6.6	98
131	Rotational spectrum and theoretical structure of the carbene HC4N. Journal of Chemical Physics, 1999, 111, 6750-6754.	1.2	22
132	Structure and Energetics of Isomers of the Interstellar Molecule C5H. Journal of the American Chemical Society, 1999, 121, 1902-1911.	6.6	54
133	Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611.	1.0	139
134	Definitive ab initio structure for the XÌƒâ€‰2Aâ€²H2PO radical and resolution of the Pâ€“O stretching mode assignment. Journal of Chemical Physics, 1998, 109, 2694-2699.	1.2	14
135	Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. , 1998, 70, 601.		6
136	Investigation of an asymmetric tripleâ€excitation correction for coupledâ€cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611.	1.0	10
137	The weakly bound dinitrogen tetroxide molecule: High level single reference wavefunctions are good enough. Journal of Chemical Physics, 1997, 106, 7178-7184.	1.2	27
138	The CÌƒâ€‰2A2 excited state of NO2: Evidence for a Cs equilibrium structure and a failure of some spin-restricted reference wavefunctions. Journal of Chemical Physics, 1997, 107, 2525-2528.	1.2	32
139	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. Journal of Chemical Physics, 1997, 107, 9980-9984.	1.2	31
140	A new spin-restricted triple excitation correction for coupled cluster theory. Journal of Chemical Physics, 1997, 107, 7943-7950.	1.2	27
141	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	1.2	142
142	A comparison of two approaches to perturbation triple excitation corrections to the coupledâ€cluster singles and doubles method for highâ€spin openâ€shell systems. Journal of Chemical Physics, 1996, 104, 6259-6264.	1.2	31
143	Aluminum monocarbonyl and aluminum isocarbonyl. Journal of Chemical Physics, 1996, 104, 3672-3675.	1.2	20
144	On the energy invariance of openâ€shell perturbation theory with respect to unitary transformations of molecular orbitals. Journal of Chemical Physics, 1996, 105, 1060-1069.	1.2	31

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145	A contribution to the understanding of the structure of xenon hexafluoride. Journal of Chemical Physics, 1995, 102, 3307-3311.	1.2	25
146	Benchmark studies of electron correlation in sixâ€electron systems. Journal of Chemical Physics, 1994, 100, 8132-8139.	1.2	19
147	The balance between theoretical method and basis set quality: A systematic study of equilibrium geometries, dipole moments, harmonic vibrational frequencies, and infrared intensities. Journal of Chemical Physics, 1993, 99, 403-416.	1.2	213
148	Rotational constants for the Cl̀ƒâ€‰2A2 state of NO2. Journal of Chemical Physics, 1993, 99, 7926-7928.	1.2	10
149	Monofluorinated hydrogen sulfide (HFS): A definitive theoretical prediction of the infrared spectrum. Journal of Chemical Physics, 1992, 96, 2044-2047.	1.2	8
150	The Hartley basis functions and transform: alternatives to plane waves and the Fourier transform. Chemical Physics Letters, 1992, 192, 45-48.	1.2	3