Henry F Schaefer

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7301362/publications.pdf

Version: 2024-02-01

1,011 papers	56,131 citations	1614 105 h-index	2332 199 g-index
1026 all docs	1026 docs citations	1026 times ranked	21258 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	An efficient reformulation of the closedâ€shell coupled cluster single and double excitation (CCSD) equations. Journal of Chemical Physics, 1988, 89, 7382-7387.	3.0	1,519
4	Atomic and Molecular Electron Affinities:â€‰ Photoelectron Experiments and Theoretical Computations. Chemical Reviews, 2002, 102, 231-282.	47.7	1,152
5	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. Journal of Chemical Physics, 1989, 90, 3700-3703.	3.0	1,065
6	<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.	5.3	961
7	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	14.6	838
8	On the evaluation of analytic energy derivatives for correlated wave functions. Journal of Chemical Physics, 1984, 81, 5031-5033.	3.0	815
9	A Stable Silicon(0) Compound with a Si=Si Double Bond. Science, 2008, 321, 1069-1071.	12.6	680
10	Extensive theoretical studies of the hydrogenâ€bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2Hâ^', and (NH3)2. Journal of Chemical Physics, 1986, 84, 2279-2289.	3.0	666
11	In pursuit of theab initiolimit for conformational energy prototypes. Journal of Chemical Physics, 1998, 108, 9751-9764.	3.0	659
12	A new implementation of the full CCSDT model for molecular electronic structure. Chemical Physics Letters, 1988, 152, 382-386.	2.6	579
13	An Introduction to Coupled Cluster Theory for Computational Chemists. Reviews in Computational Chemistry, 2007, , 33-136.	1.5	531
14	A Stable Neutral Diborene Containing a BB Double Bond. Journal of the American Chemical Society, 2007, 129, 12412-12413.	13.7	508
15	The C2H5+ O2Reaction Mechanism:Â High-Level ab Initio Characterizations. Journal of Physical Chemistry A, 2000, 104, 9823-9840.	2.5	496
16	A systematic study of molecular vibrational anharmonicity and vibrationâ€"rotation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. Chemical Physics, 1988, 123, 187-239.	1.9	476
17	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
18	The diagonal correction to the Bornâ€"Oppenheimer approximation: Its effect on the singletâ€"triplet splitting of CH2 and other molecular effects. Journal of Chemical Physics, 1986, 84, 4481-4484.	3.0	399

#	Article	IF	Citations
19	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. Journal of Chemical Physics, 1987, 87, 5361-5373.	3.0	378
20	The graphical unitary group approach to the electron correlation problem. Methods and preliminary applications. Journal of Chemical Physics, 1979, 70, 5092-5106.	3.0	351
21	Localized and Delocalized 1s Hole States of the O 2 + Molecular Ion. Journal of Chemical Physics, 1972, 56, 224-226.	3.0	323
22	Analytic Raman intensities from molecular electronic wave functions. Journal of Chemical Physics, 1986, 84, 531-532.	3.0	319
23	Toward subchemical accuracy in computational thermochemistry: Focal point analysis of the heat of formation of NCO and [H,N,C,O] isomers. Journal of Chemical Physics, 2004, 120, 11586-11599.	3.0	317
24	Electronic structure of homoleptic transition metal hydrides: TiH4, VH4, CrH4, MnH4, FeH4, CoH4, and NiH4. Journal of Chemical Physics, 1979, 71, 705-712.	3.0	316
25	The closedâ€shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. Journal of Chemical Physics, 1987, 86, 2881-2890.	3.0	316
26	Systematic study of molecular anions within the selfâ€consistentâ€field approximation: OHâ^', CNâ^', C2Hâ^', NHâ^'2, and CHâ^'3. Journal of Chemical Physics, 1985, 83, 1784-1794.	3.0	312
27	The Configuration Interaction Method: Advances in Highly Correlated Approaches. Advances in Quantum Chemistry, 1999, , 143-269.	0.8	294
28	Concerning zeroâ€point vibrational energy corrections to electronic energies. Journal of Chemical Physics, 1991, 95, 5128-5132.	3.0	284
29	Analytic gradients from correlated wave functions via the twoâ€particle density matrix and the unitary group approach. Journal of Chemical Physics, 1980, 72, 4652-4653.	3.0	279
30	Analytic evaluation and basis set dependence of intensities of infrared spectra. Journal of Chemical Physics, 1986, 84, 2262-2278.	3.0	279
31	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. Chemical Physics, 1990, 145, 427-466.	1.9	267
32	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. Journal of Chemical Physics, 2002, 116, 690-701.	3.0	262
33	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. Journal of Chemical Physics, 2007, 127, 024102.	3.0	255
34	Homonuclear 3d transition-metal diatomics: A systematic density functional theory study. Journal of Chemical Physics, 2000, 113, 690-700.	3.0	249
35	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. Journal of Chemical Physics, 1986, 85, 963-968.	3.0	245
36	Electron Affinities of the DNA and RNA Bases. Journal of the American Chemical Society, 2001, 123, 4023-4028.	13.7	236

#	Article	IF	Citations
37	Transition structures for the interchange of hydrogen atoms within the water dimer. Journal of Chemical Physics, 1990, 92, 1240-1247.	3.0	230
38	The shapeâ€driven graphical unitary group approach to the electron correlation problem. Application to the ethylene molecule. Journal of Chemical Physics, 1982, 77, 5584-5592.	3.0	222
39	Coupled cluster energy derivatives. Analytic Hessian for the closedâ€shell coupled cluster singles and doubles wave function: Theory and applications. Journal of Chemical Physics, 1990, 92, 4924-4940.	3.0	222
40	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.	3.0	213
41	High-order excitations in state-universal and state-specific multireference coupled cluster theories: Model systems. Journal of Chemical Physics, 2006, 125, 154113.	3.0	207
42	A Viable Anionic N-Heterocyclic Dicarbene. Journal of the American Chemical Society, 2010, 132, 14370-14372.	13.7	206
43	Concerning the precision of standard density functional programs: Gaussian, Molpro, NWChem, Q-Chem, and Gamess. Computational and Theoretical Chemistry, 2006, 768, 175-181.	1.5	197
44	Definitive Ab Initio Studies of Model SN2 Reactions CH3X+F (X=F, Cl, CN, OH, SH, NH2, PH2). Chemistry - A European Journal, 2003, 9, 2173-2192.	3.3	196
45	Gradient techniques for openâ€shell restricted Hartreeâ€“Fock and multiconfiguration selfâ€consistentâ€field methods. Journal of Chemical Physics, 1979, 71, 1525-1530.	3.0	195
46	Concerning the applicability of density functional methods to atomic and molecular negative ions. Journal of Chemical Physics, 1996, 105, 862-864.	3.0	194
47	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
48	The photodissociation of formaldehyde: Potential energy surface features. Journal of Chemical Physics, 1979, 70, 5117-5134.	3.0	184
49	Vinylidene: the final chapter?. Journal of the American Chemical Society, 1990, 112, 8714-8719.	13.7	184
50	Potential energy surface for the model unimolecular reaction HNC â† HCN. Journal of Chemical Physics, 1975, 62, 350.	3.0	181
51	A systematic theoretical study of harmonic vibrational frequencies: The ammonium ion NH4+and other simple molecules. Journal of Chemical Physics, 1980, 73, 2310-2318.	3.0	181
52	Remarkable Aspects of Unsaturation in Trinuclear Metal Carbonyl Clusters:Â The Triiron Species Fe3(CO)n(n= 12, 11, 10, 9). Journal of the American Chemical Society, 2006, 128, 11376-11384.	13.7	181
53	CH+5: The neverâ€ending story or the final word?. Journal of Chemical Physics, 1993, 99, 3716-3720.	3.0	177
54	Structures and stability of hydrated clusters of hydrogen chloride, HCl(H2O)n, n=1â€“5. Journal of Chemical Physics, 1998, 109, 973-977.	3.0	176

#	Article	IF	Citations
55	The protonated water dimer: Extensive theoretical studies of H5O+2. Journal of Chemical Physics, 1994, 101, 4878-4884.	3.0	174
56	Large-scale symmetry-adapted perturbation theory computations via density fitting and Laplace transformation techniques: Investigating the fundamental forces of DNA-intercalator interactions. Journal of Chemical Physics, 2011, 135, 174107.	3.0	174
57	Generalization of analytic configuration interaction (CI) gradient techniques for potential energy hypersurfaces, including a solution to the coupled perturbed Hartreeâ€“Fock equations for multiconfiguration SCF molecular wave functions. Journal of Chemical Physics, 1982, 77, 383-390.	3.0	169
58	Vinylidene: Potential energy surface and unimolecular reaction dynamics. Journal of Chemical Physics, 1984, 80, 4347-4354.	3.0	169
59	Analytic second derivatives in restricted Hartreeâ€“Fock theory. A method for highâ€spin openâ€shell molecular wave functions. Journal of Chemical Physics, 1982, 77, 5647-5654.	3.0	167
60	Mindless Chemistry. Journal of Physical Chemistry A, 2006, 110, 4287-4290.	2.5	165
61	Design of a Catalytic Active Site for Electrochemical CO₂ Reduction with Mn(I)-Tricarbonyl Species. Inorganic Chemistry, 2015, 54, 5285-5294.	4.0	163
62	The torsional conformations of butane: Definitive energetics from ab initio methods. Journal of Chemical Physics, 1997, 106, 5143-5150.	3.0	159
63	Molecular Autoionization Lifetimes and Cross Sections for Penning Ionization: Numerical Results for He* (1s2sâ€‰3S) + H(1sâ€‰2S). Journal of Chemical Physics, 1972, 56, 1347-1358.	3.0	154
64	The automated solution of second quantization equations with applications to the coupled cluster approach. Theoretica Chimica Acta, 1991, 79, 1-42.	0.8	151
65	The weakly exothermic rearrangement of methoxy radical (CH3Oâ‹…) to the hydroxymethyl radical (CH2OHâ‹…). Journal of Chemical Physics, 1983, 78, 845-853.	3.0	147
66	Theoretical Treatment of Penning Ionizationâ€”He(1s2s 1S, 3S)â€‰+â€‰H(1s 2S). Journal of Chemical Physics, 1970, 53, 1421-1427.	3.0	144
67	The optimization of molecular orbitals for coupled cluster wavefunctions. Chemical Physics Letters, 1987, 142, 354-358.	2.6	144
68	Accelerating the convergence of the coupled-cluster approach. Chemical Physics Letters, 1986, 130, 236-239.	2.6	143
69	Mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1997, 107, 141-155.	3.0	142
70	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	3.0	142
71	The malonaldehyde equilibrium geometry: A major structural shift due to the effects of electron correlation. Journal of Chemical Physics, 1985, 82, 4194-4198.	3.0	137
72	Ab Initio Calculations on 62 Lowâ€Lying States of the O2Molecule. Journal of Chemical Physics, 1968, 48, 4946-4955.	3.0	136

#	Article	IF	Citations
73	Potential energy surface for the Li+HFâ†'LiF+H reaction. Journal of Chemical Physics, 1980, 72, 4376-4393.	3.0	135
74	Carbene Rearrangements Unsurpassed:â€‰ Details of the C7H6 Potential Energy Surface Revealed. Journal of Organic Chemistry, 1996, 61, 7030-7039.	3.2	133
75	Interaction potential between two rigid HF molecules. Journal of Chemical Physics, 1974, 60, 855-865.	3.0	131
76	Binuclear Homoleptic Iron Carbonyls:Â Incorporation of Formal Ironâ^'Iron Single, Double, Triple, and Quadruple Bonds, Fe2(CO)x(x= 9, 8, 7, 6). Journal of the American Chemical Society, 2000, 122, 8746-8761.	13.7	131
77	An energetically lowâ€lying silacyclopropyne isomer of SiC2. Journal of Chemical Physics, 1984, 80, 3552-3555.	3.0	130
78	Infrared cavity ringdown spectroscopy of methanol clusters: Single donor hydrogen bonding. Journal of Chemical Physics, 1999, 110, 4258-4267.	3.0	130
79	The remarkable monobridged structure of Si2H2. Journal of Chemical Physics, 1992, 97, 7990-7998.	3.0	129
80	Potential Energy Surface Including Electron Correlation for the Chemical F + H2 â†' FH + H I. Preliminary Surface. Journal of Chemical Physics, 1972, 56, 4626-4631.	3.0	127
81	The silicon-carbon double bond: a healthy rivalry between theory and experiment. Accounts of Chemical Research, 1982, 15, 283-290.	15.6	126
82	Conformers of Gaseous Cysteine. Journal of Chemical Theory and Computation, 2009, 5, 1511-1523.	5.3	126
83	Is Mo/llerâ€"Plesset perturbation theory a convergent ab initio method?. Journal of Chemical Physics, 2000, 112, 9213-9222.	3.0	125
84	Electron Affinity of the Guanineâ^'Cytosine Base Pair and Structural Perturbations upon Anion Formation. Journal of the American Chemical Society, 2002, 124, 10163-10170.	13.7	125
85	A theory of selfâ€consistent electron pairs. Computational methods and preliminary applications. Journal of Chemical Physics, 1976, 65, 2740-2750.	3.0	124
86	The Nature of the Galliumâ^'Gallium Triple Bond. Journal of the American Chemical Society, 1998, 120, 3773-3780.	13.7	124
87	Electron Affinities of Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 524-528.	2.5	124
88	Characteristics of novel sandwiched beryllium, magnesium, and calcium dimers: C5H5BeBeC5H5, C5H5MgMgC5H5, and C5H5CaCaC5H5. Chemical Physics Letters, 2005, 402, 414-421.	2.6	124
89	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Agn (nâ©½4). Journal of Chemical Physics, 2006, 124, 184102.	3.0	124
90	Triple excitations in state-specific multireference coupled cluster theory: Application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. Journal of Chemical Physics, 2008, 128, 124104.	3.0	123

#	Article	IF	Citations
91	Electrophilic Aromatic Substitution: New Insights into an Old Class of Reactions. Accounts of Chemical Research, 2016, 49, 1191-1199.	15.6	123
92	Ab Initio Potential Curve for the X 3Î£gâ¯ State of O2. Journal of Chemical Physics, 1971, 54, 2207-2211.	3.0	122
93	The decarboxylation and dehydration reactions of monomeric formic acid. Journal of Chemical Physics, 1992, 96, 1158-1166.	3.0	119
94	Non-innocent Additives in a Palladium(II)-Catalyzed Câ€“H Bond Activation Reaction: Insights into Multimetallic Active Catalysts. Journal of the American Chemical Society, 2014, 136, 5535-5538.	13.7	119
95	Model studies of chemisorption. Interaction between atomic hydrogen and beryllium clusters. Journal of Chemical Physics, 1975, 62, 4815-4825.	3.0	118
96	Electron correlation in small metal clusters. Application of a theory of selfâ€consistent electron pairs to the Be4system. Journal of Chemical Physics, 1976, 65, 5141-5146.	3.0	118
97	Assessment of Density Functional Theory for Model SN2 Reactions:Â CH3X + F-(X = F, Cl, CN, OH, SH, NH2,) Tj ETQq1 1 0.784314 rgBT	2.5	118
98	Features of the H2CO potential energy hypersurface pertinent to formaldehyde photodissociation. Journal of Chemical Physics, 1981, 75, 3459-3465.	3.0	114
99	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	3.0	114
100	The Dichotomy of Dimetallocenes:Â Coaxial versus Perpendicular Dimetal Units in Sandwich Compounds. Journal of the American Chemical Society, 2005, 127, 2818-2819.	13.7	113
101	Analytic second derivatives for Rennerâ€“Teller potential energy surfaces. Examples of the five distinct cases. Journal of Chemical Physics, 1984, 81, 356-361.	3.0	111
102	The analytic evaluation of energy first derivatives for twoâ€configuration selfâ€consistentâ€field configuration interaction (TCSCFâ€CI) wave functions. Application to ozone and ethylene. Journal of Chemical Physics, 1987, 87, 7062-7075.	3.0	111
103	DNA Nucleosides and Their Radical Anions:Â Molecular Structures and Electron Affinities. Journal of the American Chemical Society, 2004, 126, 4404-4411.	13.7	109
104	The photodissociation of formaldehyde: A coupled cluster study including connected triple excitations of the transition state barrier height for H2COâ†'H2+CO. Journal of Chemical Physics, 1989, 90, 3629-3636.	3.0	108
105	Multiple dâ€type basis functions for molecules containing second row atoms. Journal of Chemical Physics, 1985, 83, 5721-5726.	3.0	106
106	The Adenineâ¯Thymine Base Pair Radical Anion:â€‰ Adding an Electron Results in a Major Structural Change. Journal of Physical Chemistry B, 2003, 107, 848-853.	2.6	106
107	Metalâ€“Metal (MM) Bond Distances and Bond Orders in Binuclear Metal Complexes of the First Row Transition Metals Titanium Through Zinc. Chemical Reviews, 2018, 118, 11626-11706.	47.7	106
108	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.	5.3	106

#	Article	IF	Citations
109	Valenceâ€Excited States of Carbon Monoxide. Journal of Chemical Physics, 1970, 53, 3994-4004.	3.0	105
110	Calculation of the Attractive He Pair Potential. Physical Review Letters, 1970, 25, 988-990.	7.8	105
111	A systematic theoretical study of harmonic vibrational frequencies: The single and double excitation coupled cluster (CCSD) method. Journal of Chemical Physics, 1988, 89, 360-366.	3.0	105
112	An Efficient Computational Approach for the Evaluation of Substituent Constants. Journal of Organic Chemistry, 2006, 71, 6382-6387.	3.2	105
113	Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 104103.	3.0	104
114	Stabilization of elusive silicon oxides. Nature Chemistry, 2015, 7, 509-513.	13.6	104
115	Negative Ion Thermochemistry:â€‰ The Sulfur Fluorides SFn/SFn- (n = 1â^'7). The Journal of Physical Chemistry, 1996, 100, 6061-6068.	2.9	102
116	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. Journal of Chemical Physics, 1998, 108, 7197-7201.	3.0	102
117	Theoretical Studies of the Potential Energy Surfaces and Compositions of thed-Aldo-andd-Ketohexoses. Journal of the American Chemical Society, 1998, 120, 3411-3422.	13.7	101
118	Triplet electronic states of acetylene:cisandtransstructures and energetics. Journal of Chemical Physics, 1978, 69, 1648-1654.	3.0	100
119	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. Theoretical Chemistry Accounts, 2003, 109, 140-148.	1.4	100
120	Binuclear Cyclopentadienylcobalt Carbonyls:Â Comparison with Binuclear Iron Carbonyls. Journal of the American Chemical Society, 2005, 127, 11646-11651.	13.7	100
121	Avoided intersection of potential energy surfaces: The (H+â€‰+â€‰H2,â€‰Hâ€‰+â€‰H2+) system. Journal of Chemical Physics, 1973, 59, 1286-1292.	3.0	99
122	Cleavage of Carbene-Stabilized Disilicon. Journal of the American Chemical Society, 2011, 133, 8874-8876.	13.7	98
123	Thermochemistry of CHn, SiHn(n=0â€“4), and the cations SiH+, SiH2+, and SiH3+: A converged quantum mechanical approach. Journal of Chemical Physics, 1992, 97, 8389-8406.	3.0	97
124	A new zincâ€“zinc-bonded compound with a dianionic Î±-diimine ligand: synthesis and structure of [Na(THF)2]2Â·[LZnâ€“ZnL] (L = [(2,6-iPr2C6H3)N(Me)C]22â^'). Chemical Communications, 2007, , 2363-2365.	4.1	97
125	New theoretical evidence for the nonlinearity of the triplet ground state of methylene. Journal of the American Chemical Society, 1970, 92, 4984-4985.	13.7	96
126	Perturbative triples corrections in state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2010, 132, 074107.	3.0	96

#	Article	IF	Citations
127	Theoretical Potential Energy Curves for OH, HF+, HF, HFâˆ’, NeH+, and NeH. Journal of Chemical Physics, 1972, 57, 1123-1128.	3.0	95
128	Structures and vibrational frequencies in the full configuration interaction limit: Predictions for four electronic states of methylene using a triple-zeta plus double polarization (TZ2P) basis. Journal of Chemical Physics, 1998, 108, 1040-1049.	3.0	93
129	The existence of secondary orbital interactions. Journal of Computational Chemistry, 2007, 28, 344-361.	3.3	92
130	Theoretical Study of SO2 Molecular Properties. Journal of Chemical Physics, 1970, 53, 3014-3019.	3.0	91
131	Electronic Structures and Potential Energy Curves for the Lowâ€Lying States of the CN Radical. Journal of Chemical Physics, 1971, 54, 2573-2580.	3.0	91
132	A combined crossed molecular beam and ab initio investigation of C2 and C3 elementary reactions with unsaturated hydrocarbonsÃ¢â‚¬â€pathways to hydrogen deficient hydrocarbon radicals in combustion flames. Faraday Discussions, 2001, 119, 51-66.	3.2	91
133	Relativistic and correlation effects in CuH, AgH, and AuH: Comparison of various relativistic methods. Journal of Chemical Physics, 1995, 102, 2024-2031.	3.0	90
134	Theoretical study of the H+O3â†”OH+O2â†”O+HO2 system. Journal of Chemical Physics, 1986, 84, 2691-2697.	3.0	89
135	Geometrical structures and vibrational frequencies of the energetically lowâ€lying isomers of SiC3. Journal of Chemical Physics, 1990, 93, 5046-5052.	3.0	89
136	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹…HO): The global minimum. Journal of Chemical Physics, 1993, 98, 8829-8834.	3.0	89
137	A systematic theoretical study of the harmonic vibrational frequencies for polyatomic molecules: The single, double, and perturbative triple excitation coupledâ€cluster [CCSD(T)] method. Journal of Chemical Physics, 1993, 98, 1336-1344.	3.0	89
138	Crossed beam reaction of cyano radicals with hydrocarbon molecules. I. Chemical dynamics of cyanobenzene (C6H5CN; Xâ€Š1A1) and perdeutero cyanobenzene (C6D5CN; Xâ€Š1A1) formation from reaction of CN(Xâ€Š2Î£+) with benzene C6H6(Xâ€Š1A1g), and d6-benzene C6D6(Xâ€Š1A1g). Journal of Chemical Physics, 1999, 111, 7457-7471.	3.0	89
139	NHCâ€Containing Manganese(I) Electrocatalysts for the Twoâ€Electron Reduction of CO₂. Angewandte Chemie - International Edition, 2014, 53, 5152-5155.	13.8	89
140	Analytic configuration interaction (CI) gradient techniques for potential energy hypersurfaces. A method for openâ€shell molecular wave functions. Journal of Chemical Physics, 1981, 75, 2919-2922.	3.0	88
141	The Chemical Vapor Deposition of Aluminum Nitride:Â Unusual Cluster Formation in the Gas Phase. Journal of the American Chemical Society, 1997, 119, 5668-5678.	13.7	88
142	Direct Nearâ€Hartreeâ€“Fock Calculations on the 1s Hole States of NO+. Journal of Chemical Physics, 1971, 55, 1474-1475.	3.0	87
143	Analytic energy second derivatives for general MCSCF wave functions. Journal of Chemical Physics, 1984, 80, 2660-2668.	3.0	87
144	Analytic third derivatives for selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1984, 81, 6395-6396.	3.0	86

#	Article	IF	Citations
145	A Systematic Application of Density Functional Theory to Some Carbon-Containing Molecules and Their Anions. Journal of Physical Chemistry A, 1999, 103, 4065-4077.	2.5	86
146	Electronic Splitting between the 2B1 and 2A1 States of the NH2 Radical. Journal of Chemical Physics, 1971, 55, 4798-4803.	3.0	85
147	C2Ï... Potential Energy Surfaces for Seven Lowâ€Lying States of CH2. Journal of Chemical Physics, 1971, 55, 162-169.	3.0	84
148	Electronic structure of the N4+molecular ion. Journal of Chemical Physics, 1981, 74, 550-558.	3.0	84
149	Potential energy surfaces related to the ionâ€molecule reaction C+ + H2. Journal of Chemical Physics, 1974, 61, 2507-2513.	3.0	81
150	The silicon analog of benzeneâ€“hexasilabenzene (Si6H6). Journal of Chemical Physics, 1986, 84, 1664-1669.	3.0	81
151	Use of 2h and 3hâ^'p-like coupled-cluster Tammâ€“Dancoff approaches for the equilibrium properties of ozone. Chemical Physics Letters, 2003, 378, 42-46.	2.6	81
152	Interpretation of excited state Hartreeâ€“Fock analytic derivative anomalies for NO2 and HCO2 using the molecular orbital Hessian. Journal of Chemical Physics, 1991, 95, 7466-7478.	3.0	80
153	Curve Crossing of theB3Î£uâ^' and 3Î u States of O2and Its Relation to Predissociation in the Schumannâ€"Runge Bands. Journal of Chemical Physics, 1971, 55, 4107-4113.	3.0	79
154	Ab initio calculation of reaction energies. III. Basis set dependence of relative energies on the FH2 and H2CO potential energy surfaces. Journal of Chemical Physics, 1984, 81, 1882-1893.	3.0	79
155	The H+5potential energy hypersurface: Characterization of ten distinct energetically lowâ€lying stationary points. Journal of Chemical Physics, 1987, 86, 5072-5081.	3.0	79
156	The convergence of the cluster model for the study of chemisorption: Be36H. Journal of Chemical Physics, 1983, 78, 1390-1395.	3.0	78
157	Molecular clustering about a positive ion. Structures, energetics, and vibrational frequencies of the protonated hydrogen clusters H+3, H+5, H+7, and H+9. Journal of Chemical Physics, 1983, 78, 4074-4085.	3.0	77
158	Re(I) NHC Complexes for Electrocatalytic Conversion of CO₂. Inorganic Chemistry, 2016, 55, 3136-3144.	4.0	77
159	Methane as a Numerical Experiment for Polarization Basis Function Selection. Journal of Chemical Physics, 1971, 54, 2764-2766.	3.0	76
160	Diatomic sulfur: Low lying bound molecular electronic states of S2. Journal of Chemical Physics, 1979, 70, 947.	3.0	76
161	Carbon clusters: The structure of C10 studied with configuration interaction methods. Journal of Chemical Physics, 1990, 93, 8844-8849.	3.0	76
162	Protonated Ethane. A Theoretical Investigation of C2H7+ Structures and Energies. Journal of the American Chemical Society, 1994, 116, 3483-3493.	13.7	76

#	Article	IF	Citations
163	The electron affinities of the silicon fluorides SiFn (n=1â€“5). Journal of Chemical Physics, 1996, 105, 6880-6886.	3.0	76
164	Structures, thermochemistry, and electron affinities of the PFn and PFâ¯n series, n=1â€“6. Journal of Chemical Physics, 1996, 104, 3676-3683.	3.0	76
165	Singlet-triplet energy separation, Walsh-Mulliken diagrams, and singlet d-polarization effects in methylene. Journal of the American Chemical Society, 1972, 94, 6888-6893.	13.7	74
166	A critical test of semiempirical FH2 potential energy sufaces: The barrier height for H + FH â†' HF + H. Journal of Chemical Physics, 1975, 62, 1188-1189.	3.0	74
167	6â€311G is not of valence tripleâ€zeta quality. Journal of Chemical Physics, 1989, 91, 7305-7306.	3.0	74
168	Cobaltâ¯Cobalt Multiple Bonds in Homoleptic Carbonyls? Co2(CO)x(x= 5â¯8) Structures, Energetics, and Vibrational Spectra. Inorganic Chemistry, 2001, 40, 900-911.	4.0	74
169	Geometries of the excited electronic states of HCN. Journal of Chemical Physics, 1974, 60, 2787-2793.	3.0	73
170	The structure and stability of BH5. Does correlation make it a stable molecule? Qualitative changes at high levels of theory. Journal of Chemical Physics, 1994, 101, 7625-7632.	3.0	73
171	The barrier to linearity of water. Journal of Chemical Physics, 1999, 110, 11971-11981.	3.0	73
172	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
173	Lowest-Lying Conformers of Alanine: Pushing Theory to Ascertain Precise Energetics and Semiexperimental R_e Structures. Journal of Chemical Theory and Computation, 2010, 6, 3066-3078.	5.3	73
174	Large multiconfiguration selfâ€consistentâ€field wave functions for the ozone molecule. Journal of Chemical Physics, 1981, 74, 3411-3414.	3.0	72
175	The ~X1A1 and ~a3B2 states of o-benzyne: a theoretical characterization of equilibrium geometries, harmonic vibrational frequencies, and the singlet-triplet energy gap. Journal of the American Chemical Society, 1989, 111, 3118-3124.	13.7	72
176	Electrocatalytic Reduction of Carbon Dioxide by Mn(CN)(2,2â€²-bipyridine)(CO)₃: CN Coordination Alters Mechanism. Inorganic Chemistry, 2015, 54, 8849-8856.	4.0	72
177	Synthesis, Spectroscopy, and Electrochemistry of (Î±-Diimine)M(CO)₃Br, M = Mn, Re, Complexes: Ligands Isoelectronic to Bipyridyl Show Differences in CO₂ Reduction. Organometallics, 2015, 34, 3-12.	2.3	72
178	Theoretical studies of oxygen rings: Cyclotetraoxygen, O4. Journal of Chemical Physics, 1988, 88, 7043-7049.	3.0	71
179	Equilibrium geometry of the HCCN triplet ground state: Carbene or allene? An openâ€shell coupled cluster study including connected triple excitations. Journal of Chemical Physics, 1992, 96, 4449-4452.	3.0	71
180	Homoleptic Carbonyls of the Second-Row Transition Metals:â€‰ Evaluation of Hartreeâ¯Fock and Density Functional Theory Methods. Journal of Chemical Theory and Computation, 2007, 3, 1580-1587.	5.3	71

#	Article	IF	Citations
181	Molecular structures of the two most stable conformers of free glycine. Journal of Computational Chemistry, 2007, 28, 1373-1383.	3.3	71
182	Stabilization of Siliconâ€“Carbon Mixed Oxides. Journal of the American Chemical Society, 2015, 137, 8396-8399.	13.7	71
183	Potential energy curves for diatomic zinc and cadmium. Journal of Chemical Physics, 1979, 71, 1122-1127.	3.0	70
184	On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	3.0	70
185	Germanium-germanium multiple bonds: The singlet electronic ground state of Ge2H2. Chemical Physics Letters, 1990, 165, 257-264.	2.6	69
186	Electron Correlation in the Lowest 1Î£+ State of Beryllium Oxide. Journal of Chemical Physics, 1971, 55, 176-181.	3.0	68
187	Generalization of the direct configuration interaction method to the Hartreeâ€“Fock interacting space for doublets, quartets, and openâ€shell singlets. Applications to NO2and NO2â^'. Journal of Chemical Physics, 1979, 71, 426-435.	3.0	68
188	Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. Journal of Chemical Physics, 2009, 131, 064109.	3.0	68
189	Palladiumâ€“Silver Cooperativity in an Aryl Amination Reaction through Câ€“H Functionalization. ACS Catalysis, 2016, 6, 696-708.	11.2	68
190	Complete basis set limit studies of conventional and R12 correlation methods: The silicon dicarbide (SiC[sub 2]) barrier to linearity. Journal of Chemical Physics, 2003, 118, 7353.	3.0	67
191	Reaction paths for the dissociation alƒâ€‰3Aâ€˜ CH2COâ†'XÌƒâ€‰3B1 CH2â€‰+â€‰XÌƒâ€‰1Î£+ CO. Journal of Chemical Physics, 329-344.	3.0	66
192	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813.	3.0	66
193	Exploring the effect of axial ligand substitution (X = Br, NCS, CN) on the photodecomposition and electrochemical activity of [MnX(Nâ€“C)(CO)₃] complexes. Dalton Transactions, 2015, 44, 2122-2131.	3.3	66
194	Aspects of the reaction mechanism of ethane combustion. Conformations of the ethylperoxy radical. Journal of the American Chemical Society, 1992, 114, 8239-8247.	13.7	65
195	TheXÌƒ3B1,Ã£1A1,bÌƒ1B1, andcÌƒ1A1Electronic States of CH2. The Journal of Physical Chemistry, 1996, 100, 7911-7918.	2.9	65
196	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
197	Bending Frequency of the C3 Molecule. Journal of Chemical Physics, 1972, 56, 5075-5080.	3.0	64
198	An assessment for the full coupled cluster method including all single, double, and triple excitations: The diatomic molecules LiH, Li2, BH, LiF, C2, BeO, CN+, BF, NO+, and F2. Journal of Chemical Physics, 1990, 92, 568-573.	3.0	64

#	Article	IF	Citations
199	Collisional Quenching of Metastable Hydrogen Atoms. Journal of Chemical Physics, 1971, 55, 926-932.	3.0	63
200	Generalization of analytic energy third derivatives for the RHF closedâ€shell wave function: Derivative energy and integral formalisms and the prediction of vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 1986, 85, 5132-5142.	3.0	63
201	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹…OH): The 2Aâ€˜ and 2Aâ€™ minima. Journal of Chemical Physics, 1991, 94, 2057-2062.	3.0	63
202	Chemical dynamics of d1-methyldiacetylene (CH3CCCCD; Xâ€‰1A1) and d1-ethynylallene (H2CCCH(C2D); Xâ€‰1Aâ€²) formation from reaction of C2D(Xâ€‰2Î£+) with methylacetylene, CH3CCH(Xâ€‰1A1). Journal of Chemical Physics, 2001, 114, 3488-3496.	3.0	63
203	The entrance complex, transition state, and exit complex for the F + H2O â†’ HF + OH reaction. Definitive predictions. Comparison with popular density functional methods. Physical Chemistry Chemical Physics, 2012, 14, 10891.	2.8	63
204	Linear Symmetric H4. Journal of Chemical Physics, 1972, 57, 217-220.	3.0	62
205	Hydrogen bonding between the nitrate anion (conventional and peroxy forms) and the water molecule. Journal of Chemical Physics, 1990, 93, 3379-3388.	3.0	62
206	Symmetry breaking in the NO2 Ïƒ radical: Construction of the 2A1 and 2B2 states with Cs symmetry complete active space selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1990, 93, 8105-8109.	3.0	62
207	Reaction of the ethynyl radical, C2H, with methylacetylene, CH3CCH, under single collision conditions: Implications for astrochemistry. Journal of Chemical Physics, 2001, 114, 3476-3487.	3.0	62
208	The highly anharmonic BH5 potential energy surface characterized in the ab initio limit. Journal of Chemical Physics, 2005, 122, 104302.	3.0	62
209	Firstâ€Order Wavefunctions, Orbital Correlation Energies, and Electron Affinities of Firstâ€Row Atoms. Journal of Chemical Physics, 1969, 51, 4643-4650.	3.0	61
210	Self-consistent-field wave functions, energies, multipole moments, diamagnetic susceptibility and shielding tensors, and electric field gradient tensors for nitrogen dioxide and ozone. Molecular Physics, 1971, 21, 317-327.	1.7	61
211	Electronic structure of Liâ€“H2O and related neutral molecular complexes, including Alâ€“H2O. Journal of Chemical Physics, 1978, 68, 4047-4050.	3.0	61
212	Infrared intensities of H3O+, H2DO+, HD2O+, and D3O+. Journal of Chemical Physics, 1983, 79, 1551-1552.	3.0	61
213	Aspects of the Reaction Mechanism of Ethane Combustion. 2. Nature of the Intramolecular Hydrogen Transfer. Journal of the American Chemical Society, 1994, 116, 4953-4962.	13.7	61
214	Binuclear Homoleptic Nickel Carbonyls:Â Incorporation of Niâˆ’Ni Single, Double, and Triple Bonds, Ni2(CO)x(x= 5, 6, 7). Journal of the American Chemical Society, 2000, 122, 1989-1994.	13.7	61
215	N(1Ag),T(3B1u), andV(1B1u) states of vertical ethylene. Journal of Chemical Physics, 1978, 68, 4839-4847.	3.0	60
216	A unimolecular reaction ABCâ†’A+B+C involving three product molecules and a single transition state. Photodissociation of glyoxal: HCOHCOâ†’H2+CO+CO. Journal of Chemical Physics, 1981, 75, 5828-5836.	3.0	60

#	Article	IF	Citations
217	Electrophile Affinity: A Reactivity Measure for Aromatic Substitution. Journal of the American Chemical Society, 2009, 131, 14722-14727.	13.7	60
218	On the H+F2â†'HF+F reaction. An ab initio potential energy surface. Journal of Chemical Physics, 1973, 58, 1126-1131.	3.0	59
219	The anharmonic force fields of HOF and F2O. Journal of Chemical Physics, 1988, 89, 4965-4975.	3.0	59
220	Anionic N-Heterocyclic Dicarbeneâ^'Borane Binuclear Complexes. Organometallics, 2011, 30, 1303-1306.	2.3	59
221	Geometrical structure and vibrational frequencies of several electronic states of Si2C. Journal of Chemical Physics, 1985, 82, 4126-4130.	3.0	58
222	Abinitiostudies of the lowâ€lying electronic states of ketene. Journal of Chemical Physics, 1986, 84, 2212-2225.	3.0	58
223	Is there a transition state for the unimolecular dissociation of cyclotetraoxygen (O4)?. Journal of Chemical Physics, 1992, 96, 1176-1182.	3.0	58
224	Ge2H2: a germanium-containing molecule with a low-lying monobridged equilibrium geometry. Journal of the American Chemical Society, 1993, 115, 6901-6903.	13.7	58
225	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	3.0	58
226	A possible role for triplet H2CN+ isomers in the formation of HCN and HNC in interstellar clouds. Journal of Chemical Physics, 1980, 73, 3255-3263.	3.0	57
227	Geometry and electronic structure of (CO)3NiCH2. A model transition-metal carbene. Journal of the American Chemical Society, 1981, 103, 3985-3990.	13.7	57
228	Structures and energies of singlet silacyclopropenylidene and 14 higher lying C2SiH2 isomers. Journal of the American Chemical Society, 1986, 108, 2169-2173.	13.7	57
229	The classical and nonclassical forms of protonated acetylene, C2H+3. Structures, vibrational frequencies, and infrared intensities from explicitly correlated wave functions. Journal of Chemical Physics, 1986, 85, 3437-3443.	3.0	57
230	The valence isoelectronic molecules CCO, CNN, SiCO, and SiNN in their triplet ground states: Theoretical predictions of structures and infrared spectra. Journal of Chemical Physics, 1988, 89, 3016-3027.	3.0	57
231	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â^'. Journal of Chemical Physics, 2000, 112, 4053-4063.	3.0	57
232	Is there an absence of threefold symmetry at the equilibrium geometry of the ground electronic state for NO3?. Journal of Chemical Physics, 1989, 91, 4410-4411.	3.0	56
233	The known and unknown group 13 hydride molecules M2H6: Diborane(6), dialane(6), and digallane(6). Journal of Chemical Physics, 1992, 96, 2868-2876.	3.0	56
234	Spectroscopic constants and potential energy surfaces for the possible interstellar molecules A1NC and A1CN. Molecular Physics, 1995, 86, 1331-1337.	1.7	56

#	Article	IF	Citations
235	Dinuclear versus Mononuclear Zinc Compounds from Reduction of LZnCl2 (L = Î±-Diimine Ligands): Effects of the Ligand Substituent, Reducing Agent, and Solvent. Organometallics, 2008, 27, 5800-5805.	2.3	56
236	Multiconfiguration Wavefunctions for the Water Molecule. Journal of Chemical Physics, 1971, 55, 1720-1724.	3.0	55
237	Internal rotation barrier and transition state for glyoxal. Journal of Chemical Physics, 1981, 74, 4576-4580.	3.0	55
238	Theory and applications of spin-restricted open-shell MÃ¸ller-Plesset theory. Molecular Physics, 1993, 79, 777-793.	1.7	55
239	Is there a potential minimum corresponding to singlet methylnitrene? A study of the CH3N to CH2NH rearrangement on the lowest singlet state potential energy hypersurface. Journal of Chemical Physics, 1994, 100, 481-489.	3.0	55
240	Toward resolution of the silicon dicarbide (SiC2) saga:Ab initioexcursions in the web of polytopism. Journal of Chemical Physics, 1997, 107, 1195-1211.	3.0	55
241	Structure and Energetics of Isomers of the Interstellar Molecule C5H. Journal of the American Chemical Society, 1999, 121, 1902-1911.	13.7	54
242	Theab initiolimit quartic force field of BH3. Journal of Computational Chemistry, 2005, 26, 1106-1112.	3.3	54
243	The alkaline earth dimer cations (Be₂ ⁺, Mg₂ ⁺,) Tj ETQq1 1 0.784314 rgBT /Over Coupled cluster and full configuration interaction studies^{â€}. Molecular Physics, 2013, 111, 2292-2298.	1.7	54
244	Hexalithiobenzene: a D6h equilibrium geometry with six lithium atoms in bridging positions. Chemical Physics Letters, 1991, 179, 563-567.	2.6	53
245	Is the oxywater radical cation more stable than neutral oxywater?. Journal of Chemical Physics, 1996, 104, 7615-7623.	3.0	53
246	The structures, electron affinities, and energetic stabilities of TiOn and TiOnâ' (n=1â€“3). Journal of Chemical Physics, 1999, 110, 5224-5230.	3.0	53
247	DFT Modeling of Chemical Vapor Deposition of GaN from Organogallium Precursors. 1. Thermodynamics of Elimination Reactions. Journal of Physical Chemistry A, 2001, 105, 3240-3248.	2.5	53
248	Binding energies of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2004, 120, 4683-4689.	3.0	53
249	Is silver a mere terminal oxidant in palladium catalyzed Câ€“H bond activation reactions?. Chemical Science, 2020, 11, 208-216.	7.4	53
250	The uncoupled symmetric stretching frequency of H3+. Journal of Chemical Physics, 1978, 68, 3951-3952.	3.0	52
251	The efficient evaluation of configuration interaction analytic energy second derivatives: Application to hydrogen thioperoxide, HSOH. Journal of Chemical Physics, 1986, 85, 3930-3938.	3.0	52
252	Microhydration of cytosine and its radical anion: Cytosineâ™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2007, 126, 064301.	3.0	52

#	Article	IF	Citations
253	Symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method: Improving upon CCSD(T) and CCSD(T)Î›: Preliminary application. Journal of Chemical Physics, 2012, 136, 204114.	3.0	52
254	Mn-NHC Electrocatalysts: Increasing Ï€ Acidity Lowers the Reduction Potential and Increases the Turnover Frequency for CO₂ Reduction. Inorganic Chemistry, 2016, 55, 9509-9512.	4.0	52
255	Tungsten hexahydride (WH6). An equilibrium geometry far from octahedral. Journal of Chemical Physics, 1993, 98, 508-521.	3.0	51
256	The unimolecular dissociation of H2CO on the lowest triplet potential-energy surface. Journal of Chemical Physics, 1998, 108, 5281-5288.	3.0	51
257	Binuclear Homoleptic Manganese Carbonyls:â€‰ Mn2(CO)x (x = 10, 9, 8, 7). Inorganic Chemistry, 2003, 42, 5219-5230.	4.0	51
258	PES-Learn: An Open-Source Software Package for the Automated Generation of Machine Learning Models of Molecular Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 4386-4398.	5.3	51
259	Saddle point geometry and barrier height for H + F2 â†' HF + F. Journal of Chemical Physics, 1974, 60, 3707-3708.	3.0	50
260	Vibrational frequencies of the cyanocarbene (HCCN) molecule. A near degeneracy between bent cyanocarbene and linear allene-related geometries. Journal of the American Chemical Society, 1983, 105, 4148-4154.	13.7	50
261	Investigating the Effects of Basis Set on Metalâ€“Metal and Metalâ€“Ligand Bond Distances in Stable Transition Metal Carbonyls: Performance of Correlation Consistent Basis Sets with 35 Density Functionals. Journal of Chemical Theory and Computation, 2013, 9, 2930-2938.	5.3	50
262	Why does Togni's reagent I exist in the high-energy hypervalent iodine form? Re-evaluation of benziodoxole based hypervalent iodine reagents. Chemical Communications, 2016, 52, 5371-5374.	4.1	50
263	Theoretical Description of Molecular Rydberg States: B 1Î£+ and Lowest 3Î£+ States of BH. Journal of Chemical Physics, 1971, 55, 5235-5241.	3.0	49
264	Tetrahedral Be4. Journal of Chemical Physics, 1976, 64, 905-906.	3.0	49
265	Analytic force constants for postâ€Hartreeâ€“Fock wave functions: The simplest case. Journal of Chemical Physics, 1983, 78, 1607-1608.	3.0	49
266	The singletâ€“triplet separation in dichlorocarbene: A surprising difference between theory and experiment. Journal of Chemical Physics, 2000, 112, 6515-6516.	3.0	49
267	The second-order MÃ¸llerâ€“Plesset limit for the barrier to linearity of water. Journal of Chemical Physics, 2001, 114, 2875-2878.	3.0	49
268	Establishment of the C2H5+O2 reaction mechanism: A combustion archetype. Journal of Chemical Physics, 2008, 128, 074308.	3.0	49
269	A Stable Anionic Dithiolene Radical. Journal of the American Chemical Society, 2017, 139, 6859-6862.	13.7	49
270	Sulfur oxide: Lowâ€lying bound molecular electronic states of SO. Journal of Chemical Physics, 1979, 71, 3761-3769.	3.0	48

#	Article	IF	Citations
271	An examination of the 2â€‰1A1 states of formaldehyde and ketene including analytic configuration interaction energy first derivatives for singlet excited electronic states of the same symmetry as the ground state. Journal of Chemical Physics, 1987, 87, 7076-7095.	3.0	48
272	High level ab initio study on the ground state potential energy hypersurface of the HCO+â€“COH+ system. Journal of Chemical Physics, 1994, 101, 8945-8954.	3.0	48
273	Are Neutralâ€Neutral Reactions Effective for the Carbonâ€Chain Growth of Cyanopolyynes and Polyacetylenes in Interstellar Space?. Astrophysical Journal, 1998, 505, 278-285.	4.5	48
274	Unsaturation in Binuclear Cyclopentadienyliron Carbonyls. Inorganic Chemistry, 2006, 45, 3384-3392.	4.0	48
275	Energy separation between the open (C2v) and closed (D3h) forms of ozone. Journal of Chemical Physics, 1977, 67, 848-849.	3.0	47
276	Structures and energetics of planar and tetrahedral dilithiomethane. A near degeneracy of singlet and triplet electronic states. Journal of the American Chemical Society, 1978, 100, 5972-5973.	13.7	47
277	The radical anions and the electron affinities of perfluorinated benzene, naphthalene and anthraceneElectronic supplementary information (ESI) available: calculated energies and electron affinities for perfluorinated benzene, naphthalene and anthracene and their anions. Calculated structures for perfluorinated naphthalene and anthracene and their anions. See http://www.rsc.org/suppdata/cc/b2/b208831m/. Chemical Communications, 2003, , 102-103.	4.1	47
278	Vibrational frequencies for silaacetylene and its silylidene and vinylidene isomers. Journal of the American Chemical Society, 1983, 105, 1084-1088.	13.7	46
279	Characterization of the bifurcated structure of the water dimer. Journal of Chemical Physics, 1991, 95, 1825-1828.	3.0	46
280	On apparent quantized transition-state thresholds in the photofragmentation of acetaldehyde. Journal of Chemical Physics, 2000, 112, 5585-5592.	3.0	46
281	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. Journal of Computational Chemistry, 2001, 22, 1574-1589.	3.3	46
282	Radicals Derived from Adenine:Â Prediction of Large Electron Affinities with a Considerable Spread. Journal of Physical Chemistry A, 2004, 108, 3565-3571.	2.5	46
283	Reactions of carbynes. Potential energy surfaces for the doublet and quartet methylidyne (CH) reactions with molecular hydrogen. Journal of Chemical Physics, 1977, 67, 5146-5151.	3.0	45
284	The infrared spectrum of cyclotetraoxygen, O4: A theoretical investigation employing the single and double excitation coupled cluster method. Journal of Chemical Physics, 1990, 92, 6077-6080.	3.0	45
285	Structures, thermochemistry, and electron affinities of the germanium fluorides, GeFn/GeFnâ^'(n=1â€“5). Journal of Chemical Physics, 1999, 111, 7945-7953.	3.0	45
286	New Approach to Electronic Structure Calculations for Diatomic Molecules: Application to F2and Cl2. Journal of Chemical Physics, 1970, 52, 6241-6247.	3.0	44
287	A multiconfiguration selfâ€consistentâ€field (MCSCF) study of the bent and linear conformations of HCCN. Journal of Chemical Physics, 1987, 86, 7051-7053.	3.0	44
288	Formyl fluoride photodissociation: Potential energy surface features of singlet HFCO. Journal of Chemical Physics, 1990, 93, 4907-4915.	3.0	44

#	Article	IF	Citations
289	Vibrational frequencies of the HF dimer from the coupled cluster method including all single and double excitations plus perturbative connected triple excitations. Journal of Chemical Physics, 1995, 103, 6051-6056.	3.0	44
290	Crossed beam reaction of cyano radicals with hydrocarbon molecules. II. Chemical dynamics of 1-cyano-1-methylallene (CNCH3CCCH2; Xâ€‰1Aâ€²) formation from reaction of CN(Xâ€‰2Î£+) with dimethylacetylene CH3CCCH3â€Š(Xâ€‰1A1â€²). Journal of Chemical Physics, 1999, 111, 7472-7479.	3.0	44
291	Electron affinities of the oxides of aluminum, silicon, phosphorus, sulfur, and chlorine. Journal of Chemical Physics, 1999, 110, 6240-6245.	3.0	44
292	The reaction of benzene with a ground state carbon atom, C(3Pj). Journal of Chemical Physics, 2000, 113, 4250-4264.	3.0	44
293	Evaluation of two-electron integrals for explicit r12 theories. Journal of Chemical Physics, 2000, 113, 3990-3995.	3.0	44
294	Role of Electron Correlation ina PrioriPredictions of the Electronic Ground State of BeO. Journal of Chemical Physics, 1972, 56, 3938-3942.	3.0	43
295	Carbonylâ€“water hydrogen bonding: The H2COâ€“H2O prototype. Journal of Chemical Physics, 1994, 100, 4347-4354.	3.0	43
296	Can Oxywater Be Made?. The Journal of Physical Chemistry, 1996, 100, 6076-6080.	2.9	43
297	Compact Variational Wave Functions Incorporating Limited Triple and Quadruple Substitutions. The Journal of Physical Chemistry, 1996, 100, 6069-6075.	2.9	43
298	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. Journal of Chemical Physics, 2014, 140, 184101.	3.0	43
299	DFT Modeling of Chemical Vapor Deposition of GaN from Organogallium Precursors. 2. Structures of the Oligomers and Thermodynamics of the Association Processesâ€. Journal of Physical Chemistry A, 2001, 105, 3249-3258.	2.5	42
300	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	5.3	42
301	Molecular properties of excited electronic states: TheÃ£3Aâ€³andÃƒ1Aâ€³states of formaldehyde. Journal of Chemical Physics, 1974, 61, 3039-3042.	3.0	41
302	Formulation of the direct configuration interaction method for triplet spin states. Applications to glyoxal. Journal of Chemical Physics, 1978, 68, 769-774.	3.0	41
303	The prototype aluminumâ€“carbon single, double, and triple bonds: Alâ€“CH3, Al=CH2, and Alâ‰¡CH. Journal of Chemical Physics, 1980, 73, 3246-3254.	3.0	41
304	Striking similarities between elementary silicon and aluminum compounds: monobridged, dibridged, trans-bent, and vinylidene isomers of aluminum hydride (Al2H2). Journal of the American Chemical Society, 1993, 115, 1936-1943.	13.7	41
305	Molecules for materials: Germanium hydride neutrals and anions. Molecular structures, electron affinities, and thermochemistry of GeHn/GeHâ€‰nâ^' (n = 0-4) and Ge2Hn/Ge2Hâ€‰nâ^' (n = 0-6). Journal of Computational Chemistry, 2002, 23, 1642-1655.	3.3	41
306	The small planarization barriers for the amino group in the nucleic acid bases. Journal of Chemical Physics, 2006, 124, 044303.	3.0	41

#	Article	IF	Citations
307	Effects of microsolvation on uracil and its radical anion: Uracilâˆ™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2006, 125, 144305.	3.0	41
308	Enthalpy of formation and anharmonic force field of diacetylene. Journal of Chemical Physics, 2009, 130, 044301.	3.0	41
309	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. Journal of Chemical Theory and Computation, 2018, 14, 1333-1350.	5.3	41
310	Krypton Monofluoride and Its Positive Ion. Journal of Chemical Physics, 1971, 55, 2369-2374.	3.0	40
311	Configuration Interaction Study of the X 3Î£â^', a 1Î", and b 1Î£+ States of NH. Journal of Chemical Physics, 1971, 55, 394-401.	3.0	40
312	Ab initio SCF and CI studies of three states of NH2. Journal of Chemical Physics, 1977, 67, 5173-5177.	3.0	40
313	Ordering of the Oâ€“O stretching vibrational frequencies in ozone. Journal of Chemical Physics, 1989, 90, 5635-5637.	3.0	40
314	Ammonia alane. Journal of Chemical Physics, 1992, 96, 5310-5317.	3.0	40
315	Benchmark configuration interaction spectroscopic constants for Xâ€‰1Î£g+â€‰C2 and Xâ€‰1Î£+â€‰CN+. Journal of Chemical Physics, 1998, 108, 6717-6721.	3.0	40
316	Odd Carbon Long Linear Chains HC2n+1H (n= 4â^'11): Properties of the Neutrals and Radical Anions. Journal of the American Chemical Society, 2002, 124, 14716-14720.	13.7	40
317	The arsenic clusters Asn (n = 1-5) and their anions: Structures, thermochemistry, and electron affinities. Journal of Computational Chemistry, 2004, 25, 907-920.	3.3	40
318	Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy. Physical Chemistry Chemical Physics, 2018, 20, 7479-7491.	2.8	40
319	Analytic evaluation of infrared intensities and polarizabilities by two-configuration self-consistent field wave functions. Theoretica Chimica Acta, 1986, 69, 337-352.	0.8	39
320	The infrared spectrum of the acetylene radical cation C2H+2. A theoretical study using SCF, MCSCF, and CI methods. Journal of Chemical Physics, 1987, 86, 3051-3053.	3.0	39
321	Natural orbitals from single and double excitation configuration interaction wave functions: their use in secondâ€order configuration interaction and wave functions incorporating limited triple and quadruple excitations. Journal of Chemical Physics, 1992, 96, 6850-6856.	3.0	39
322	Low-lying triplet electronic states of acetylene:cis 3 B 2 and3 A 2,trans 3 B u and3 A u. Theoretica Chimica Acta, 1993, 86, 97-113.	0.8	39
323	Isomerization reactions on the lowest potential energy hypersurface of triplet vinylidene and triplet acetylene. Journal of Chemical Physics, 1993, 98, 4766-4776.	3.0	39
324	Molecular geometry and vibrational frequencies of ozone from compact variational wave functions explicitly including triple and quadruple substitutions. Journal of Chemical Physics, 1997, 107, 9059-9062.	3.0	39

#	Article	IF	Citations
325	A combined crossed-beam, ab initio, and Riceâ€“Ramspergerâ€“Kasselâ€“ Marcus investigation of the reaction of carbon atoms C(3Pj) with benzene, C6H6(Xâ€Š1A1g) and d6-benzene, C6D6(Xâ€Š1A1g). Journal of Chemical Physics, 2002, 116, 3248-3262.	3.0	39
326	Low-lying electronic states of FeNC and FeCN: A theoretical journey into isomerization and quartet/sextet competition. Journal of Chemical Physics, 2004, 120, 4726-4741.	3.0	39
327	Homonuclear transition-metal trimers. Journal of Chemical Physics, 2005, 123, 074321.	3.0	39
328	Hydroxyl Radical Reactions with Adenine: Reactant Complexes, Transition States, and Product Complexes. Chemistry - A European Journal, 2010, 16, 11848-11858.	3.3	39
329	The Inherent Competition between Addition and Substitution Reactions of Br₂ with Benzene and Arenes. Angewandte Chemie - International Edition, 2011, 50, 6809-6813.	13.8	39
330	7Î£+ and 7Î states of manganese hydride. Journal of Chemical Physics, 1973, 58, 1844-1848.	3.0	38
331	A Hartreeâ€“Fock interaction potential between a rigid asymmetric top and a spherical atom: (H2CO,He). Journal of Chemical Physics, 1975, 63, 1449-1454.	3.0	38
332	Vibrational frequencies and infrared intensities for H2CN+, protonated HCN. Journal of Chemical Physics, 1984, 80, 2977-2978.	3.0	38
333	Efficient use of Jacobi rotations for orbital optimization and localization. Theoretica Chimica Acta, 1993, 86, 149-165.	0.8	38
334	Dodecahedral and smaller arsenic clusters: Asn, n=2, 4, 12, 20. Journal of Chemical Physics, 1994, 101, 2261-2266.	3.0	38
335	The electron affinities of the perfluorocarbons C2Fn, n=1â€“6. Journal of Chemical Physics, 1997, 107, 8536-8544.	3.0	38
336	The infrared spectrum of the nitric oxide dimer cation: Problems for density functional theory and a muddled relationship to experiment. Journal of Chemical Physics, 1999, 111, 2532-2541.	3.0	38
337	Electron attachment induced proton transfer in a DNA nucleoside pair: 2â€²-deoxyguanosine-2â€²-deoxycytidine. Journal of Chemical Physics, 2007, 127, 155107.	3.0	38
338	Arenium ions are not obligatory intermediates in electrophilic aromatic substitution. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10067-10072.	7.1	38
339	Potential Curves for the Valenceâ€Excited States of Silicon Monoxide. A Theoretical Study. Journal of Chemical Physics, 1972, 56, 958-968.	3.0	37
340	Parallel algorithms for quantum chemistry. I. Integral transformations on a hypercube multiprocessor. Journal of Chemical Physics, 1987, 86, 2185-2193.	3.0	37
341	Silaketene: A product of the reaction between silylene and carbon monoxide?. Journal of Chemical Physics, 1989, 90, 1031-1035.	3.0	37
342	Assignment of the infrared spectra of the methanol trimer. Journal of Chemical Physics, 1999, 111, 3027-3034.	3.0	37

#	Article	IF	Citations
343	Flat Potential Energy Surface of the Saturated Binuclear Homoleptic Chromium Carbonyl Cr2(CO)11 with One, Two, and Three Bridging Carbonyls:â€‰ Comparison with the Well-Known [HCr2(CO)10]- Anion and the Related [(Î¼-H)2Cr2(CO)9]2- and [(Î¼-H)2Cr2(CO)8]2- Dianions. Journal of Physical Chemistry A, 2001, 105, 11134-11143.	2.5	37
344	Energetics and Structures of Adamantane and the 1- and 2-Adamantyl Radicals, Cations, and Anions. Journal of Physical Chemistry A, 2003, 107, 9479-9485.	2.5	37
345	Excited singlet electronic states of acetylene:cisandtransstructures and energetics. Journal of Chemical Physics, 1980, 73, 5706-5710.	3.0	36
346	The effects of triple and quadruple excitations in configuration interaction procedures for the quantum mechanical prediction of molecular properties. Journal of Chemical Physics, 1988, 89, 408-422.	3.0	36
347	Aluminumâ^'Phosphorus Compounds with Low Coordination Numbers:â€‰ Structures, Energies, and Vibrational Frequencies of the AlPH2, AlPH3, and AlPH4 Isomers and the H3Alâ^'PH3 Adduct. Journal of Physical Chemistry A, 1997, 101, 3135-3142.	2.5	36
348	Protonated High Energy Density Materials:â€‰ N4 Tetrahedron and N8 Octahedron. Journal of Physical Chemistry A, 1997, 101, 4460-4464.	2.5	36
349	Bond length and bond multiplicity: Ïƒ-bond prevents short Ï€-bonds. Chemical Communications, 2006, , 2164-2166.	4.1	36
350	Correlation diagram for He + He â†' Be. Journal of Chemical Physics, 1974, 61, 4921-4925.	3.0	35
351	Role of different isomers of the H2CN+ ion in the formation of interstellar HCN and HNC. Nature, 1978, 274, 456-457.	27.8	35
352	Singletâ€“triplet energy separation for silaethylene. Journal of Chemical Physics, 1978, 68, 2985.	3.0	35
353	Near degenerate rearrangement between the radical cations of formaldehyde and hydroxymethylene. Journal of Chemical Physics, 1981, 74, 617-621.	3.0	35
354	Cyclopropyne and Silacyclopropyne:Â A World of Difference. Journal of the American Chemical Society, 1996, 118, 7158-7163.	13.7	35
355	Do Linear-Chain Perfluoroalkanes Bind an Electron?. Journal of Physical Chemistry A, 2004, 108, 9428-9434.	2.5	35
356	The barrier height, unimolecular rate constant, and lifetime for the dissociation of HN2. Journal of Chemical Physics, 2010, 132, 064308.	3.0	35
357	A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment. Organic Letters, 2017, 19, 6502-6505.	4.6	35
358	Reduction of Dinitrogen via 2,3â€²-Bipyridine-Mediated Tetraboration. Journal of the American Chemical Society, 2020, 142, 6244-6250.	13.7	35
359	Simplest halogen atom plus alkali dimer potential surface: F+Li2â†'LiF+Li. Journal of Chemical Physics, 1973, 58, 5358-5363.	3.0	34
360	Geometry of the LiO2 radical. Journal of Chemical Physics, 1973, 59, 3608-3611.	3.0	34

#	Article	IF	Citations
361	Effects of electron correlation on the geometrical structure of cyanomethylene. Journal of the American Chemical Society, 1979, 101, 1072-1076.	13.7	34
362	Tetrasilatetrahedrane. Journal of the American Chemical Society, 1986, 108, 4344-4346.	13.7	34
363	Cyclic isomers of singlet Si4H4 related to tetrasilacyclobutadiene. Chemical Physics Letters, 1988, 143, 421-427.	2.6	34
364	Potential new high energy density materials: Cyclooctaoxygen O8, including comparisons with the wellâ€known cycloâ€S8molecule. Journal of Chemical Physics, 1990, 92, 1887-1892.	3.0	34
365	A high level theoretical investigation of the cyclic hydrogen fluoride trimer. Journal of Chemical Physics, 1997, 106, 9627-9633.	3.0	34
366	The gas-phase acidity of H3PO4. Journal of Chemical Physics, 1997, 106, 3545-3547.	3.0	34
367	Exploring the intermediates of photochemical CO₂reduction: reaction of Re(dmb)(CO)₃ COOH with CO₂. Chemical Communications, 2012, 48, 6797-6799.	4.1	34
368	An Experimentally Established Key Intermediate in Benzene Nitration with Mixed Acid. Angewandte Chemie - International Edition, 2015, 54, 14123-14127.	13.8	34
369	Relation between electronic structure and the chemiluminescence arising from collisions between alkaline earth atoms and halogen molecules. Molecular Physics, 1973, 26, 941-952.	1.7	33
370	Classical and nonclassical forms of the vinyl cation: A coupled cluster study. Journal of Chemical Physics, 1990, 92, 3653-3658.	3.0	33
371	Quantum mechanical frequencies and matrix assignments to Al2H2. Journal of Chemical Physics, 1997, 107, 119-123.	3.0	33
372	Xìƒ 3B1, Ã£ 1A1, bìƒ 1B1, and cìƒ 1 Electronic States of. Journal of Physical Chemistry A, 1998, 102, 3999-4006.	2.5	33
373	Molecular structure of the methyl anion CHâ¯3. An investigation of the effects of electron correlation using the theory of self-consistent electron pairs (SCEP). Journal of Chemical Physics, 1999, 67, 4071.	3.0	33
374	Atomic and molecular hydrogen elimination in the crossed beam reaction of d1-ethinyl radicals C2D(X) Tj ETQq0 0 0 rgBT /Overlock 10 T formationPresented at the XIX International Symposium on Molecular Beams, Rome, 3â€“8 June, 2001.. Physical Chemistry Chemical Physics, 2002, 4, 2950-2958.	2.8	33
375	The germanium clusters Gen(n= 1â€“6) and their anions: structures, thermochemistry and electron affinities. Molecular Physics, 2004, 102, 579-598.	1.7	33
376	Noncovalent Interactions of a Benzo[a]pyrene Diol Epoxide with DNA Base Pairs: Insight into the Formation of Adducts of (+)-BaP DE-2 with DNA. Journal of Physical Chemistry A, 2010, 114, 2038-2044.	2.5	33
377	Free Cyclooctatetraene Dianion: Planarity, Aromaticity, and Theoretical Challenges. Journal of Chemical Theory and Computation, 2013, 9, 4436-4443.	5.3	33
378	Semi-exact concentric atomic density fitting: Reduced cost and increased accuracy compared to standard density fitting. Journal of Chemical Physics, 2014, 140, 064109.	3.0	33

#	Article	IF	Citations
379	Weak attraction between water and methane. Journal of the American Chemical Society, 1974, 96, 7898-7901.	13.7	32
380	The experimental vibrational spectra, vibrational assignment, and normal coordinate analysis of thiiraneâ€h4and â€d4andcisâ€•andtransâ€1,2â€dideuteriothiirane:Abinitiotheoretical IR spectra of thiirane, thiirene, and isotopically substituted derivatives. Journal of Chemical Physics, 1986, 84, 4211-4227.	3.0	32
381	The Cl̀fâ€‰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.	3.0	32
382	Experimental and ab initio study of the infrared spectra of ionic species derived from SF6 and SF4 and trapped in solid neon. Journal of Chemical Physics, 1998, 108, 9639-9650.	3.0	32
383	Crossed beam reaction of phenyl radicals with unsaturated hydrocarbon molecules. I. Chemical dynamics of phenylmethylacetylene (C6H5CCCH3;Xâ€Š1Aâ€²) formation from reaction of C6H5(Xâ€Š2A1) with methylacetylene, CH3CCH(Xâ€Š1A1). Journal of Chemical Physics, 2000, 112, 4994-5001.	3.0	32
384	Fragmentation path for hydrogen atom dissociation from methoxy radical. Journal of Chemical Physics, 2002, 116, 10229-10237.	3.0	32
385	The microwave and infrared spectroscopy of benzaldehyde: Conflict between theory and experimental deductions. Journal of Chemical Physics, 2004, 120, 4247-4250.	3.0	32
386	CO₂ reduction with Re(<scp>i</scp>)â€“NHC compounds: driving selective catalysis with a silicon nanowire photoelectrode. Chemical Communications, 2016, 52, 14258-14261.	4.1	32
387	Can cyclopropyne really be made?. Journal of the American Chemical Society, 1980, 102, 3239-3240.	13.7	31
388	The electronic spectrum of sâ€tetrazine: Structures and vibrational frequencies of the ground and excited electronic states. Journal of Chemical Physics, 1987, 87, 3539-3556.	3.0	31
389	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.	3.0	31
390	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.	3.0	31
391	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. Journal of Chemical Physics, 1997, 107, 9980-9984.	3.0	31
392	The XËœ 1 A 1 , aËœ 3 B 1 , aËœ 1 BËœ 1 , and BËœ 1 A 1 electronic states of SiH 2. Theoretical Chemistry Accounts, 1997, 97, 341-349.	1.4	31
393	Structureâ€“reactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 37-55.	14.6	31
394	Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach. Journal of Physical Chemistry A, 2017, 121, 6090-6103.	2.5	31
395	Interaction Potential between Ground State Helium Atom and theB1Î£u+State of the Hydrogen Molecule. Journal of Chemical Physics, 1972, 56, 1219-1223.	3.0	30
396	Model studies of Ï€-bonded organometallic systems Mn-C2H2 and Mn-C2H4. Molecular Physics, 1977, 34, 1037-1048.	1.7	30

#	Article	IF	Citations
397	Sodium Pentaphosphacyclopentadienide (NaP5) and the Pentaphosphacyclopentadienide Ion (P5?) : Theoretical Predictions of Molecular Structures, Infrared and Raman Spectra. Angewandte Chemie International Edition in English, 1989, 28, 485-486.	4.4	30
398	Toward the observation of silanone (H2SiO) and hydroxysilylene (HSiOH) via microwave spectroscopy. Journal of Chemical Physics, 1994, 101, 2734-2739.	3.0	30
399	Coupled-cluster electronic spectra for the Ca+â€“acetylene Ï€ complex and comparisons to its alkaline earth analogs. Journal of Chemical Physics, 2000, 113, 701-706.	3.0	30
400	Metalâ^'Metal Quintuple and Sextuple Bonding in Bent Dimetallocenes of the Third Row Transition Metals. Journal of Chemical Theory and Computation, 2010, 6, 735-746.	5.3	30
401	Ground and excited state properties of photoactive platinum(iv) diazido complexes: Theoretical considerations. Dalton Transactions, 2011, 40, 7571.	3.3	30
402	In search of the next Holy Grail of polyoxide chemistry: Explicitly correlated ab initio full quartic force fields for HOOH, HOOOH, HOOOOH, and their isotopologues. Journal of Chemical Physics, 2012, 136, 084302.	3.0	30
403	Fluorine peroxide (FOOF): A problem molecule for theoretical structural predictions. Journal of Chemical Physics, 1978, 68, 2507-2508.	3.0	29
404	Communication: Some critical features of the potential energy surface for the Cl + H2O â†' HCl + OH forward and reverse reactions. Journal of Chemical Physics, 2013, 139, 041101.	3.0	29
405	Some Features of the CH3NCâ†'CH3CN Potential Surface. Journal of Chemical Physics, 1972, 57, 4509-4511.	3.0	28
406	The acetyl cation and its geometrical isomers. Journal of Chemical Physics, 1975, 63, 4317-4328.	3.0	28
407	A multiconfiguration selfâ€consistentâ€field formalism utilizing the twoâ€particle density matrix and the unitary group approach. Journal of Chemical Physics, 1980, 72, 3837-3838.	3.0	28
408	Mechanism of the H+O3 reaction. Journal of Chemical Physics, 1981, 74, 2938-2944.	3.0	28
409	Vibrational frequencies for the classical and nonclassical forms of protonated acetyleneâ€“C2H+3. Journal of Chemical Physics, 1984, 81, 4034-4037.	3.0	28
410	Nitrogen quadrupole coupling constants for HCN and H2CN+: Explanation of the absence of fine structure in the microwave spectrum of interstellar H2CN+. Journal of Chemical Physics, 1986, 84, 5711-5714.	3.0	28
411	Tetrasilacyclobutadiylidene: The lowest energy cyclic isomer of singlet Si4H4?. Chemical Physics Letters, 1989, 155, 563-571.	2.6	28
412	How stable is cyclobutyne? The activation energy for the unimolecular rearrangement to butatriene. Journal of the American Chemical Society, 1992, 114, 5344-5348.	13.7	28
413	Ga2H2: planar dibridged, vinylidene-like, monobridged, and trans equilibrium geometries. Chemical Physics Letters, 1993, 203, 195-200.	2.6	28
414	Acetylene: Synergy between theory and experiment. Journal of Chemical Physics, 1993, 98, 8384-8391.	3.0	28

#	Article	IF	Citations
415	1-Silavinylidene: The First Unsaturated Silylene. The Journal of Physical Chemistry, 1995, 99, 1949-1952.	2.9	28
416	The Ã¹Aâ€‰1Au state and the T2 potential surface of acetylene: Implications for triplet perturbations in the fluorescence spectra of the Ã¹A state. Journal of Chemical Physics, 1996, 104, 8507-8515.	3.0	28
417	Conformational Stability of 3-Fluoropropene:â€‰ A Challenging Problem for Both Theory and Experiment. Journal of Physical Chemistry A, 2002, 106, 3625-3628.	2.5	28
418	Chromiumâ^'Chromium Multiple Bonding in Cr2(CO)9. Journal of Physical Chemistry A, 2003, 107, 10118-10125.	2.5	28
419	Interplay between Two-Electron and Four-Electron Donor Carbonyl Groups in Oxophilic Metal Systems:Â Highly Unsaturated Divanadocene Carbonyls. Journal of the American Chemical Society, 2007, 129, 3433-3443.	13.7	28
420	The lowest-lying electronic singlet and triplet potential energy surfaces for the HNOâ€“NOH system: Energetics, unimolecular rate constants, tunneling and kinetic isotope effects for the isomerization and dissociation reactions. Journal of Chemical Physics, 2012, 136, 164303.	3.0	28
421	Infrared Laser Spectroscopy of the CH₃OO Radical Formed from the Reaction of CH₃ and O₂ within a Helium Nanodroplet. Journal of Physical Chemistry A, 2012, 116, 5299-5304.	2.5	28
422	Orbital-optimized density cumulant functional theory. Journal of Chemical Physics, 2013, 139, 204110.	3.0	28
423	Using an iterative eigensolver and intertwined rank reduction to compute vibrational spectra of molecules with more than a dozen atoms: Uracil and naphthalene. Journal of Chemical Physics, 2018, 149, 064108.	3.0	28
424	A comparison between hydrogen and halogen bonding: the hypohalous acidâ€“water dimers, HOXâ‹¯H₂O (X = F, Cl, Br). Physical Chemistry Chemical Physics, 2019, 21, 6160-6170.	2.8	28
425	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. Proceedings of the Combustion Institute, 2021, 38, 375-384.	3.9	28
426	The gas phase structure of transition metal dihydrides. Journal of Chemical Physics, 1980, 72, 311-315.	3.0	27
427	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: A comparison with configuration interaction (CCSD,CISDT, andCISDTQ) results for the harmonic vibrational frequencies, infrared intensities, dipole moment, and inversion barrier of ammonia. International Journal of Quantum Chemistry, 1987, 32, 495-501.	2.0	27
428	Benzyne: higher-level theoretical evidence for the weak triple bond. Chemical Physics Letters, 1991, 177, 471-476.	2.6	27
429	The weakly bound dinitrogen tetroxide molecule: High level single reference wavefunctions are good enough. Journal of Chemical Physics, 1997, 106, 7178-7184.	3.0	27
430	A new spin-restricted triple excitation correction for coupled cluster theory. Journal of Chemical Physics, 1997, 107, 7943-7950.	3.0	27
431	Stable Hexacoordinated Neutral Complexes between Silyl Halides and Two Water or Two Ammonia Molecules:â€‰ SiX4Y2 (X = H, F, Cl; Y = H2O, NH3). Journal of Physical Chemistry A, 2001, 105, 7665-7671.	2.5	27
432	A theoretical approach to the single-source precursor concept: quantum chemical modeling of gas-phase reactions. Journal of Crystal Growth, 2001, 222, 170-182.	1.5	27

#	Article	IF	Citations
433	Three-â€‰versusâ€‰four-coordinateâ€‰phosphorusâ€‰inâ€‰theâ€‰gasâ€‰phaseâ€‰andâ€‰inâ€‰solution: Treacherous re for phosphine oxide and phosphinousâ€‰acid. Journal of Chemical Physics, 2002, 116, 112.	3.0	27
434	The thymine radicals and their respective anions: molecular structures and electron affinities. Molecular Physics, 2003, 101, 3277-3284.	1.7	27
435	Bis(cycloheptatrienyl) Derivatives of the First-Row Transition Metals: Variable Hapticity of the Cycloheptatrienyl Ring. European Journal of Inorganic Chemistry, 2008, 2008, 3698-3708.	2.0	27
436	Analytic configuration interaction gradient studies of SH4, sulfurane. Journal of Chemical Physics, 1981, 74, 1855-1863.	3.0	26
437	Naked organosulfur clusters: The infrared spectrum of the C2S molecule. Journal of Chemical Physics, 1992, 96, 3714-3717.	3.0	26
438	Singlet C2H2Li2: Acetylenic and 1,2-Dilithioethene Isomers. A Remarkably Congested Potential Energy Hypersurface for a Simple Organometallic System. Journal of the American Chemical Society, 1994, 116, 9602-9612.	13.7	26
439	Spectroscopic constants and potential energy surfaces for silanone (H2SiO), hydroxysilylene (HSiOH), the hydroxysilylene dimer, and the disilynyl radical (Si2H). Journal of Chemical Physics, 1996, 105, 5731-5736.	3.0	26
440	The ClO4 radical: Experiment versus theory. Journal of Chemical Physics, 1997, 106, 4028-4037.	3.0	26
441	Subtle basis set effects on hydrogen bonded systems. Molecular Physics, 1999, 96, 493-504.	1.7	26
442	Isomerization of the interstellar molecule silicon cyanide to silicon isocyanide through two transition states. Journal of Chemical Physics, 2003, 119, 12946-12955.	3.0	26
443	Unsaturated Binuclear Cyclopentadienylmanganese Carbonyl Derivatives Related to Cymantrene. Organometallics, 2008, 27, 61-66.	2.3	26
444	Density cumulant functional theory: First implementation and benchmark results for the DCFT-06 model. Journal of Chemical Physics, 2010, 133, 174122.	3.0	26
445	The ethyl radical in superfluid helium nanodroplets: Rovibrational spectroscopy and ab initio computations. Journal of Chemical Physics, 2013, 138, 194303.	3.0	26
446	Quantification of Aromaticity Based on Interaction Coordinates: A New Proposal. Journal of Physical Chemistry A, 2016, 120, 2894-2901.	2.5	26
447	Pushâ€“Pull Stabilization of Parent Monochlorosilylenes. Journal of the American Chemical Society, 2016, 138, 9799-9802.	13.7	26
448	Stabilizing a different cyclooctatetraene stereoisomer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9803-9808.	7.1	26
449	Multiconfiguration selfâ€consistentâ€field study of the importance of triply and quadruply excited electronic configurations in the water molecule. Journal of Chemical Physics, 1980, 73, 1765-1769.	3.0	25
450	A contribution to the understanding of the structure of xenon hexafluoride. Journal of Chemical Physics, 1995, 102, 3307-3311.	3.0	25

#	Article	IF	Citations
451	Analyses of the ScOâ^' and ScO2â^' photoelectron spectra. Journal of Chemical Physics, 2000, 113, 567-572.	3.0	25
452	Unsaturated binuclear homoleptic metal carbonyls M2(CO)x (M = Fe, Co, Ni; x = 5, 6, 7, 8). Are multiple bonds between transition metals possible for these molecules?. Pure and Applied Chemistry, 2001, 73, 1059-1073.	1.9	25
453	From ?Parasitic? Association Reactions toward the Stoichiometry Controlled Gas Phase Synthesis of Nanoparticles: A Theoretically Driven Challenge for Experimentalists. Chemical Record, 2002, 2, 319-338.	5.8	25
454	Neâ€"Hâ€"H potential energy surface including electron correlation. Journal of Chemical Physics, 1975, 63, 1741-1747.	3.0	24
455	Seven isomers of protonated nitrosyl fluoride. Journal of Chemical Physics, 1990, 93, 1215-1220.	3.0	24
456	Structure and energetics of the lowest 1A1 and 1B1 states of dichlorocarbene. Journal of Chemical Physics, 1991, 94, 2063-2067.	3.0	24
457	Investigation of XNO and XON (where X=Cl or Br) and their protonated isomers. Journal of Chemical Physics, 1992, 96, 480-488.	3.0	24
458	The XÌƒ AlOHâ€"XÌƒ HAlO isomerization potential energy hypersurface. Journal of Chemical Physics, 1993, 98, 8704-8709.	3.0	24
459	The hydroperoxyl radical dimer: Triplet ring or singlet string?. Journal of Chemical Physics, 1997, 106, 5102-5108.	3.0	24
460	Binuclear Homoleptic Copper Carbonyls Cu2(CO)x(x= 1â^'6):Â Remarkable Structures Contrasting Metalâ^'Metal Multiple Bonding with Low-Dimensional Copper Bonding Manifolds. Inorganic Chemistry, 2001, 40, 5842-5850.	4.0	24
461	Coupled-cluster characterization of the ground and excited states of the CH2N and CH2P radicals. Journal of Chemical Physics, 2001, 114, 3055-3064.	3.0	24
462	The Î½5 vibrational frequency of the vinyl radical: Conflict between theory and experiment. Journal of Chemical Physics, 2002, 117, 7914-7916.	3.0	24
463	Understanding Electron Attachment to the DNA Double Helix:â€‰ The Thymidine Monophosphateâ^'Adenine Pair in the Gas Phase and Aqueous Solution. Journal of Physical Chemistry B, 2006, 110, 19696-19703.	2.6	24
464	Metalâ€"Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. Inorganic Chemistry, 2018, 57, 8778-8787.	4.0	24
465	Singlet cyclobutyne: a relative minimum on the C4H4 potential-energy hypersurface?. Journal of the American Chemical Society, 1983, 105, 690-695.	13.7	23
466	The silaformyl radical HSiO and its energetically lowerâ€lying isomer SiOH. Journal of Chemical Physics, 1985, 82, 4585-4587.	3.0	23
467	The dissociation mechanism of triplet formaldehyde. Journal of Chemical Physics, 1990, 93, 8798-8807.	3.0	23
468	What is the lowest energy structure of the NS2molecule?. Journal of Chemical Physics, 1990, 92, 3683-3687.	3.0	23

#	Article	IF	Citations
469	The infrared spectrum of difluorovinylidene, F2C=C:. Journal of Chemical Physics, 1990, 93, 865-866.	3.0	23
470	The siliconâ€“carbon symmetric stretching fundamental Î½1 of Si2C: Nonintuitive theoretical behavior. Journal of Chemical Physics, 1992, 97, 5586-5591.	3.0	23
471	Sulfur clusters: structure, infrared, and Raman spectra of cyclo-S6and comparison with the hypothetical cyclo-O6molecule. Molecular Physics, 1992, 76, 537-546.	1.7	23
472	XÌƒÂ1A1, Ã£Â3B1, ÃƒÂ1B1, and BÌƒÂ1A1Electronic States of. Journal of Physical Chemistry A, 1997, 101, 6955-6963.	2.5	23
473	Structural isomerization of cyclopropane: a new mechanism through propylidene. Chemical Communications, 1999, , 1515-1516.	4.1	23
474	The global minimum structure of SiC3: The controversy continues. Journal of Chemical Physics, 2002, 116, 9151-9153.	3.0	23
475	The rule breaking Cr2(CO)10. A 17 electron Cr system or a Crî€Cr double bond?. Faraday Discussions, 2003, 124, 315-329.	3.2	23
476	Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861.	2.8	23
477	Easy chairs: the conformational preferences of polyfluorocyclohexanes. RSC Advances, 2013, 3, 6572.	3.6	23
478	Experimental Measurement and Theory of Substituent Effects in Ï€-Hydrogen Bonding: Complexes of Substituted Phenols with Benzene. Journal of Organic Chemistry, 2014, 79, 6823-6831.	3.2	23
479	Exploring mechanisms of a tropospheric archetype: CH3O2 + NO. Journal of Chemical Physics, 2015, 143, 234302.	3.0	23
480	The Symmetric Exchange Reaction OH + H2O â†' H2O + OH: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2016, 120, 10223-10230.	2.5	23
481	Stable Boron Dithiolene Radicals. Angewandte Chemie - International Edition, 2018, 57, 7865-7868.	13.8	23
482	Ionâ€Molecule Reactions Producing HC documentclass{aastex} usepackage{amsbsy} usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace} usepackage{amsmath,amsxtra} usepackage[OT2,OT1]{fontenc} ewcommandcyr{ enewcommandmdefault{wncyr} enewcommandsfdefault{wncyss} enewcommandencodingdefault{OT2} ormalfont selectfont} DeclareTextFontCommand{extcyr}	4.5	23
483	The HO+2 molecular ion. Geometrical structure and vibrational frequencies. Journal of Chemical Physics, 1984, 80, 319-324.	3.0	22
484	The open chain or chemically bonded structure of H2O4: The hydroperoxyl radical dimer. Journal of Chemical Physics, 1985, 83, 6275-6282.	3.0	22
485	The equilibrium geometry of F₂⁺in its ground electronic state. A simple example of the effects of symmetry breaking on an observable molecular property. International Reviews in Physical Chemistry, 1986, 5, 229-237.	2.3	22
486	The Aìƒ 1Aâ€˜ state of isocyanogen (CNCN). Journal of Chemical Physics, 1994, 100, 8920-8924.	3.0	22

#	Article	IF	Citations
487	Comparative energy derivative analyses of the HBOâ€“BOH and AlOHâ€“HAlO potential energy hypersurfaces. Journal of Chemical Physics, 1994, 101, 3006-3017.	3.0	22
488	The structures, energies, vibrational, and rotational frequencies, and dissociation energy of GeH+5. Journal of Chemical Physics, 1994, 101, 2141-2147.	3.0	22
489	Fragmentation surface of triplet ketene. Faraday Discussions, 1998, 110, 23-50.	3.2	22
490	Quantum chemistry in the 21st century (Special topic article). Pure and Applied Chemistry, 2000, 72, 1405-1423.	1.9	22
491	3Î£â¯ and 3Î states of GeC and GeSi: The problematic dissociation energy of GeC. Journal of Chemical Physics, 2003, 119, 8266-8275.	3.0	22
492	Quantification of Aromaticity of Heterocyclic Systems Using Interaction Coordinates. Journal of Physical Chemistry A, 2018, 122, 6953-6960.	2.5	22
493	Electron correlation effects on the excitation energies of the lowest triplet states of glyoxal. Journal of Chemical Physics, 1977, 67, 2422.	3.0	21
494	Correlated wavefunctions for the water molecule. Journal of Chemical Physics, 1978, 68, 5292-5294.	3.0	21
495	Molecular structures and energetics for the lowest triplet states of glyoxal. Journal of Chemical Physics, 1985, 83, 1741-1745.	3.0	21
496	Analytic energy derivative methods for excited singlet states of the same symmetry as the electronic ground state. Journal of Chemical Physics, 1985, 83, 1162-1167.	3.0	21
497	The ring and superoxide isomers of SO2. Journal of Chemical Physics, 1995, 102, 4177-4183.	3.0	21
498	Electron attachment to PCl3 and POCl3, 296â€“552 K. Journal of Chemical Physics, 1998, 109, 578-584.	3.0	21
499	The SF6â¯ enigma for density functional theory: is the KMLYP functional a reasonable solution for this problematic anion?. Chemical Physics Letters, 2003, 381, 123-128.	2.6	21
500	Ionization potentials of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2005, 122, 204328.	3.0	21
501	Periodane: A wealth of structural possibilities revealed by the Kick procedure. International Journal of Quantum Chemistry, 2007, 107, 2220-2223.	2.0	21
502	Are isomers of the vinyl cyanide ion missing links for interstellar pyrimidine formation?. Journal of Chemical Physics, 2009, 131, 074303.	3.0	21
503	Theoretical Support for the Assignment of X-ogen to the HCO+ Molecular Ion. Nature: Physical Science, 1973, 246, 4-5.	0.8	20
504	The cyclic, twoâ€hydrogen bond form of the HO2 dimer. Journal of Chemical Physics, 1984, 81, 362-367.	3.0	20

#	Article	IF	Citations
505	Electronic symmetry breaking in polyatomic molecules. Multiconfiguration selfâ€consistent field study of the cyclopropenyl radical C3H3. Journal of Chemical Physics, 1984, 80, 338-343.	3.0	20
506	Peroxy and cyclic isomers of NO2 and NOâ˜2. Journal of Chemical Physics, 1991, 94, 1317-1326.	3.0	20
507	An ab initio study on the ground state HBOâ€“BOH system. Journal of Chemical Physics, 1995, 102, 1280-1287.	3.0	20
508	Aluminum monocarbonyl and aluminum isocarbonyl. Journal of Chemical Physics, 1996, 104, 3672-3675.	3.0	20
509	Scratching the surface of the water dication. Journal of Chemical Physics, 1999, 110, 11856-11864.	3.0	20
510	Remarkable electron accepting properties of the simplest benzenoid cyanocarbons: hexacyanobenzene, octacyanonaphthalene and decacyanoanthracene. Chemical Communications, 2006, , 758.	4.1	20
511	The Beryllium tetramer: Profiling an elusive molecule. Journal of Chemical Physics, 2011, 134, 074110.	3.0	20
512	F + (H2O)2 Reaction: The Second Water Removes the Barrier. Journal of Physical Chemistry A, 2013, 117, 11979-11982.	2.5	20
513	Transitionâ€Metalâ€Mediated Cleavage of a Sïï£¾Si Double Bond. Angewandte Chemie - International Edition, 2015, 54, 10267-10270.	13.8	20
514	CO₂ Reduction Pathways on MnBr(N-C)(CO)₃ Electrocatalysts. Organometallics, 2018, 37, 337-342.	2.3	20
515	Reaction mechanisms of a cyclic ether intermediate: Ethyloxirane. International Journal of Chemical Kinetics, 2021, 53, 43-59.	1.6	20
516	Magnetic Hyperfine Structure of NO2. Journal of Chemical Physics, 1971, 54, 1423-1424.	3.0	19
517	1,1-Dilithioethylene. A ground-state triplet olefin with nearly free rotation about the double bond. Journal of the American Chemical Society, 1979, 101, 7184-7188.	13.7	19
518	The nuclear quadrupole moment of 14N. A theoretical prediction from full valence shell and full configuration interaction atomic wave functions. Journal of Chemical Physics, 1987, 87, 4020-4024.	3.0	19
519	Vertical electronic spectrum of NO3: 2Aâ€™2, 2Eâ€˜(2A2,2B1), and 2Eâ€™ states. Journal of Chemical Physics, 1988, 88, 3204-3210.	3.0	19
520	The infrared spectrum of silacyclopropenylidene. Journal of the American Chemical Society, 1991, 113, 3192-3193.	13.7	19
521	Benchmark studies of electron correlation in sixâ€electron systems. Journal of Chemical Physics, 1994, 100, 8132-8139.	3.0	19
522	The ethylenedione anion: Elucidation of the intricate potential energy hypersurface. Journal of Chemical Physics, 1995, 102, 6525-6536.	3.0	19

#	Article	IF	Citations
523	The 3A2, 1A2, 3B2, and 1B2 electronic states of CH2: Small bond angle states. Journal of Chemical Physics, 1997, 106, 1819-1826.	3.0	19
524	COMPUTATIONAL ANALYSES OF PROTOTYPE CARBENE STRUCTURES AND REACTIONS. , 1997, , 89-170.		19
525	The barrier height for decomposition of HN2. Journal of Chemical Physics, 1998, 108, 8029-8030.	3.0	19
526	An L-shaped equilibrium geometry for germanium dicarbide (GeC2)? Interesting effects of zero-point vibration, scalar relativity, and coreâ€“valence correlation. Journal of Chemical Physics, 2002, 117, 10008-10018.	3.0	19
527	Characterization of the three lowest-lying singlet electronic states of AlOH. Journal of Chemical Physics, 2003, 119, 12830-12841.	3.0	19
528	Energetics of the low-lying isomers of HCCO. Chemical Physics Letters, 2004, 383, 266-269.	2.6	19
529	In search of definitive signatures of the elusive NCCO radical. Journal of Chemical Physics, 2007, 127, 014306.	3.0	19
530	Molecular Structures and Energetics Associated with Hydrogen Atom Addition to the Guanineâ^'Cytosine Base Pair. Journal of Chemical Theory and Computation, 2007, 3, 115-126.	5.3	19
531	Unsaturation in Binuclear Cyclobutadiene Iron Carbonyls: Triplet Structures, Four-Electron Bridging Carbonyl Groups, and Perpendicular Structures. Organometallics, 2008, 27, 3113-3123.	2.3	19
532	Infrared laser spectroscopy of the n-propyl and i-propyl radicals: Stretch-bend Fermi coupling in the alkyl CH stretch region. Journal of Chemical Physics, 2016, 145, 224304.	3.0	19
533	The addition of methanol to Criegee intermediates. Physical Chemistry Chemical Physics, 2019, 21, 17760-17771.	2.8	19
534	Walsh's Rules and the Small Bond Angle States of Triatomic Dihydride Molecules. Israel Journal of Chemistry, 1980, 19, 127-131.	2.3	18
535	Protonated disilyne, Si2H+3: Molecular structures, vibrational frequencies, and infrared intensities. Journal of Chemical Physics, 1990, 93, 7230-7242.	3.0	18
536	Simple mixed hydrides of boron, aluminum, and gallium: AlBH6, AlGaH6, and BGaH6. Journal of Chemical Physics, 1991, 95, 1160-1167.	3.0	18
537	Structure, Spectra, and Reaction Energies of the Aluminumâ^'Nitrogen (HAlâ^'NH)2and (H2Alâ^'NH2)2Rings and the (HAlâ^'NH)4Cluster. Inorganic Chemistry, 1998, 37, 2291-2295.	4.0	18
538	Electron affinities of the bromine oxides BrOn,n= 1-4. Molecular Physics, 2000, 98, 879-890.	1.7	18
539	Molecular Structures and Electron Affinities for the Chlorine Oxides ClOO, ClOOO, and ClO3(C3v). Journal of Physical Chemistry A, 2002, 106, 12324-12330.	2.5	18
540	Binuclear Alkaline Earth Metal Compounds (Be, Mg, Ca, Sr, Ba) with Î±-Diimine Ligands: A Computational Study. Organometallics, 2011, 30, 3113-3118.	2.3	18

#	Article	IF	Citations
541	Analytic gradients for density cumulant functional theory: The DCFT-06 model. Journal of Chemical Physics, 2012, 137, 054105.	3.0	18
542	Structural Isomerization of the Gasâ€Phase 2â€Norbornyl Cation Revealed with Infrared Spectroscopy and Computational Chemistry. Angewandte Chemie - International Edition, 2014, 53, 5888-5891.	13.8	18
543	Proton-transfer in hydrogenated guanineâ€“cytosine trimer neutral species, cations, and anions embedded in B-form DNA. Physical Chemistry Chemical Physics, 2014, 16, 6717.	2.8	18
544	Additionâ€“Elimination versus Direct Substitution Mechanisms for Arene Chlorination. European Journal of Organic Chemistry, 2014, 2014, 6918-6924.	2.4	18
545	Benchmarking the Electron Affinity of Uracil. Journal of Chemical Theory and Computation, 2014, 10, 609-612.	5.3	18
546	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. Journal of Chemical Physics, 2015, 142, 154106.	3.0	18
547	High-level theoretical characterization of the vinoxy radical (â€¢CH2CHO) + O2 reaction. Journal of Chemical Physics, 2018, 148, 184308.	3.0	18
548	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO₂ by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	2.5	18
549	A model transition metal-carbene system MnCH2. Molecular Physics, 1977, 34, 193-213.	1.7	17
550	Isomeric structures of CH2LiF, the prototype carbenoid. Journal of Chemical Physics, 1982, 77, 6103-6108.	3.0	17
551	Variational studies of the importance of triple and quadruple excitations on the barrier height for F+H2â†'FH+H. Journal of Chemical Physics, 1988, 88, 7024-7026.	3.0	17
552	Use of canonical orbital energy derivatives for closedâ€shell selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1993, 98, 8749-8760.	3.0	17
553	Excited electronic states of carbon disulphide. Molecular Physics, 1999, 96, 693-704.	1.7	17
554	Two-Electron Aromatics with Classical and Non-Classical Homobridges. Journal of Molecular Modeling, 2000, 6, 257-271.	1.8	17
555	The silaketenylidene (SiCO) molecule: Characterization of the XÌƒâ€Š3Î£â^' and Ãƒâ€Š3Î states. Journal of Chemical Physics, 2000, 112, 3201-3207.	3.0	17
556	Synthesis and molecular structure of an unusual â€“Gaâ€“Gaâ€“Gaâ€“ linked organometallic. Chemical Communications, 2000, , 453-454.	4.1	17
557	The puzzling infrared spectra of the nitric oxide dimer radical cation: a systematic application of Brueckner methods. Molecular Physics, 2000, 98, 955-959.	1.7	17
558	Group 13â^'Group 16 Heterocubanes [RM(Î¼3-E)]4 (R = H, CH3; M = Al, Ga, In; E = O, S, Se, Te) and Group 13 Cubanes [RM(Î¼3-M)]4 (R = F, Cl, CH3, NO2; M = Al, Ga, In):â€‰ A Structural Study. Organometallics, 2002, 21, 3605-3609.	2.3	17

#	Article	IF	Citations
559	Silylidene (SiCH2) and its isomers: Anharmonic rovibrational analyses for silylidene, silaacetylene, and silavinylidene. Journal of Molecular Structure, 2012, 1009, 103-110.	3.6	17
560	Density cumulant functional theory: The DC-12 method, an improved description of the one-particle density matrix. Journal of Chemical Physics, 2013, 138, 024107.	3.0	17
561	Is Pd^{II}â€Promoted Ïƒâ€Bond Metathesis Mechanism Operative for the Pdï£¿PEPPSI Complexâ€Catalyzed Amination of Chlorobenzene with Aniline? Experiment and Theory. Chemistry - A European Journal, 2015, 21, 4153-4161.	3.3	17
562	The fate of the tert-butyl radical in low-temperature autoignition reactions. Journal of Chemical Physics, 2017, 146, 194304.	3.0	17
563	Facile Conversion of Bis-Silylene to Cyclic Silylene Isomers: Unexpected Câ€“N and Câ€“H Bond Cleavage. Journal of the American Chemical Society, 2017, 139, 16109-16112.	13.7	17
564	Câ€“HÂ·Â·Â·O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. Journal of Chemical Theory and Computation, 2017, 13, 5379-5395.	5.3	17
565	Nucleophilic Influences and Origin of the S N 2 Allylic Effect. Chemistry - A European Journal, 2018, 24, 11637-11648.	3.3	17
566	Isomerâ€dependent reaction mechanisms of cyclic ether intermediates: cisâ€2,3â€dimethyloxirane and transâ€2,3â€dimethyloxirane. International Journal of Chemical Kinetics, 2021, 53, 127-145.	1.6	17
567	Where to look for the electronic spectrum of hydrogen isocyanide, HNC. Journal of Chemical Physics, 1984, 80, 3069-3072.	3.0	16
568	Radiative decay lifetimes of CHâ˜2. Journal of Chemical Physics, 1987, 86, 3807-3815.	3.0	16
569	The SiOH+â€“HSiO+ system: A high level ab initio quantum mechanical study. Journal of Chemical Physics, 1995, 102, 5327-5334.	3.0	16
570	The GaOHâ€“HGaO potential energy hypersurface and the necessity of correlating the 3d electrons. Journal of Chemical Physics, 1996, 104, 8516-8523.	3.0	16
571	Isomerization pathway of the aluminum monocarbonyl/isocarbonyl pair, AlCO/AlOC: Evidence of a cyclic minimum. Journal of Chemical Physics, 1998, 108, 9398-9403.	3.0	16
572	Structure and Conformations of Cyclopentasilane, Si5H10. Journal of Physical Chemistry A, 1999, 103, 5581-5584.	2.5	16
573	Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. Journal of Physical Chemistry A, 2003, 107, 6311-6316.	2.5	16
574	Triplet states of cyclopropenylidene and its isomers. Journal of Chemical Physics, 2010, 132, 044308.	3.0	16
575	Applying a Smolyak collocation method to Cl₂CO. Molecular Physics, 2017, 115, 1775-1785.	1.7	16
576	Ethyl + O₂ in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical. Journal of Physical Chemistry A, 2019, 123, 3558-3568.	2.5	16

#	Article	IF	Citations
577	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie - International Edition, 2020, 59, 8864-8867.	13.8	16
578	Arbitrary-Order Derivatives of Quantum Chemical Methods via Automatic Differentiation. Journal of Physical Chemistry Letters, 2021, 12, 3232-3239.	4.6	16
579	Selfâ€consistentâ€field wavefunctions using a symmetryâ€restricted annihilation of singleâ€excitations procedure. Journal of Chemical Physics, 1976, 64, 981-986.	3.0	15
580	The infrared spectrum of silaethylene. Journal of Chemical Physics, 1986, 85, 4563-4566.	3.0	15
581	Natriumpentaphosphacyclopentadienid NaP₅ und das Pentaphosphacyclopentadienidâ€Ion P: Theoretische Studien zu MolekÃ¼lstruktur, IRâ€und Ramanâ€Spektren. Angewandte Chemie, 1989, 101, 500-501.	2.0	15
582	The structures and vibrational frequencies of the NNO analogs NPO and PNO and their protonated forms. Journal of Chemical Physics, 1990, 92, 5417-5421.	3.0	15
583	The silaformyl radical HSiO and its SiOH isomer. Journal of Chemical Physics, 1990, 93, 1196-1199.	3.0	15
584	The infrared spectrum of trimethylenemethane. Predictions of inâ€plane vibrational frequencies from correlated wave functions. Journal of Chemical Physics, 1990, 92, 1174-1179.	3.0	15
585	First and second energy derivative analyses of the vinylidene and acetylene triplet state potential energy hypersurfaces. Journal of Chemical Physics, 1994, 100, 4969-4980.	3.0	15
586	Can AlH5 exist?. Journal of Chemical Physics, 1995, 103, 5565-5569.	3.0	15
587	Brillouinâ€“Wigner coupled cluster theory. Fock-space approach. Journal of Chemical Physics, 2002, 117, 9580-9587.	3.0	15
588	The 2â€˜-Deoxyadenosine-5â€˜-phosphate Anion, the Analogous Radical, and the Different Hydrogen-Abstracted Radical Anions:Â Molecular Structures and Effects on DNA Damage. Journal of Physical Chemistry B, 2005, 109, 22053-22060.	2.6	15
589	Binuclear Vanadium Carbonyls:Â The Limits of the 18-Electron Rule. Inorganic Chemistry, 2007, 46, 1803-1816.	4.0	15
590	Unsaturation in Binuclear (Cyclobutadiene)cobalt Carbonyls with Axial and Perpendicular Structures:â€‰ Comparison with Isoelectronic Binuclear Cyclopentadienyliron Carbonyls. Organometallics, 2007, 26, 1393-1401.	2.3	15
591	Unsaturation and Variable Hapticity in Binuclear Azulene Iron Carbonyl Complexes. Organometallics, 2010, 29, 630-641.	2.3	15
592	Possibilities for Titaniumâ€˜Titanium Multiple Bonding in Binuclear Cyclopentadienyltitanium Carbonyls: 16-Electron Metal Configurations and Four-Electron Donor Bridging Carbonyl Groups as Alternatives. Inorganic Chemistry, 2010, 49, 1961-1975.	4.0	15
593	The Quest for Metalâ€“Metal Quadruple and Quintuple Bonds in Metal Carbonyl Derivatives: Nb2(CO)9 and Nb2(CO)8. Journal of Chemical Theory and Computation, 2012, 8, 862-874.	5.3	15
594	Hydrogen bondâ€“aromaticity cooperativity in selfâ€assembling 4â€pyridone chains. Journal of Computational Chemistry, 2016, 37, 59-63.	3.3	15

#	Article	IF	Citations
595	Spinâ€“Orbit Coupling via Four-Component Multireference Methods: Benchmarking on p-Block Elements and Tentative Recommendations. Journal of Chemical Theory and Computation, 2018, 14, 1235-1246.	5.3	15
596	The low-lying electronic states of nickel cyanide and isocyanide: A theoretical investigation. Journal of Chemical Physics, 2006, 124, 034310.	3.0	15
597	On the convergence of Z-averaged perturbation theory. Journal of Chemical Physics, 2008, 128, 074107.	3.0	15
598	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
599	Excited electronic states of HNC, hydrogen isocyanide. Journal of Chemical Physics, 1975, 63, 569-572.	3.0	14
600	Structures, Energetics and Vibrational Frequencies of Cyclopropyne. Israel Journal of Chemistry, 1983, 23, 93-96.	2.3	14
601	The description of elementary organoaluminum fragments: AlCHx (x=1,2,3). Journal of Chemical Physics, 1991, 95, 1834-1837.	3.0	14
602	The titane molecule (TiH4): Equilibrium geometry, infrared and Raman spectra of the first spectroscopically characterized transition metal tetrahydride. Journal of Chemical Physics, 1992, 96, 6857-6861.	3.0	14
603	High-Levelab InitioCalculation of the Rotationâ^'Vibration Energies in the cl̀ƒ1A1State of Methylene, CH2. The Journal of Physical Chemistry, 1996, 100, 18088-18092.	2.9	14
604	The Rovibrational Energy Levels of Quasilinearc1A1Methylene. Journal of Molecular Spectroscopy, 1996, 179, 263-268.	1.2	14
605	The SiOHâ€“HSiO system: A high level quantum mechanical study. Journal of Chemical Physics, 1996, 105, 1951-1958.	3.0	14
606	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.	3.0	14
607	Interlocking Triplet Electronic States of Isocyanic Acid:Â Sources of Nonadiabatic Photofragmentation Dynamicsâ€. Journal of Physical Chemistry A, 2001, 105, 2716-2730.	2.5	14
608	Structures, thermochemistry, and electron affinities of the disilicon fluorides, Si2Fn/Si2Fâ^'n(n= 1â€“6). Molecular Physics, 2001, 99, 1053-1074.	1.7	14
609	The ability of silylenes to bind excess electrons: Electron affinities of SiX2, and SiXY species (X,Y=H,CH3,SiH3,F,Cl,Br). Journal of Chemical Physics, 2004, 121, 9361-9367.	3.0	14
610	The low-lying electronic excited states of NiCO. Journal of Chemical Physics, 2004, 121, 1412-1418.	3.0	14
611	The Highly Unsaturated Binuclear Chromium Carbonyl Cr2(CO)8. Journal of Physical Chemistry A, 2004, 108, 6879-6885.	2.5	14
612	Hydrogen bridging in the compounds X2H (X=Al,Si,P,S). Journal of Chemical Physics, 2006, 125, 164322.	3.0	14

#	Article	IF	Citations
613	A laboratory and theoretical study of protonated carbon disulfide, HSCS+. Journal of Chemical Physics, 2009, 130, 234304.	3.0	14
614	Binuclear and Trinuclear Chromium Carbonyls with Linear Bridging Carbonyl Groups: Isocarbonyl versus Carbonyl Bonding of Carbon Monoxide Ligands. Journal of Physical Chemistry A, 2010, 114, 4672-4679.	2.5	14
615	Binuclear iron boronyl carbonyls isoelectronic with the well-known decacarbonyldimanganese. New Journal of Chemistry, 2012, 36, 1022.	2.8	14
616	A new type of sandwich compound: homoleptic bis(trimethylenemethane) complexes of the first row transition metals. New Journal of Chemistry, 2013, 37, 1545.	2.8	14
617	Coaxial versus perpendicular structures for a range of binuclear cyclopentadienylpalladium derivatives. New Journal of Chemistry, 2013, 37, 775.	2.8	14
618	Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O4+. Journal of Chemical Physics, 2014, 141, 074111.	3.0	14
619	Toward Understanding the Decomposition of Carbonyl Diazide (N₃)₂Câ•O and Formation of Diazirinone cycl-N₂CO: Experiment and Computations. Journal of Physical Chemistry A, 2015, 119, 8903-8911.	2.5	14
620	Protonation of carbene-stabilized diphosphorus: complexation of HP₂⁺. Chemical Communications, 2016, 52, 5746-5748.	4.1	14
621	The methylsulfinyl radical CH₃SO examined. Physical Chemistry Chemical Physics, 2016, 18, 22293-22299.	2.8	14
622	Analytic Energy Gradients for Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4113-4122.	5.3	14
623	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. Journal of Chemical Physics, 2018, 148, .	3.0	14
624	Acceleration Effect of Bases on Mn Pincer Complex-Catalyzed CO₂ Hydroboration. Inorganic Chemistry, 2022, 61, 3970-3980.	4.0	14
625	Some features of the potential energy surfaces for the F++H2 ionâ€“molecule reaction. Journal of Chemical Physics, 1978, 68, 781-782.	3.0	13
626	Reaction barrier for the methyldiazenyl radical decomposition (CH3N2â†'CH3+N2). Journal of Chemical Physics, 1994, 101, 1289-1292.	3.0	13
627	Equilibrium geometry of isocyanomethylene (HCNC) and comparison to the troublesome isomer cyanomethylene (HCCN). Journal of Chemical Physics, 1994, 101, 430-435.	3.0	13
628	The electron affinity of CF. Journal of Chemical Physics, 1994, 101, 10191-10192.	3.0	13
629	Revision of the experimental electron affinity of BO. Journal of Chemical Physics, 1997, 106, 8278-8279.	3.0	13
630	The hydroxyethynyl radical (CCOH): an accessible isomer of the ketenyl radical (HCCO)?. Chemical Physics Letters, 1998, 291, 509-516.	2.6	13

#	Article	IF	Citations
631	A comparison between the CISD[TQ] wave function and other highly correlated methods: Molecular geometry and harmonic vibrational frequencies of MgH2. Journal of Chemical Physics, 1998, 108, 7511-7515.	3.0	13
632	Three Lowest-Lying Electronic States of NH2. Journal of Physical Chemistry A, 1999, 103, 7701-7708.	2.5	13
633	Coupled-cluster studies of the hyperfine splitting constants of the thioformyl radical. Journal of Chemical Physics, 2000, 112, 6245-6254.	3.0	13
634	The 2-Silaketenylidene (CSiO) Radical:Â Electronic Structure of the XÌƒ3Î£-and Ãƒ3Î Statesâ€. Journal of Physical Chemistry A, 2000, 104, 10165-10172.	2.5	13
635	Electron affinities of cyano-substituted ethylenes. Molecular Physics, 2001, 99, 663-675.	1.7	13
636	Coupled cluster study of the XÌƒâ€Š2Î and Ãƒâ€Š2Î£+ electronic states of the HCGe radical: Rennerâ€“Teller splitting and the effects of relativistic corrections. Journal of Chemical Physics, 2001, 115, 5932-5942.	3.0	13
637	Characterization of the XÌƒ2A1 and Ã£4A2 electronic states of CH2+. Chemical Physics Letters, 2002, 352, 505-510.	2.6	13
638	Protonated carbonyl sulfide: Prospects for the spectroscopic observation of the elusive HSCO+ isomer. Journal of Chemical Physics, 2006, 124, 044322.	3.0	13
639	The subtleties of explicitly correlated Z-averaged perturbation theory: Choosing an R12 method for high-spin open-shell molecules. Journal of Chemical Physics, 2009, 131, 244116.	3.0	13
640	Binuclear Cobalt Thiocarbonyl Carbonyl Derivatives: Comparison with Homoleptic Binuclear Cobalt Carbonyls. Inorganic Chemistry, 2009, 48, 5973-5982.	4.0	13
641	Mononuclear and binuclear manganese carbonyl hydrides: the preference for bridging hydrogens over bridging carbonyls. Dalton Transactions, 2009, , 3774.	3.3	13
642	Silacyclopropenylidene and Its Most Important SiC₂H₂ Isomers. Journal of Physical Chemistry C, 2010, 114, 5447-5457.	3.1	13
643	Is There an Entrance Complex for the F+NH₃ Reaction?. Chemistry - an Asian Journal, 2011, 6, 3152-3156.	3.3	13
644	Conformational Preferences of Gas-Phase Helices: Experiment and Theory Struggle to Agree: The Seven-Residue Peptide Ac-Phe-(Ala)5-Lys-H+. Chemistry - A European Journal, 2012, 18, 12941-12944.	3.3	13
645	Fundamental vibrational frequencies and spectroscopic constants for the methylperoxyl radical, CH₃O₂, and related isotopologues ¹³CH₃OO, CH₃ ¹⁸O¹⁸O, and CD₃OO. Molecular Physics, 2012, 110, 2419-2427.	1.7	13
646	Isoguanine Formation from Adenine. Chemistry - A European Journal, 2012, 18, 4877-4886.	3.3	13
647	Benchmark Study of Density Cumulant Functional Theory: Thermochemistry and Kinetics. Journal of Chemical Theory and Computation, 2014, 10, 2389-2398.	5.3	13
648	Spinâ€“orbit corrected potential energy surface features for the I (2P3/2) + H2O â†' HI + OH forward and reverse reactions. Physical Chemistry Chemical Physics, 2014, 16, 2641.	2.8	13

#	Article	IF	Citations
649	Examining the ground and first excited states of methyl peroxy radical with high-level coupled-cluster theory. Molecular Physics, 2015, 113, 2992-2998.	1.7	13
650	Can Density Cumulant Functional Theory Describe Static Correlation Effects?. Journal of Chemical Theory and Computation, 2015, 11, 2487-2495.	5.3	13
651	NMR chemical shielding surface ofN-Acetyl-N?-Methylalaninamide: A density functional study. Journal of Computational Chemistry, 1997, 18, 126-138.	3.3	12
652	XÌƒ3Î£-and Ãƒ3Î Electronic States of Ketenylidene (CCO):Â Analysis of the Renner Effect in the Upper Stateâ€. Journal of Physical Chemistry A, 2000, 104, 3603-3612.	2.5	12
653	Electron affinities, molecular structures, and thermochemistry of the fluorine, chlorine and bromine substituted methyl radicals. Molecular Physics, 2002, 100, 3615-3648.	1.7	12
654	Molecules for Materials: Structures, Thermochemistry, and Electron Affinities of the Digermanium Fluorides Ge2Fn/Ge2Fn- (n=1-6): A Wealth of Unusual Structures. ChemPhysChem, 2002, 3, 179-194.	2.1	12
655	Molecular structures, thermochemistry, and electron affinities for the dichlorine oxides: Cl2On/Cl2Oâ€‰â”n (n= 1-4). International Journal of Quantum Chemistry, 2003, 95, 731-757.	2.0	12
656	Gas Phase Complexes MX3Â·4,4â€˜BpyÂ·Mâ€˜X3 (M,Mâ€˜ = Al, Ga; X = Cl, Br):â€‰ Experiment and Theory. Journal of Physical Chemistry B, 2004, 108, 9561-9563.	2.6	12
657	Structures, thermochemistry, vibrational frequencies and integrated infrared intensities of SF5CF3and SF5, with implications for global temperature patterns. Molecular Physics, 2004, 102, 1415-1439.	1.7	12
658	The Vinyl Radical and Fluorinated Vinyl Radicals, C2H3-nFn (n = 0â”3), and Corresponding Anions:â€‰ Comparison with the Isoelectronic Complexes [XÂ·Â·Â·YCâ‰¡CZ]-. Journal of Physical Chemistry A, 2004, 108, 1608-1615.	2.5	12
659	The diazocarbene (CNN) molecule: Characterization of the XÌƒâ€‚3Î£â” and Ãƒâ€‚3Î electronic states. Journal of Chemical Physics, 2004, 120, 9536-9546.	3.0	12
660	Beyond the metalâ€“metal triple bond in binuclear cyclopentadienylchromium carbonyl chemistry. Dalton Transactions, 2008, , 4805.	3.3	12
661	Binuclear Cyclopentadienylmetal Carbonyl Derivatives of the Oxophilic Metal Niobium. Organometallics, 2009, 28, 6410-6424.	2.3	12
662	Trifluorophosphine as a Bridging Ligand in Homoleptic Binuclear Nickel Complexes^{â€}. Journal of Physical Chemistry A, 2010, 114, 8896-8901.	2.5	12
663	Designing new Togni reagents by computation. Chemical Communications, 2019, 55, 5667-5670.	4.1	12
664	Redox chemistry of an anionic dithiolene radical. Dalton Transactions, 2019, 48, 3543-3546.	3.3	12
665	Terminal vs bridge bonding of methylene to metal systems: Al2CH2as a model system. Journal of Chemical Physics, 1983, 78, 328-338.	3.0	11
666	The treatment of triple excitations within the coupled cluster description of molecular electronic structure. Journal of Chemical Physics, 1985, 83, 703-712.	3.0	11

#	Article	IF	Citations
667	Ab initio prediction of the structure, harmonic vibrational frequencies, and dissociation energy of the H2â€“GeH+3â€“H2 cluster ion. Journal of Chemical Physics, 1995, 102, 3667-3673.	3.0	11
668	THE CHEMICAL APPLICABILITY OF STANDARD METHODS IN AB INITIO MOLECULAR QUANTUM MECHANICS. Advanced Series in Physical Chemistry, 1995, , 3-54.	1.5	11
669	The 3d Rydberg (3A2) electronic state observed by Herzberg and Shoosmith for methylene. Journal of Chemical Physics, 1997, 106, 8753-8759.	3.0	11
670	Structure, Spectra, and Reaction Energies of the Aluminumâˆ’Phosphorus Rings (HAlâˆ’PH)2and (H2Alâˆ’PH2)2and the (HAlâˆ’PH)4Cluster. Journal of Physical Chemistry A, 1997, 101, 5707-5711.	2.5	11
671	An ab initio study on the four electronically lowest-lying states of CH2 using the state-averaged complete active space second-order configuration interaction method. Chemical Physics, 1997, 225, 23-31.	1.9	11
672	Formation of CF3Oâˆ’ in the gas phase. Journal of Chemical Physics, 1999, 110, 8436-8442.	3.0	11
673	The equilibrium structure of the ammonium radical Rydberg ground state. Journal of Chemical Physics, 2001, 114, 9863-9865.	3.0	11
674	III: PROPERTIES OF COMPLEX SYSTEMS. Molecular Physics, 2003, 101, 211-225.	1.7	11
675	The Binuclear Cyclopentadienylvanadium Carbonyls (Î·5-C5H5)2V2(CO)7 and (Î·5-C5H5)2V2(CO)6: Comparison with Homoleptic Chromium Carbonyls. European Journal of Inorganic Chemistry, 2007, 2007, 1599-1605.	2.0	11
676	(Acetylene)dicobalt Carbonyl Derivatives: Decarbonylation of the H₂C₂Co₂(CO)₆Tetrahedrane. Organometallics, 2009, 28, 3390-3394.	2.3	11
677	Binuclear homoleptic rhodium carbonyls: Structures, energetics, and vibrational spectra. Dalton Transactions, 2009, , 2599.	3.3	11
678	Chromium-Chromium Bonding in Binuclear Azulene Chromium Carbonyl Complexes. European Journal of Inorganic Chemistry, 2010, 2010, 5161-5173.	2.0	11
679	Vertical detachment energies of anionic thymidine: Microhydration effects. Journal of Chemical Physics, 2010, 133, 144305.	3.0	11
680	Does the metalâ€“metal sextuple bond exist in the bimetallic sandwich compounds Cr₂(C₆H₆)₂, Mo₂(C₆H₆)₂, and W₂(C₆H₆)₂?^{â€}. Molecular Physics, 2013, 111, 2523-2535.	1.7	11
681	Dinickelametallocenes: Sandwich Compounds of the First-Row Transition Metals (M = Fe, Co, Ni) with Two Pentahapto Planar Nickelacycle Ligands. Organometallics, 2014, 33, 4410-4416.	2.3	11
682	From Gasâ€Phase to Liquidâ€Water Chemical Reactions: The Fluorine Atom Plus Water Trimer System. Angewandte Chemie - International Edition, 2015, 54, 11223-11226.	13.8	11
683	Molecular Mechanics (MM4) Studies on Unusually Long Carbonâ€“Carbon Bond Distances in Hydrocarbons. Journal of Chemical Theory and Computation, 2016, 12, 2774-2778.	5.3	11
684	Spin-Adapted Formulation and Implementation of Density Cumulant Functional Theory with Density-Fitting Approximation: Application to Transition Metal Compounds. Journal of Chemical Theory and Computation, 2016, 12, 4833-4842.	5.3	11

#	Article	IF	Citations
685	Structural Distortions Accompanying Noncovalent Interactions: Methaneâ€“Water, the Simplest Câ€“H Hydrogen Bond. Journal of Chemical Theory and Computation, 2017, 13, 1478-1485.	5.3	11
686	The Hydrogen Abstraction Reaction H₂S + OH â†' H₂O + SH: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2017, 121, 9136-9145.	2.5	11
687	Dispersion Effects in Stabilizing Organometallic Compounds: Tetra-1-norbornyl Derivatives of the First-Row Transition Metals as Exceptional Examples. Journal of Physical Chemistry A, 2019, 123, 9514-9519.	2.5	11
688	Characterization of the 2-methylvinoxy radical + O2 reaction: A focal point analysis and composite multireference study. Journal of Chemical Physics, 2019, 151, 124302.	3.0	11
689	Riddles of the structure and vibrational dynamics of HO3 resolved near the ab initio limit. Journal of Chemical Physics, 2019, 151, 094304.	3.0	11
690	Multi-fidelity Gaussian process modeling for chemical energy surfaces. Chemical Physics Letters: X, 2019, 737, 100022.	2.1	11
691	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C₆₀ and cyclopentadiene. Physical Chemistry Chemical Physics, 2019, 21, 5039-5048.	2.8	11
692	A Stable Naked Dithiolene Radical Anion and Synergic THF Ring-Opening. Journal of the American Chemical Society, 2020, 142, 17301-17305.	13.7	11
693	Reduced Density Matrix Cumulants: The Combinatorics of Size-Consistency and Generalized Normal Ordering. Journal of Chemical Theory and Computation, 2020, 16, 6150-6164.	5.3	11
694	Coupled Cluster Externally Corrected by Adaptive Configuration Interaction. Journal of Chemical Theory and Computation, 2021, 17, 182-190.	5.3	11
695	Some characteristics of the intravalence tripletâ€“triplet electronic transition in HCN. Journal of Chemical Physics, 1980, 73, 1470-1472.	3.0	10
696	SiLiF: The competition between electronic effects favoring singlet and triplet ground states. A case study. Journal of Chemical Physics, 1985, 83, 4581-4584.	3.0	10
697	The bending frequency ΠNS of dinitrogen sulfide (N2S): A theoretical analysis demonstrating the importance of Coriolis coupling terms. Journal of Chemical Physics, 1993, 98, 4777-4782.	3.0	10
698	Rotational constants for the Cl̃ƒâ€‰2A2 state of NO2. Journal of Chemical Physics, 1993, 99, 7926-7928.	3.0	10
699	The electron affinities of PF and PF2. Journal of Chemical Physics, 1998, 108, 1050-1054.	3.0	10
700	The not-so-peculiar case of calcium oxide: a weakness in atomic natural orbital basis sets for calcium. Molecular Physics, 2000, 98, 1227-1231.	1.7	10
701	The ground and two lowest-lying singlet excited electronic states of copper hydroxide (CuOH). Journal of Chemical Physics, 2005, 123, 014313.	3.0	10
702	Effects of Fluorine on the Structures and Energetics of the Propynyl and Propargyl Radicals and Their Anions. Journal of Organic Chemistry, 2005, 70, 8676-8686.	3.2	10

#	Article	IF	Citations
703	Characterization of the HSiNî—¸HNSi system in its electronic ground state. Journal of Chemical Physics, 2009, 130, 104301.	3.0	10
704	The mixed sandwich compounds C5H5MC7H7of the first row transition metals: variable hapticity of the seven-membered ring. Molecular Physics, 2010, 108, 883-894.	1.7	10
705	Stabilization of Binuclear Chromium Carbonyls by Substitution of Thiocarbonyl Groups for Carbonyl Groups: Nearly Linear Structures for Cr₂(CS)₂(CO)₉. Journal of Physical Chemistry A, 2010, 114, 486-497.	2.5	10
706	Reaction Energetics for the Abstraction Process C₂H₃ + H₂ â†' C₂H₄ + H. Journal of Physical Chemistry Letters, 2011, 2, 2587-2592.	4.6	10
707	Telluroformaldehyde and its derivatives: structures, ionization potentials, electron affinities and singletâ€"triplet gaps of the X2CTe and XYCTe (X,YÂ=ÂH, F, Cl, Br, I and CN) species. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	10
708	Anchoring the potential energy surface for the BrÂ+ÂH2OÂâ†'ÂHBrÂ+ÂOH reaction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	10
709	Mechanistic Investigations of the AuCl₃-Catalyzed Nitrene Insertion into an Aromatic Câ€"H Bond of Mesitylene. Journal of Organic Chemistry, 2015, 80, 5795-5803.	3.2	10
710	Intricate Internal Rotation Surface and Fundamental Infrared Transitions of the n-Propyl Radical. Journal of Physical Chemistry B, 2015, 119, 728-735.	2.6	10
711	Peroxyacetyl radical: Electronic excitation energies, fundamental vibrational frequencies, and symmetry breaking in the first excited state. Journal of Chemical Physics, 2015, 142, 054303.	3.0	10
712	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. Journal of Computational Chemistry, 2018, 39, 889-900.	3.3	10
713	Calculation of Spin Densities for Light Atoms. Journal of Chemical Physics, 1968, 49, 469-470.	3.0	9
714	The BERKELEY system. III. General configuration-interaction methods for open-shell molecular electronic states. International Journal of Quantum Chemistry, 1978, 14, 603-612.	2.0	9
715	Does Singlet 1,1-Dilithioethene Really Prefer a Perpendicular Structure?. The Journal of Physical Chemistry, 1995, 99, 17551-17557.	2.9	9
716	The anomalous behavior of the Zeeman anticrossing spectra of Alƒâ€‰1Au acetylene: Theoretical considerations. Journal of Chemical Physics, 1996, 104, 1774-1778.	3.0	9
717	A Systematic Study of the Xlƒ 2B1, Ãƒ 2A1, and Blƒ 2B2 States of the Neutral Radical PH2. Journal of Physical Chemistry A, 2001, 105, 5037-5045.	2.5	9
718	Elusive electron affinity of ClF. Journal of Chemical Physics, 2003, 119, 11615-11619.	3.0	9
719	The singlet electronic ground state isomers of dialuminum monoxide: AlOAl, AlAlO, and the transition state connecting them. Journal of Chemical Physics, 2005, 122, 094304.	3.0	9
720	Binuclear Iron Carbonyl Nitrosyls: Bridging Nitrosyls versus Bridging Carbonyls. Inorganic Chemistry, 2008, 47, 3045-3055.	4.0	9

#	Article	IF	Citations
721	Homoleptic tetranuclear osmium carbonyls: from the rhombus via the butterfly to the tetrahedron. Dalton Transactions, 2008, , 1366.	3.3	9
722	Vanadium Carbonyl Nitrosyl Compounds: The Carbonyl Nitrosyl Chemistry of an Oxophilic Early Transition Metal. European Journal of Inorganic Chemistry, 2009, 2009, 1647-1656.	2.0	9
723	Mononuclear and binuclear cobalt carbonyl nitrosyls: comparison with isoelectronic nickel carbonyls. New Journal of Chemistry, 2009, 33, 2090.	2.8	9
724	Binuclear manganesecarbonyl thiocarbonyls: metalâ€“metal multiple bonds versus four-electron donorthiocarbonyl groups. New Journal of Chemistry, 2010, 34, 92-102.	2.8	9
725	Open chains versus closed rings: comparison of binuclear butadiene iron carbonyls with their cyclobutadiene analogues. New Journal of Chemistry, 2011, 35, 920.	2.8	9
726	Binuclear Pentalene Iron Carbonyl Complexes. European Journal of Inorganic Chemistry, 2011, 2011, 2746-2755.	2.0	9
727	Structures and Energetics of the tertâ€Butyl Cation: The Final Answer or a Neverâ€Ending Story?. Chemistry - A European Journal, 2011, 17, 10552-10555.	3.3	9
728	Carbonyl migration from phosphorus to the metal in binuclear phosphaketenyl metal carbonyl complexes to give bridging diphosphido complexes. New Journal of Chemistry, 2015, 39, 1390-1403.	2.8	9
729	The Recently Synthesized Dimagnesiabutadiene and the Analogous Dimetallaâ€Beryllium, â€Calcium, â€Strontium, and â€Barium Compounds. Chemistry - A European Journal, 2016, 22, 15019-15026.	3.3	9
730	Vibrational frequencies, structures, and energetics of the highly challenging alkali metal trifluorides MF3 (M = Li, Na, K, Rb, and Cs). Physical Chemistry Chemical Physics, 2018, 20, 18986-18994.	2.8	9
731	Janus: An Extensible Open-Source Software Package for Adaptive QM/MM Methods. Journal of Chemical Theory and Computation, 2019, 15, 4362-4373.	5.3	9
732	Lewis base-complexed magnesium dithiolenes. Chemical Communications, 2019, 55, 8087-8089.	4.1	9
733	Contrasting the Mechanism of H₂Activation by Monomeric and Potassiumâ€Stabilized Dimeric Al^IComplexes: Do Potassium Atoms Exert any Cooperative Effect?. Chemistry - A European Journal, 2021, 27, 17369-17378.	3.3	9
734	Structure and energetics of realistic carbynes: (carbohydroxy)carbyne (HOCOC.tplbond.). Journal of the American Chemical Society, 1982, 104, 1457-1461.	13.7	8
735	The HO2 + ion. Molecular Physics, 1989, 68, 1095-1109.	1.7	8
736	The silyl anion (SiHâ¯3): Harmonic vibrational frequencies and infrared intensities predicted at the SCF, CISD, and CCSD levels of theory with substantial basis sets. Journal of Chemical Physics, 1990, 93, 8098-8104.	3.0	8
737	Monofluorinated hydrogen sulfide (HFS): A definitive theoretical prediction of the infrared spectrum. Journal of Chemical Physics, 1992, 96, 2044-2047.	3.0	8
738	The structure of the bitetrahedryl molecule?A major shift due to electron correlation: Effects of carbonyl substituents, implications for the structure of coupled tricyclo[3.1.0.02,6]hexyl, and extension to cubylcubane. International Journal of Quantum Chemistry, 1992, 42, 953-963.	2.0	8

#	Article	IF	Citations
739	Ethynylvinylidene. Israel Journal of Chemistry, 1993, 33, 317-321.	2.3	8
740	A study of the silagermylyne (SiGeH2) molecule: A new monobridged structure. International Journal of Quantum Chemistry, 1995, 56, 593-604.	2.0	8
741	Chromium dihydride (CrH2): theoretical evidence for a bent5B2ground state. Molecular Physics, 1995, 84, 1109-1126.	1.7	8
742	Examination of the Stabilities of Group 14 (C, Si, Ge, Sn, Pb) Congeners of Dihydroxycarbene and Dioxirane. Comparison to Formic Acid and Hydroperoxycarbene Congeners. Inorganic Chemistry, 1999, 38, 6271-6277.	4.0	8
743	Ring structure of the NO dimer radical cation: A possible new assignment of the mysterious IR absorption at 1424 cmâ˜1. Journal of Chemical Physics, 2002, 117, 9727-9732.	3.0	8
744	Low-lying quartet electronic states of nitrogen dioxide. Journal of Chemical Physics, 2007, 127, 174303.	3.0	8
745	A Carbonyl Group Bridging Four Metal Atoms in a Homoleptic Carbonylmetal Cluster: The Remarkable Case of ÂCo4(CO)11. European Journal of Inorganic Chemistry, 2008, 2008, 2158-2164.	2.0	8
746	Binuclear manganese and rhenium carbonyls M2(CO)n (n = 10, 9, 8, 7): comparison of first row and third row transition metal carbonyl structures. Dalton Transactions, 2008, , 2495.	3.3	8
747	Unsaturation in Binuclear Benzene Manganese Carbonyls: Comparison with Isoelectronic Cyclopentadienyliron and Cyclobutadienecobalt Derivatives. Organometallics, 2008, 27, 4572-4579.	2.3	8
748	Hypervalent molecules, sulfuranes, and persulfuranes: review and studies related to the recent synthesis of the first persulfurane with all substituents carbon-linked. Theoretical Chemistry Accounts, 2009, 124, 151-159.	1.4	8
749	Formation of a four-electron donor carbonyl group in the decarbonylation of the unsaturated H2C2Fe2(CO)6 tetrahedrane as an alternative to an ironâ€“iron triple bond. Journal of Organometallic Chemistry, 2010, 695, 244-248.	1.8	8
750	Coordination Properties of Bridging Diazene Ligands in Unusual Diiron Complexes. Organometallics, 2010, 29, 3271-3280.	2.3	8
751	Mononuclear bis(pentalene) sandwich compounds of the first-row transition metals: variable hapticity of the pentalene rings and intramolecular coupling reactions. New Journal of Chemistry, 2011, 35, 1718.	2.8	8
752	Anharmonic rovibrational analysis for disilacyclopropenylidene (Si2CH2). Journal of Chemical Physics, 2011, 134, 164101.	3.0	8
753	Binuclear pentalene manganese carbonyl complexes: conventionaltransand unconventionalcisstructures. Molecular Physics, 2012, 110, 1637-1650.	1.7	8
754	Reducing and Reversing the Diphospheneâ€“Diphosphinylidene Energy Separation. Journal of Chemical Theory and Computation, 2012, 8, 1663-1670.	5.3	8
755	Metallametallocenes: Sandwich Compounds of the Firstâ€Row Transition Metals (M, Mâ€² = Fe, Co, Ni) Containing a Metallacyclopentadiene Ring. European Journal of Inorganic Chemistry, 2013, 2013, 2070-2077.	2.0	8
756	The exothermic HCl + OHÂ·(H2O) reaction: Removal of the HCl + OH barrier by a single water molecule. Journal of Chemical Physics, 2014, 140, 124316.	3.0	8

#	Article	IF	Citations
757	Twisted Triplet Ethylene: Anharmonic Frequencies and Spectroscopic Parameters for C₂H₄, C₂D₄, and ¹³C₂H₄. Journal of Physical Chemistry A, 2014, 118, 7560-7567.	2.5	8
758	The Design of â€œNeutralâ€•Carbanions with Intramolecular Charge Compensation. Journal of Organic Chemistry, 2016, 81, 1885-1898.	3.2	8
759	Alkali-Metal Trihalides: M+X3â€“Ion Pair or MXâ€“X2Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353.	2.6	8
760	Substituent effects on the aromaticity of benzeneâ€”An approach based on interaction coordinates. Journal of Chemical Physics, 2019, 150, 214108.	3.0	8
761	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. Journal of Chemical Physics, 2020, 152, 024302.	3.0	8
762	High level ab initio investigation of the catalytic effect of water on formic acid decomposition and isomerization. Physical Chemistry Chemical Physics, 2020, 22, 25638-25651.	2.8	8
763	The atmospheric importance of methylamine additions to Criegee intermediates. Physical Chemistry Chemical Physics, 2020, 22, 22555-22566.	2.8	8
764	Fermi.jl: A Modern Design for Quantum Chemistry. Journal of Chemical Theory and Computation, 2022, 18, 677-686.	5.3	8
765	The electronic spectra of SNS. Lowâ€lying doublet states. Journal of Chemical Physics, 1990, 93, 5053-5061.	3.0	7
766	The silyl anion (SiHâ¯3): Cubic/quartic force field and anharmonic contributions to the fundamental vibrational frequencies. Journal of Chemical Physics, 1991, 94, 8112-8121.	3.0	7
767	The inversion barrier in NF+â‹…3. Journal of Chemical Physics, 1994, 100, 4459-4466.	3.0	7
768	The GeOH+â€“HGeO+ system: A detailed quantum mechanical study. Journal of Chemical Physics, 1995, 103, 7975-7982.	3.0	7
769	The GeOHâ€“HGeO system: Are the 3d electrons core or valence?. Journal of Chemical Physics, 1996, 104, 9841-9847.	3.0	7
770	Is SH4, the simplest 10-S-4 sulfurane, observable?. Physical Chemistry Chemical Physics, 2000, 2, 2239-2244.	2.8	7
771	What is the true electronic ground state of the disilaethynyl radical (SiSiH):â€Š2B1 or 2A1?. Journal of Chemical Physics, 2001, 115, 2157-2164.	3.0	7
772	Theoretical characterization of the disilaethynyl anion (Si[sub 2]H[sup â¯]). Journal of Chemical Physics, 2003, 118, 7256.	3.0	7
773	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.	3.0	7
774	Nonacarbonyldivanadium:Â Alternatives to Metalâ¯Metal Quadruple Bonding. Journal of Physical Chemistry A, 2005, 109, 11064-11072.	2.5	7

#	Article	IF	Citations
775	Dimetallocene carbonyls: The limits of the 18-electron rule and metalâ€“metal multiple bonding in highly unsaturated molecules of the early transition metals. Journal of Molecular Structure, 2008, 890, 184-191.	3.6	7
776	Binuclear fluoroborylene manganese carbonyls. Inorganica Chimica Acta, 2010, 363, 3538-3549.	2.4	7
777	Unsaturation and variable hapticity in binuclear azulene manganese carbonyl complexes. Dalton Transactions, 2010, 39, 10702.	3.3	7
778	Binuclear Nickel Carbonyl Thiocarbonyls: Metalâ^'Metal Multiple Bonds versus Four-Electron Donor Thiocarbonyl Groups. Journal of Physical Chemistry A, 2010, 114, 2365-2375.	2.5	7
779	Hydration of the Lowest Triplet States of the DNA/RNA Pyrimidines. Journal of Chemical Theory and Computation, 2010, 6, 930-939.	5.3	7
780	Structures, Energetics, and Aromaticities of the Tetrasilacyclobutadiene Dianion and Related Compounds: (Si4H4)2â€“, (Si4H4)2â€“Â·2Li+, [Si4(SiH3)4]2â€“Â·2Li+, [Si4(SiH3)4]2â€“Â·2Na+, and [Si4(SiH3)4]2â€“Â·2K+. Journal of Physical Chemistry A, 2011, 115, 5478-5487.	2.5	7
781	1-Germavinylidene (Geâ•CH₂), Germyne (HGeCH), and 2-Germavinylidene (H₂Geâ•C) Molecules and Isomerization Reactions among Them: Anharmonic Rovibrational Analyses. Journal of Physical Chemistry A, 2012, 116, 4578-4589.	2.5	7
782	Electron Attachment to Solvated dGpdG: Effects of Stacking on Baseâ€Centered and Phosphateâ€Centered Valenceâ€Bound Radical Anions. Chemistry - A European Journal, 2012, 18, 5232-5238.	3.3	7
783	Features of the potential energy surface for the SiO + OH â†' SiO2+ H reaction: relationship to oxygen isotopic partitioning during gas phase SiO2formation. RSC Advances, 2014, 4, 47163-47168.	3.6	7
784	Investigating the ground-state rotamers of n-propylperoxy radical. Journal of Chemical Physics, 2016, 145, 174301.	3.0	7
785	Chlorine peroxide (Cl₂O₂) and its isomers: structures, spectroscopy, formation and thermochemistry. Molecular Physics, 2016, 114, 1135-1147.	1.7	7
786	Prediction and Characterization of Alkalineâ€Earth (M=Be, Mg, Ca, Sr, and Ba) Metallacyclopentadienes and Relevant Derivatives. ChemistrySelect, 2017, 2, 1442-1453.	1.5	7
787	Astrophysical sulfur in diffuse and dark clouds: The fundamental vibrational frequencies and spectroscopic constants of hydrogen sulfide cation (H2S+). Monthly Notices of the Royal Astronomical Society, 2018, 480, 3483-3490.	4.4	7
788	tert-Butyl peroxy radical: ground and first excited state energetics and fundamental frequencies. Physical Chemistry Chemical Physics, 2019, 21, 9747-9758.	2.8	7
789	Ï€-Hydrogen Bonding Probes the Reactivity of Aromatic Compounds: Nitration of Substituted Benzenes. Journal of Physical Chemistry A, 2019, 123, 1069-1076.	2.5	7
790	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C₃H₂): the importance of numerical stability. Molecular Physics, 2020, 118, e1589007.	1.7	7
791	Conclusive determination of ethynyl radical hydrogen abstraction energetics and kinetics*. Molecular Physics, 2020, 118, e1769214.	1.7	7
792	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. Journal of Computational Chemistry, 2001, 22, 1574-1589.	3.3	7

#	Article	IF	Citations
793	Theoretical methods and their application to ketenes and allenes. , 0, , 1-44.		6
794	Analytic energy third derivatives for pairedâ€excited multiconfiguration selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1989, 90, 334-345.	3.0	6
795	The electronic spectrum of NS2: Lowâ€lying quartet states. Journal of Chemical Physics, 1991, 94, 1277-1287.	3.0	6
796	The fundamental vibrational frequencies of the silyl anion (SiH-3). Molecular Physics, 1992, 76, 467-474.	1.7	6
797	The remarkable enneahydridorhenate dianion: ReH2-9. Molecular Physics, 1992, 76, 995-1007.	1.7	6
798	Is F3+ viable? A high-level ab initio comparison of F3+ and Cl3+. Journal of Chemical Physics, 1998, 109, 1772-1780.	3.0	6
799	Structure and reactivity of the vinylcyclopropane radical cation. Journal of Molecular Structure, 2001, 599, 95-116.	3.6	6
800	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	3.0	6
801	Novel bromine oxyfluorides: structures, thermochemistry and electron affinities of BrOFn/BrO (nâ€‰=â€‰1â€“5). Molecular Physics, 2005, 103, 1995-2008.	1.7	6
802	Octacarbonyldivanadium: a highly unsaturated binuclear metal carbonyl. Molecular Physics, 2006, 104, 763-775.	1.7	6
803	Coupled cluster investigation on the low-lying electronic states of CuCN and CuNC and the ground state barrier to isomerization. Journal of Chemical Physics, 2007, 127, 154324.	3.0	6
804	Formal chromiumâ€“chromium triple bonds and bent rings in the binuclear cycloheptatrienylchromium carbonyls (C7H7)2Cr2(CO)n (n=6,5,4,3,2,1,0): A density functional theory study. Journal of Organometallic Chemistry, 2008, 693, 3201-3212.	1.8	6
805	Local Hybrid Divide-and-Conquer Method for the Computation of Medium and Large Molecules. Journal of Chemical Theory and Computation, 2008, 4, 2049-2056.	5.3	6
806	The highly unsaturated dimetal hexacarbonyls of manganese and rhenium: Alternatives to a formal metalâ€“metal quintuple bond. International Journal of Quantum Chemistry, 2009, 109, 3082-3092.	2.0	6
807	Binuclear Cyclopentadienylmanganese Carbonyl Thiocarbonyls: Four-Electron Donor Bridging Thiocarbonyl Groups of Two Types and a Bridging Acetylenedithiolate Ligand. European Journal of Inorganic Chemistry, 2010, 2010, 4175-4186.	2.0	6
808	Neutral homoleptic tetranuclear iron carbonyls: why havenâ€™t they been synthesized as stable molecules?. New Journal of Chemistry, 2010, 34, 208-214.	2.8	6
809	Fe3(BF)3(CO)8 structures with face-semibridging fluoroborylene ligands and a bicapped tetrahedral Fe3B3 cluster isoelectronic with Os6(CO)18. New Journal of Chemistry, 2010, 34, 2813.	2.8	6
810	Binuclear methylaminobis(difluorophosphine) iron carbonyls: phosphorusâ€“nitrogen bond cleavage in preference to ironâ€“iron multiple bond formation. New Journal of Chemistry, 2013, 37, 3294.	2.8	6

#	Article	IF	Citations
811	Tetragermacyclobutadiene: Energetically Disfavored with Respect to Its Structural Isomers. Chemistry - A European Journal, 2013, 19, 7487-7495.	3.3	6
812	Modeling intermediates in carbon monoxide coupling reactions using cyclooctatetraene thorium derivatives. New Journal of Chemistry, 2014, 38, 6031-6040.	2.8	6
813	The reactions of Cr(CO)₆, Fe(CO)₅, and Ni(CO)₄ with O₂ yield viable oxoâ€•metal carbonyls. Journal of Computational Chemistry, 2014, 35, 998-1009.	3.3	6
814	Surprising Quenching of the Spinâ€“Orbit Interaction Significantly Diminishes H₂OÂ·Â·Â·X [X = F, Cl, Br, I] Dissociation Energies. Journal of Physical Chemistry A, 2014, 118, 11956-11961.	2.5	6
815	Structures, Bonding, and Energetics of Potential Triatomic Circumstellar Molecules Containing Group 15 and 16 Elements. Journal of Physical Chemistry A, 2015, 119, 11693-11700.	2.5	6
816	Bis(azulene) â€œsubmarineâ€•metal dimer sandwich compounds (C₁₀H₈)₂M₂ (Mâ€‰=â€‰Ti, V, Cr, Mn, Fe, Co, Ni): Parallel and opposed orientations. Journal of Computational Chemistry, 2016, 37, 250-260.	3.3	6
817	Ligand conformations and spin states in open metallocenes of the first row transition metals having U-shaped 2,4-dimethylpentadienyl ligands. New Journal of Chemistry, 2016, 40, 8511-8521.	2.8	6
818	From gas-phase to liquid water chemical reactions: The F + (H2O) , n= 1â€“4 systems. Chemical Physics Letters, 2016, 648, 1-7.	2.6	6
819	Thioformaldehyde S-Sulfide, Sulfur Analogue of the Criegee Intermediate: Structures, Energetics, and Rovibrational Analysis. Journal of Physical Chemistry A, 2017, 121, 998-1006.	2.5	6
820	Radicals derived from acetaldehyde and vinyl alcohol. Physical Chemistry Chemical Physics, 2017, 19, 27275-27287.	2.8	6
821	Hyperconjugative effects in ï€â€hydrogen bonding: Theory and experiment. Journal of Computational Chemistry, 2018, 39, 527-534.	3.3	6
822	Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues. ChemPhysChem, 2018, 19, 3257-3265.	2.1	6
823	Stable Boron Dithiolene Radicals. Angewandte Chemie, 2018, 130, 7991-7994.	2.0	6
824	Unusual Î·¹â€Coordinated Alkyne and Alkene Complexes. Chemistry - A European Journal, 2019, 25, 15628-15633.	3.3	6
825	Binding modes of cabazitaxel with the different human Î²-tubulin isotypes: DFT and MD studies. Journal of Molecular Modeling, 2020, 26, 162.	1.8	6
826	Substituted Ortho-Benzynes: Properties of the Triple Bond. Journal of Organic Chemistry, 2020, 85, 9905-9914.	3.2	6
827	Catalyzed reaction of isocyanates (RNCO) with water. Physical Chemistry Chemical Physics, 2021, 23, 18535-18546.	2.8	6
828	Carbonylic-Carbon-Centered Mechanism for Catalytic Î±-Methylation. Organometallics, 2021, 40, 2420-2429.	2.3	6

#	Article	IF	Citations
829	Carbeneâ€Stabilized Dithiolene (L⁰) Zwitterions. Angewandte Chemie - International Edition, 2021, 60, 22706-22710.	13.8	6
830	The reaction of methane with molecular oxygen: A semiquantitative estimate of the activation energy. Journal of Chemical Physics, 1989, 90, 6391-6394.	3.0	5
831	Coupled-cluster vibrational frequencies for open, ring and superoxide sulfur dioxide. Theoretical Chemistry Accounts, 1997, 96, 7-10.	1.4	5
832	What to do about unpaired electrons? A hydrocarbon hexaradical with three Closs diradicals linked by 1,3,5-trimethylbenzene as ferromagnetic coupler. Journal of Chemical Physics, 2002, 117, 7147-7152.	3.0	5
833	Structures and electron affinities of the di-arsenic fluorides As2Fn/As2Fâ€‰nâˆ’ (n= 1-8). Journal of Computational Chemistry, 2005, 26, 411-435.	3.3	5
834	The lowest triplet electronic states of polyacenes and perfluoropolyacenes. Molecular Physics, 2007, 105, 2743-2752.	1.7	5
835	Unexpected Direct Ironâ€Fluorine Bonds in Trifluorophosphane Iron Complexes: An Alternative to Bridging Trifluorophosphane and Difluorophosphido Groups. Chemistry - A European Journal, 2008, 14, 11149-11157.	3.3	5
836	Binuclear Cyclopentadienylmolybdenum Carbonyl Derivatives: Where is the Missing Moâ•Mo Double-Bonded Species Cp₂Mo₂(CO)₅?. Organometallics, 2009, 28, 2818-2829.	2.3	5
837	Dimerization of a fluorocarbyne complex to a tetrahedrane derivative: Fluorocarbyne and difluoroacetylene cobalt carbonyl complexes. Dalton Transactions, 2010, 39, 5242.	3.3	5
838	The quest for trifluorophosphine as a bridging ligand in homoleptic binuclear and tetranuclear cobalt complexes. Molecular Physics, 2010, 108, 2477-2489.	1.7	5
839	The Remarkable Nb2(CO)12with Seven-Coordinate Niobium: Decarbonylation to Nb2(CO)11and Nb2(CO)10. Journal of Chemical Theory and Computation, 2011, 7, 2112-2125.	5.3	5
840	Spin-Restriction in Explicitly Correlated Coupled Cluster Theory: The Z-Averaged CCSD(2)_{<ovl>R12</ovl>} Approach. Journal of Chemical Theory and Computation, 2011, 7, 2416-2426.	5.3	5
841	Binuclear Cyclopentadienylmetal Cyclooctatetraene Derivatives of the First Row Transition Metals: Effects of Ring Conformation on the Bonding of an Eight-Membered Carbocyclic Ring to a Pair of Metal Atoms. Journal of Physical Chemistry A, 2011, 115, 3133-3143.	2.5	5
842	Anharmonic vibrational analyses for the 1-silacyclopropenylidene molecule and its three isomers. Molecular Physics, 2012, 110, 783-800.	1.7	5
843	Characterization of the t-Butyl Radical and Its Elusive Anion. Journal of Chemical Theory and Computation, 2012, 8, 4323-4329.	5.3	5
844	The Beryllium Pentamer: Trailing an Uneven Sequence of Dissociation Energies. ChemPhysChem, 2012, 13, 1255-1260.	2.1	5
845	Binuclear dimethylaminoborole iron carbonyls: ironâ€“iron multiple bonding versus nitrogenÂâ†'Âiron dative bonding. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
846	The cis- and trans-formylperoxy radical: fundamental vibrational frequencies and relative energies of the XÌƒ 2Aâ€²â€² and Ãƒ 2Aâ€² states. RSC Advances, 2015, 5, 107254-107265.	3.6	5

#	Article	IF	Citations
847	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. Molecular Physics, 2017, 115, 2065-2076.	1.7	5
848	The Structure and Clâ€“O Dissociation Energy of the ClOO Radical: Finally, the Right Answers for the Right Reason. Journal of Physical Chemistry A, 2018, 122, 2604-2610.	2.5	5
849	Butadiene as a ligand in open sandwich compounds. Physical Chemistry Chemical Physics, 2018, 20, 5683-5691.	2.8	5
850	Reinterpreting the infrared spectrum of H + HCN: Methylene amidogen radical and its coproducts. Journal of Chemical Physics, 2018, 148, 014305.	3.0	5
851	The non-covalently bound SOâ‹¯H₂O system, including an interpretation of the differences between SOâ‹¯H₂O and O₂â‹¯H₂O. Physical Chemistry Chemical Physics, 2018, 20, 28840-28847.	2.8	5
852	Energetics and mechanisms for the acetonyl radical + O2 reaction: An important system for atmospheric and combustion chemistry. Journal of Chemical Physics, 2020, 152, 114301.	3.0	5
853	Four isomers of In ₂ H ₂ : a careful comparison between theory and experiment. Molecular Physics, 2021, 119, .	1.7	5
854	Kinetic Stability of Pentazole. Journal of Physical Chemistry A, 2021, 125, 9092-9098.	2.5	5
855	The search for the lowâ€lying states of the silicon carbide cluster cation Si2C+2. Journal of Chemical Physics, 1995, 103, 7025-7029.	3.0	4
856	Comparison between molecular geometry and harmonic vibrational frequency predictions from CISD[TQ] and CISDTQ wave functions for hydrogen sulfide. Journal of Chemical Physics, 1997, 107, 10616-10619.	3.0	4
857	The XÌƒ1A1,Ã£3B1and Ãƒ1B1Electronic States of the Aluminum Dihydride Anion. Journal of Physical Chemistry A, 1999, 103, 1886-1893.	2.5	4
858	Dimethyldioxirane, Carbonyl Oxide, and the Transition State Connecting Them:Â Electronic Structures, Relative Energies, and Vibrational Frequencies. Journal of Physical Chemistry A, 2000, 104, 7892-7897.	2.5	4
859	The treacherous potential energy hypersurface of AgSiO. Journal of Chemical Physics, 2003, 118, 10623-10630.	3.0	4
860	Assessing Alkyl-, Silyl-, and Halo-Substituent Effects on the Electron Affinities of Silyl Radicals. Journal of Physical Chemistry A, 2005, 109, 10100-10105.	2.5	4
861	Comparison of Isoelectronic Heterometallic and Homometallic Binuclear Cyclopentadienylmetal Carbonyls: The Ironâ€“Nickel vs. the Dicobalt Systems. European Journal of Inorganic Chemistry, 2008, 2008, 1219-1225.	2.0	4
862	Toward the observation of quartet states of the ozone radical cation: Insights from coupled cluster theory. Journal of Chemical Physics, 2008, 128, 214302.	3.0	4
863	The ten chemically transparent dinitronaphthalene isomers and their radical anions. Molecular Physics, 2010, 108, 2491-2509.	1.7	4
864	Anharmonic Vibrational Analysis for the Propadienylidene Molecule (H2Câ•Câ•C:). Journal of Chemical Theory and Computation, 2010, 6, 3122-3130.	5.3	4

#	Article	IF	Citations
865	Terminal versus bridging cyclobutadiene rings in binuclear nickel carbonyl derivatives: A cube-antiprism twist of the cyclobutadiene rings in the perpendicular structures. New Journal of Chemistry, 2010, 34, 1885.	2.8	4
866	Unsaturation in homoleptic tetranuclear iridium carbonyls: a comparison of density functional theory with the MP2 method in metal cluster structures. Theoretical Chemistry Accounts, 2011, 130, 393-400.	1.4	4
867	Structural and electronic property responses to the arsenic/phosphorus exchange in GCâ€related DNA of the Bâ€form. Journal of Computational Chemistry, 2012, 33, 817-821.	3.3	4
868	New Structural Features in Tetranuclear Iron Carbonyl Thiocarbonyls: Exotriangular Iron Atoms and Sixâ€Electronâ€Donating Thiocarbonyl Groups Bridging Four Iron Atoms. European Journal of Inorganic Chemistry, 2012, 2012, 1104-1113.	2.0	4
869	Moving on from F+H₂: The More Challenging Reaction between Atomic Fluorine and Methylamine. ChemPhysChem, 2013, 14, 896-899.	2.1	4
870	How Small Can a Catenane Be?. Journal of Chemical Theory and Computation, 2014, 10, 1511-1517.	5.3	4
871	Binuclear iron carbonyl complexes of thialene. RSC Advances, 2016, 6, 82661-82668.	3.6	4
872	Toward unsaturated stannylenes Y₂Zî€Sn: and related compounds with triplet electronic ground states. RSC Advances, 2016, 6, 53749-53759.	3.6	4
873	Ïƒ Bond activation through tunneling: formation of the boron hydride cations BH_n⁺ (n = 2, 4, 6). Physical Chemistry Chemical Physics, 2016, 18, 4063-4070.	2.8	4
874	Ethylperoxy radical: approaching spectroscopic accuracy via coupled-cluster theory. Physical Chemistry Chemical Physics, 2017, 19, 15715-15723.	2.8	4
875	Phosgene at the complete basis set limit of CCSDT(Q): Molecular structure and rovibrational analysis. Chemical Physics Letters, 2017, 683, 12-17.	2.6	4
876	Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. Journal of Physical Chemistry A, 2018, 122, 9498-9511.	2.5	4
877	Tris(butadiene) Metal Complexes of the First-Row Transition Metals versus Coupling of Butadiene to Eight- and Twelve-Carbon Hydrocarbon Chains. Journal of Physical Chemistry A, 2019, 123, 5542-5554.	2.5	4
878	Convergent energies and anharmonic vibrational spectra of Ca₂H₂ and Ca₂H₄ constitutional isomers. Physical Chemistry Chemical Physics, 2019, 21, 10914-10922.	2.8	4
879	Labile Imidazolium Cyclopentadienides. Organometallics, 2019, 38, 4578-4584.	2.3	4
880	The reaction of alkyl hydropersulfides (RSSH, R = CH₃ and ^tBu) with H₂S in the gas phase and in aqueous solution. Physical Chemistry Chemical Physics, 2019, 21, 537-545.	2.8	4
881	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie, 2020, 132, 8949-8952.	2.0	4
882	Heteroatom (N, P, As, Sb, Bi) Effects on the Resonance-Stabilized 2-, 3-, and 4-Picolyl Radicals. Inorganic Chemistry, 2021, 60, 5860-5867.	4.0	4

#	Article	IF	Citations
883	Lanternâ€Type Divanadium Complexes with Bridging Ligands: Short Metalâ€Metal Bonds with High Multiple Bond Orders. ChemPhysChem, 2021, 22, 2014-2024.	2.1	4
884	Group 15 and 16 Nitreneâ€Like Pnictinidenes. Chemistry - A European Journal, 2021, 27, 14461-14471.	3.3	4
885	Energetics and kinetics of various cyano radical hydrogen abstractions. Physical Chemistry Chemical Physics, 2021, 23, 3389-3400.	2.8	4
886	Binuclear Cobalt Paddlewheel-Type Complexes: Relating Metalâ€“Metal Bond Lengths to Formal Bond Orders. Inorganic Chemistry, 2021, 60, 584-596.	4.0	4
887	ClF2: Structure and infrared spectra of a weakly bound triatomic molecule. Journal of Chemical Physics, 1993, 98, 8051-8056.	3.0	3
888	Silacyanogen. Journal of Chemical Physics, 1997, 107, 5776-5779.	3.0	3
889	An analysis of the conformers of 1,5-hexadiene. Molecular Physics, 2002, 100, 441-446.	1.7	3
890	Does GaH5 exist?. Journal of Chemical Physics, 2005, 123, 204303.	3.0	3
891	High electron affinities of bicyclo[n,n, 0]perfluoroalkanes. Molecular Physics, 2006, 104, 1311-1324.	1.7	3
892	(Cyclopentadienyl)nitrosylmanganese Compounds: The Original Molecules Containing Bridging Nitrosyl Groups. European Journal of Inorganic Chemistry, 2009, 2009, 3982-3992.	2.0	3
893	From two-electron via four-electron to six-electron donor carbonyl groups in trinuclear derivatives of the oxophilic metal niobium. Dalton Transactions, 2009, , 3748.	3.3	3
894	From acetylene complexes to vinylidene structures: The GeC₂H₂ system. Journal of Computational Chemistry, 2011, 32, 15-22.	3.3	3
895	Protonated Digermane, Distannane, and Diplumbane: Can They Be Made in the Laboratory?. European Journal of Inorganic Chemistry, 2014, 2014, 5015-5020.	2.0	3
896	The LiÂ·Â·Â·HF van der Waals minimum and the barrier to the deep HFâ€“Li potential well. Molecular Physics, 2014, 112, 770-773.	1.7	3
897	From spiropentane to butterfly and tetrahedral structures in tetranuclear iron carbonyl carbide chemistry. New Journal of Chemistry, 2014, 38, 3762-3769.	2.8	3
898	Novel germanetellones: XYGeî€Te (X, Y = H, F, Cl, Br, I and CN) â€“ structures and energetics. Comparison with the first synthetic successes. Dalton Transactions, 2014, 43, 4151.	3.3	3
899	Streptococcal Hyaluronate Lyase Reveals the Presence of a Structurally Significant Cï£¿Hâ‹…â‹…â‹…O Hydrogen Bond. Chemistry - A European Journal, 2014, 20, 990-998.	3.3	3
900	Triple decker sandwiches and related compounds of the first row transition metals with cyclopentadienyl and hexafluorobenzene rings: remarkable effects of fluorine substitution. Physical Chemistry Chemical Physics, 2015, 17, 20100-20113.	2.8	3

#	Article	IF	Citations
901	Catenanes: A molecular mechanics analysis of the (C₁₃H₂₆)₂ Structure 13â€13 D2. Journal of Computational Chemistry, 2016, 37, 124-129.	3.3	3
902	I + (H₂O)₂ â†' HI + (H₂O)OH Forward and Reverse Reactions. CCSD(T) Studies Including Spinâ€"Orbit Coupling. Journal of Physical Chemistry B, 2016, 120, 1743-1748.	2.6	3
903	The Reaction between Bromine and the Water Dimer and the Highly Exothermic Reverse Reaction. Journal of Computational Chemistry, 2016, 37, 177-182.	3.3	3
904	The water dimer reaction OH + (H2O)2 â†' (H2O)â€"OH + H2O. Physical Chemistry Chemical Physics, 2017, 19, 18279-18287.	2.8	3
905	Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: Hâ€"HÂ·Â·Fâ€"M (M = Li,) Tj ETQq1 1 0.784314 rgBT Computation, 2018, 14, 5118-5127.	5.3	3
906	Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners. Inorganic Chemistry, 2018, 57, 7851-7859.	4.0	3
907	Prototypical Transition-Metal Carbenes. (CO)₅Cr•CH₂, (CO)₄Feâ•CH₂, (CO)₃Niâ•CH₂, (CO)₅Moâ•CH₂, (CO)₄Ruâ•CH₂, (CO)₃Pdâ•CH₂, (CO)₅Wâ•CH₂, (CO)₄Osâ•CH₂, and (CO)₃Ptâ•CH₂: Challenge to Experiment. Journal of Physical Chemistry A, 2018, 122, 6570-6577.	2.5	3
908	Student-Friendly Guide to Molecular Integrals. Journal of Chemical Education, 2018, 95, 1572-1578.	2.3	3
909	The bismuth tetramer Bi4: the Î½3 key to experimental observation. Physical Chemistry Chemical Physics, 2018, 20, 21881-21889.	2.8	3
910	A remarkable case of basis set dependence: the false convergence patterns of the methyl anion. Molecular Physics, 2019, 117, 1069-1077.	1.7	3
911	Cyclobutyne: Minimum or Transition State?. Journal of Organic Chemistry, 2019, 84, 5548-5553.	3.2	3
912	Important features of the potential energy surface of the methylamine plus O(¹D) reaction. Physical Chemistry Chemical Physics, 2019, 21, 24194-24205.	2.8	3
913	Relatives of cyanomethylene: replacement of the divalent carbon by B^{â^'}, N⁺, Al^{â^'}, Si, P⁺, Ga^{â^'}, Ge, and As⁺. Physical Chemistry Chemical Physics, 2019, 21, 26438-26452.	2.8	3
914	Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides Be₂H₂, Mg₂H₂, Ca₂H₂, Sr₂H₂, and Ba₂H₂. Proposals for Observations. Inorganic Chemistry, 2020, 59, 10404-10408.	4.0	3
915	Carbene-mediated synthesis of a germanium tris(dithiolene)dianion. Chemical Communications, 2021, 57, 2543-2546.	4.1	3
916	Hydrogen bonding as a probe of electron density Variations: Substituted pyridines. Chemical Physics Letters, 2022, 791, 139378.	2.6	3
917	The synchronous thermal decomposition mechanism of azoisopropane. Molecular Physics, 1995, 85, 769-779.	1.7	2
918	The disilaketenyl radical (HSiSiO) in its ground and first excited electronic states. Journal of Chemical Physics, 1999, 111, 227-234.	3.0	2

#	Article	IF	Citations
919	The molecular structure and infrared and Raman spectra of SCCCS. Computational and Theoretical Chemistry, 1999, 460, 117-121.	1.5	2
920	THE EXOTHERMIC PNC â†' PCN REACTION. Journal of Theoretical and Computational Chemistry, 2006, 05, 281-297.	1.8	2
921	Vibrational energy levels for the electronic ground state of the diazocarbene (CNN) molecule. Molecular Physics, 2008, 106, 357-365.	1.7	2
922	Inhibition of Alkyne Cyclotrimerization to Arenes on a Metal Site by Fourâ€Electron Donation through Simultaneous Sigma and Pi Bonding: The Tris(alkyne)Tungsten Carbonyls. European Journal of Inorganic Chemistry, 2009, 2009, 5439-5448.	2.0	2
923	Quantum Mechanical Modeling for the GeX2/GeHX + GeH4 Reactions (X = H, F, Cl, and Br). Journal of Physical Chemistry A, 2010, 114, 4210-4223.	2.5	2
924	Edgeâ€Bridging and Faceâ€Bridging Hydrogen Atoms in Trinuclear Rhenium Carbonyl Hydrides. European Journal of Inorganic Chemistry, 2011, 2011, 4626-4636.	2.0	2
925	Arbitrary order El'yashevichâ€"WilsonBtensor formulas for the most frequently used internal coordinates in molecular vibrational analyses. Journal of Chemical Physics, 2012, 137, 164103.	3.0	2
926	Dicyanogermylenes: A Tale of Isomers and Interconversions. Inorganic Chemistry, 2012, 51, 12152-12164.	4.0	2
927	Metal triangles versus metal chains and terminal versus bridging hydrogen atoms in trinuclear osmium carbonyl hydride chemistry. New Journal of Chemistry, 2014, 38, 1433-1440.	2.8	2
928	Conical Intersections and Lowâ€Lying Electronic States of Tetrafluoroethylene. ChemPhysChem, 2014, 15, 2359-2366.	2.1	2
929	The Energy Difference between the Triply-Bridged and All-Terminal Structures of Co₄(CO)₁₂, Rh₄(CO)₁₂, and Ir₄(CO)₁₂: A Difficult Test for Conventional Density Functional Methods. Journal of Chemical Theory and Computation, 2015, 11, 940-949.	5.3	2
930	New Titanium Carbonyls: Ti2(CO)10, Ti2(CO)11, and Ti2(CO)12. Journal of Physical Chemistry A, 2015, 119, 5224-5232.	2.5	2
931	Binuclear cyclopentadienylrhenium hydride chemistry: terminal versus bridging hydride and cyclopentadienyl ligands. Journal of Molecular Modeling, 2015, 21, 7.	1.8	2
932	Theoretical studies on the desulfurization of benzothiophene (thianaphthene) and thienothiophene (thiophthene) by carbonâ€"sulfur bond cleavage: binuclear iron carbonyl intermediates. New Journal of Chemistry, 2015, 39, 7040-7045.	2.8	2
933	1,1â€Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure. ChemPhysChem, 2016, 17, 1623-1629.	2.1	2
934	Characterizing a nonclassical carbene with coupled cluster methods: cyclobutylidene. Physical Chemistry Chemical Physics, 2016, 18, 24560-24568.	2.8	2
935	Pathways for the OH + Br2 â†' HOBr + Br and HOBr + Br â†' HBr + BrO Reactions. Journal of Physical Chemistry A, 2016, 120, 805-816.	2.5	2
936	Positional selectivity in the interaction of toluene with nitronium ion. Molecular Physics, 2017, 115, 2782-2788.	1.7	2

#	Article	IF	Citations
937	Binuclear Cyclopentadienylmetal Methylene Sulfur Dioxide Complexes of Rhodium and Iridium Related to a Photochromic Metal Dithionite Complex. Inorganic Chemistry, 2017, 56, 14486-14493.	4.0	2
938	1,3,2-Diazaborole-derived carbene complexes of boron. Dalton Transactions, 2018, 47, 41-44.	3.3	2
939	Ï€â€Hydrogen Bonding Probes Chemical Reactivity: Bromination of a CC Double Bond and Electrophilic Aromatic Benzylation. ChemistrySelect, 2019, 4, 10934-10942.	1.5	2
940	Alternative modes of bonding of C4F8 units in mononuclear and binuclear iron carbonyl complexes. New Journal of Chemistry, 2019, 43, 6932-6942.	2.8	2
941	The conformational preferences of polychlorocyclohexanes. New Journal of Chemistry, 2019, 43, 18546-18558.	2.8	2
942	Stabilizing Borinium Cations [Xâ€“Bâ€“X]⁺ through Conjugation and Hyperconjugation Effects. Inorganic Chemistry, 2019, 58, 243-249.	4.0	2
943	Hydrogen Abstraction Reaction H2Se + OH â†' H2O + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. Inorganic Chemistry, 2019, 58, 2069-2079.	4.0	2
944	Comparative Study of the Thermal Stabilities of the Experimentally Known High-Valent Fe(IV) Compounds Fe(1-norbornyl)4 and Fe(cyclohexyl)4. Journal of Physical Chemistry A, 2020, 124, 6867-6876.	2.5	2
945	Assessing the orbital-optimized unitary Ansatz for density cumulant theory. Journal of Chemical Physics, 2020, 153, 244102.	3.0	2
946	C5 Metalation of Imidazole-Based Monothiolates en Route to Selenothiolates. Organometallics, 2020, 39, 4178-4182.	2.3	2
947	Unusual Structures of the Parent Molecules Diarsene, Distibene, and Dibismuthene: Toward Their Observation. Chemistry - A European Journal, 2020, 26, 14159-14166.	3.3	2
948	Perfluoroolefin complexes versus perfluorometallacycles and perfluorocarbene complexes in cyclopentadienylcobalt chemistry. Physical Chemistry Chemical Physics, 2020, 22, 7616-7624.	2.8	2
949	The water trimer reaction OH + (H₂O)₃ â†' (H₂O)₂OH + H₂O. Physical Chemistry Chemical Physics, 2020, 22, 9767-9774.	2.8	2
950	Fluorine Migration from Carbon to Iron and Fluorineâ€“Iron Dative Bonds in Octafluorocyclohexadiene Iron Carbonyl Chemistry. Organometallics, 2021, 40, 397-407.	2.3	2
951	Highly Strained Pn(CH)3 (Pn = N, P, As, Sb, Bi) Tetrahedranes: Theoretical Characterization. Journal of Physical Chemistry A, 2021, 125, 2612-2621.	2.5	2
952	Synthesis of Methanesulfonic Acid Directly from Methane: The Cation Mechanism or the Radical Mechanism?. Journal of Physical Chemistry Letters, 2021, 12, 6486-6491.	4.6	2
953	Excited electronic states of carbon disulphide. Molecular Physics, 1999, 96, 693-704.	1.7	2
954	Potential energy profile for the Cl + (H2O)3 â†' HCl + (H2O)2OH reaction. A CCSD(T) study. Physical Chemistry Chemical Physics, 2021, 23, 26837-26842.	2.8	2

#	Article	IF	Citations
955	Mini-Review on Structureâ€“Reactivity Relationship for Aromatic Molecules: Recent Advances. ACS Omega, 2022, 7, 8199-8208.	3.5	2
956	John A. Pople - Computational Chemistry Pioneer. Israel Journal of Chemistry, 1993, 33, 240-242.	2.3	1
957	John A. Pople â€" Computational Chemistry Pioneer. Israel Journal of Chemistry, 1993, 33, 354-356.	2.3	1
958	First and second energy derivative analyses for open-shell self-consistent field wavefunctions. Molecular Physics, 1994, 82, 713-733.	1.7	1
959	Structurally-Rich Potential Energy Surface of the Alagallylyne (AlGaH2) Molecule. The Journal of Physical Chemistry, 1996, 100, 7372-7379.	2.9	1
960	The 1-silaketenyl radical (HSiCO): Ground and first excited electronic states. Journal of Chemical Physics, 2000, 112, 2168-2175.	3.0	1
961	Triplet states of carbenium and silylium cations. Chemical Physics Letters, 2001, 337, 158-168.	2.6	1
962	CHARACTERIZATION OF THE $ilde{X},^2 Pi$ AND Ãƒ2Î£+ ELECTRONIC STATES OF THE PHOSPHAETHYNE CATION (HCP+). Journal of Theoretical and Computational Chemistry, 2005, 04, 707-724.	1.8	1
963	The Perfluoroadamantyl Radicals C10F15and Their Anions. Journal of Chemical Theory and Computation, 2005, 1, 279-285.	5.3	1
964	Elementary constituents of microdevices: The Ge2H fragment. Journal of Chemical Physics, 2006, 125, 164317.	3.0	1
965	Characterization of the XÌƒA12, AÌƒB12, and XÌƒÎ2 electronic states of the Ga2H molecule and the XÌƒAâ€²2 and AÌƒAâ€³2 isomerization transition states connecting the three minima. Journal of Chemical Physics, 2006, 124, 044309.	3.0	1
966	Elementary Energetic Effects of Radiation Damage to DNA and RNA Subunits. AIP Conference Proceedings, 2007, , .	0.4	1
967	Characterization of the BNNO Radical. Journal of Chemical Theory and Computation, 2010, 6, 1915-1923.	5.3	1
968	¹³C NMR relaxation and computational study of anisole and derivatives in the solution state. Journal of Physical Organic Chemistry, 2012, 25, 1374-1379.	1.9	1
969	Theoretical investigation of the cyclopropene radical cation c-C₃H^{+â€¢}₄: structure, energetics and spectroscopic properties^{â€}. Molecular Physics, 2013, 111, 2306-2313.	1.7	1
970	Molecular orbital interpretation of the metalâ€“metal multiple bonding in coaxial dibenzene dimetal compounds of iron, manganese, and chromium. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	1
971	Major differences between trifluorophosphine and carbonyl ligands in binuclear cyclopentadienyliron complexes. New Journal of Chemistry, 2015, 39, 3708-3718.	2.8	1
972	Nickelacyclopentadienylchromium Tricarbonyl Unit as a Bulky Pseudohalogen in Cyclopentadienylchromium Complexes Leading to Low-Energy High-Spin Structures. Inorganic Chemistry, 2015, 54, 5309-5315.	4.0	1

#	Article	IF	Citations
973	Reductive coupling of carbon monoxide to glycolaldehyde and hydroxypyruvaldehyde polyanions in binuclear cyclopentadienyl lanthanum and lutetium derivatives: analogies to cyclooctatetraene thorium chemistry. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	1
974	Intermolecular interactions and proton transfer in the hydrogen halideâ€“superoxide anion complexes. Physical Chemistry Chemical Physics, 2016, 18, 6201-6208.	2.8	1
975	Structures of dimetallocenes M₂(C₅H₅)₂ (M = Zn, Cu,) Tj ETQq1 1 0.784314 rgBT	2.8	1
976	Enhanced Relative Stability of Metallabenzenes versus Metallocenes upon Ring Perfluorination: Nickel, Palladium, and Platinum Systems. European Journal of Inorganic Chemistry, 2017, 2017, 4714-4721.	2.0	1
977	Carbonâ€“Hydrogen Activation in Zerovalent Bis(1,5-cyclooctadiene) Complexes of the First Row Transition Metals: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 3280-3286.	2.5	1
978	Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (H2CN). Journal of Chemical Physics, 2018, 149, 094302.	3.0	1
979	Higher spin states in some low-energy bis(tetramethyl-1,2-diaza-3,5-diborolyl) sandwich compounds of the first row transition metals: boraza analogues of the metallocenes. New Journal of Chemistry, 2019, 43, 4497-4505.	2.8	1
980	The Nature of Lithium Bonding in C₂H₂Li₂, C₆Li₆, and Lithium Halide Dimers. Organometallics, 2019, 38, 4708-4716.	2.3	1
981	Assessing the Viability of the Methylsulfinyl Radicalâ€Ozone Reaction. ChemPhysChem, 2020, 21, 1289-1294.	2.1	1
982	A Reflection on Norman Louis Allinger. Journal of Chemical Theory and Computation, 2021, 17, 2013-2013.	5.3	1
983	Subtle basis set effects on hydrogen bonded systems. Molecular Physics, 1999, 96, 493-504.	1.7	1
984	Substituent Effects on Aluminyl Anions and Derived Systems: A High-Level Theory. Journal of Physical Chemistry A, 2021, 125, 10379-10391.	2.5	1
985	An Undergraduate Chemistry Lab Exploring Computational Cost and Accuracy: Methane Combustion Energy. Journal of Chemical Education, 2022, 99, 1479-1487.	2.3	1
986	Lanternâ€type dinickel complexes: An exploration of possibilities for nickelâ€“nickel bonding with bridging bidentate ligands. Journal of Computational Chemistry, 0, , .	3.3	1
987	Phosphine-Mediated Cleavage of Sulfurâ€“Sulfur Bonds. Organometallics, 2022, 41, 3099-3103.	2.3	1
988	John A. Pople Special Issue. Molecular Physics, 1996, 88, 1425-1425.	1.7	0
989	John A. Pople Special Issue. Molecular Physics, 1996, 88, 1155-1155.	1.7	0
990	Characterization of the [Xtilde] 1Î£+Ãƒ3Î and Ãƒ1Î electronic states of BBO. Molecular Physics, 2003, 101, 1273-1283.	1.7	0

#	Article	IF	Citations
991	Generalization of the direct configuration interaction method to the hartree-fock interacting space for doublets, quartets, and open-shell singlets. International Journal of Quantum Chemistry, 2009, 16, 471-471.	2.0	0
992	The interplay between metalâ€“metal bonds, fourâ€electron donor carbonyl groups, and fiveâ€electron donor nitrosyl groups in highly unsaturated binuclear rhenium carbonyl nitrosyls. International Journal of Quantum Chemistry, 2009, 109, 2273-2285.	2.0	0
993	Copper formal oxidation states above +1 in organometallic chemistry: the possibility of synthesizing cyclopentadienylcopper chlorides by oxidative addition reactions. Theoretical Chemistry Accounts, 2011, 128, 367-376.	1.4	0
994	Some â€œremarkably stableâ€•chalcogen(ii) dications, including comparisons with their structurally distinct monocations and neutrals. New Journal of Chemistry, 2012, 36, 2000.	2.8	0
995	Introduction to proceedings of Molecular Quantum Mechanics 2013: electron correlation: theÂmany-body problem at the heart of chemistry. Molecular Physics, 2014, 112, 557-558.	1.7	0
996	Prototypical metalâ€“oxo bonds: the reactions of Cr(PF3)6, Fe(PF3)5, and Ni(PF3)4 with oxygen. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	0
997	Effect of metal complexation on the equilibrium between methylphosphepine and methylphosphanorcaradiene and their benzo analogues. New Journal of Chemistry, 2016, 40, 7804-7813.	2.8	0
998	Metalâ€“metal bonding in biscycloheptatrienyl dimetal compounds of the secondâ€row transition metals. International Journal of Quantum Chemistry, 2017, 117, e25374.	2.0	0
999	Unsaturation in binuclear iron carbonyl complexes of the split (3 + 2) fiveâ€electron donor hydrocarbon ligand bicyclo[3.2.1]octaâ€2,6â€dienâ€4â€yl: Role of agostic hydrogen atoms. International Journal of Quantum Chemistry, 2019, 119, e26010.	2.0	0
1000	Agostic Hydrogens in 1â€Norbornyl Metal Cyclopentadienyl Structures. European Journal of Inorganic Chemistry, 2020, 2020, 4180-4188.	2.0	0
1001	Unusual effects of the bulky 1-norbornyl group in cobalt carbonyl chemistry: low-energy structures with agostic hydrogen atoms. New Journal of Chemistry, 2020, 44, 8986-8995.	2.8	0
1002	Increasing the Ligand Field Strength in Butadiene Open Sandwich Compounds from the First to the Second Row Transition Metals. ChemistrySelect, 2020, 5, 6350-6359.	1.5	0
1003	The HOXâ‹¯SO‹sub›2‹/sub› (X=F, Cl, Br, I) Binary Complexes: Implications for Atmospheric Chemistry. ChemPhysChem, 2021, 22, 112-126.	2.1	0
1004	Tris(Butadiene) Compounds versus Butadiene Oligomerization in Second-Row Transition Metal Chemistry: Effects of Increased Ligand Fields. Molecules, 2021, 26, 2220.	3.8	0
1005	The isomerisation of H2XY to HXYH (X, Y = O, S, and Se)*. Molecular Physics, 0, , .	1.7	0
1006	Carbeneâ€Stabilized Dithiolene (L 0) Zwitterions. Angewandte Chemie, 2021, 133, 22888.	2.0	0
1007	Cumulants as the Variables of Density Cumulant Theory: A Path to Hermitian Triples. Journal of Chemical Physics, 2021, 155, 244105.	3.0	0
1008	Substituent, Solvent, and Dispersion Effects on the Zwitterionic Character and Dimerization Thermochemistry of the Group 6 Fulvene Metal Tricarbonyl Complexes. Journal of Physical Chemistry A, 2022, 126, 365-372.	2.5	0

#	Article	IF	Citations
1009	A Cationic Magnesium-Based Dithiolene Radical. Organometallics, 2022, 41, 527-531.	2.3	0
1010	Adiabatic Electron Detachment Energies, Reaction Barriers, Chemical Balance, and Ligand Effects on the Nucleophilicities of Metal Carbonyl Monoanions. Organometallics, 2022, 41, 1147-1157.	2.3	0
1011	The noncovalent interaction between water and the ³P ground state of the oxygen atom*. Molecular Physics, 0, , .	1.7	0