Timothy J Lee

List of Publications by Year
in descending order

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278 papers	16,919 citations	13099 68 h-index	20961 115 g-index
282 all docs	282 docs citations	282 times ranked	6735 citing authors

#	Article	IF	Citations
1	A diagnostic for determining the quality of single-reference electron correlation methods. International Journal of Quantum Chemistry, 1989, 36, 199-207.	2.0	902
2	A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. Chemical Physics Letters, 1994, 219, 21-29.	2.6	610
3	The anharmonic force field of ethylene, C2H4, by means of accurate ab initio calculations. Journal of Chemical Physics, 1995, 103, 2589-2602.	3.0	381
4	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
5	Comparison of coupledâ€cluster methods which include the effects of connected triple excitations. Journal of Chemical Physics, 1990, 93, 5851-5855.	3.0	326
6	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
7	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
8	Comparison of the quadratic configuration interaction and coupled-cluster approaches to electron correlation including the effect of triple excitations. The Journal of Physical Chemistry, 1990, 94, 5463-5468.	2.9	311
9	Theoretical investigations of molecules composed only of fluorine, oxygen and nitrogen: determination of the equilibrium structures of FOOF, (NO)2 and FNNF and the transition state structure for FNNF cis-trans isomerization. Theoretica Chimica Acta, 1989, 75, 81-98.	0.8	309
10	Achieving Chemical Accuracy with Coupled-Cluster Theory. , 1995, , 47-108.		259
11	Formulation and implementation of a relativistic unrestricted coupledâ€cluster method including noniterative connected triples. Journal of Chemical Physics, 1996, 105, 8769-8776.	3.0	254
12	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
13	An accurate ab initio quartic force field and vibrational frequencies for CH4 and isotopomers. Journal of Chemical Physics, 1995, 102, 254-261.	3.0	212
14	Comparison of the T1 and D1 diagnostics for electronic structure theory: a new definition for the open-shell D1 diagnostic. Chemical Physics Letters, 2003, 372, 362-367.	2.6	211
15	Time-dependent density functional study on the electronic excitation energies of polycyclic aromatic hydrocarbon radical cations of naphthalene, anthracene, pyrene, and perylene. Journal of Chemical Physics, 1999, 111, 8904-8912.	3.0	208
16	The atomization energy and proton affinity of NH3. An ab initio calibration study. Chemical Physics Letters, 1996, 258, 136-143.	2.6	185
17	Coupledâ€cluster theory employing approximate integrals: An approach to avoid the input/output and storage bottlenecks. Journal of Chemical Physics, 1994, 101, 400-408.	3.0	183
18	Openâ€shell coupledâ€cluster theory. Journal of Chemical Physics, 1993, 98, 9734-9747.	3.0	182

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19	On the necessity offbasis functions for bending frequencies. Journal of Chemical Physics, 1988, 88, 3187-3195.	3.0	174
20	Ab initiocalculation of a global potential, vibrational energies, and wave functions for HCN/HNC, and a simulation of theAÌƒâ€“XÌƒ emission spectrum. Journal of Chemical Physics, 1993, 99, 308-323.	3.0	174
21	Analytic gradients for coupledâ€cluster energies that include noniterative connected triple excitations: Application to cisâ€•and transâ€HONO. Journal of Chemical Physics, 1991, 94, 6229-6236.	3.0	172
22	The vibrational frequencies of ozone. Journal of Chemical Physics, 1990, 93, 489-494.	3.0	152
23	Electronic Absorption Spectra of Neutral Perylene (C20H12), Terrylene (C30H16), and Quaterrylene (C40H20) and Their Positive and Negative Ions:â€‰ Ne Matrix-Isolation Spectroscopy and Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry A, 2003, 107, 3660-3669.	2.5	151
24	An open-shell restricted Hartreeâ€"Fock perturbation theory based on symmetric spin orbitals. Chemical Physics Letters, 1993, 201, 1-10.	2.6	150
25	A procedure for computing accurate ab initio quartic force fields: Application to HO2+ and H2O. Journal of Chemical Physics, 2008, 129, 044312.	3.0	148
26	Accelerating the convergence of the coupled-cluster approach. Chemical Physics Letters, 1986, 130, 236-239.	2.6	143
27	Highly Accurate Quartic Force Fields, Vibrational Frequencies, and Spectroscopic Constants for Cyclic and Linear C₃H₃⁺. Journal of Physical Chemistry A, 2011, 115, 5005-5016.	2.5	138
28	Accurate ab initio quartic force fields for NH2â^ and CCHâ^ and rovibrational spectroscopic constants for their isotopologs. Journal of Chemical Physics, 2009, 131, .	3.0	129
29	A purely ab initio spectroscopic quality quartic force field for acetylene. Journal of Chemical Physics, 1998, 108, 676-691.	3.0	128
30	Prebiotic Astrochemistry and the Formation of Molecules of Astrobiological Interest in Interstellar Clouds and Protostellar Disks. Chemical Reviews, 2020, 120, 4616-4659.	47.7	128
31	Theoretical characterization of tetrahedral N4. Journal of Chemical Physics, 1991, 94, 1215-1221.	3.0	127
32	An accurate ab initio quartic force field for ammonia. Journal of Chemical Physics, 1992, 97, 8361-8371.	3.0	122
33	Total internal partition sums for 166 isotopologues of 51 molecules important in planetary atmospheres: Application to HITRAN2016 and beyond. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 70-87.	2.3	122
34	An efficient closed-shell singles and doubles coupled-cluster method. Chemical Physics Letters, 1988, 150, 406-415.	2.6	119
35	Extended ab Initio and Theoretical Thermodynamics Studies of the Bergman Reaction and the Energy Splitting of the Singlet o-, m-, and p-Benzynes. Journal of the American Chemical Society, 1995, 117, 7186-7194.	13.7	116
36	The trans-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301.	3.0	116

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37	An Accurate ab Initio Quartic Force Field for Formaldehyde and Its Isotopomers. Journal of Molecular Spectroscopy, 1993, 160, 105-116.	1.2	115
38	The structure and energetics of the HCN â†' HNC transition state. Chemical Physics Letters, 1991, 177, 491-497.	2.6	112
39	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
40	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
41	The determination of accurate dipole polarizabilities Î± and Î³ for the noble gases. Journal of Chemical Physics, 1991, 94, 4972-4979.	3.0	111
42	Charged polycyclic aromatic hydrocarbon clusters and the galactic extended red emission. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5274-5278.	7.1	109
43	Toward the laboratory identification of cyclopropenylidene. Journal of the American Chemical Society, 1985, 107, 137-142.	13.7	107
44	Quartic force field predictions of the fundamental vibrational frequencies and spectroscopic constants of the cations HOCO+ and DOCO+. Journal of Chemical Physics, 2012, 136, 234309.	3.0	105
45	Kramers-restricted closed-shellCCSD theory. International Journal of Quantum Chemistry, 1995, 56, 411-419.	2.0	103
46	Rovibrational spectra of ammonia. I. Unprecedented accuracy of a potential energy surface used with nonadiabatic corrections. Journal of Chemical Physics, 2011, 134, 044320.	3.0	100
47	An accurate quartic force field and vibrational frequencies for HNO and DNO. Journal of Chemical Physics, 1994, 101, 5853-5859.	3.0	93
48	Openâ€shell restricted Hartreeâ€"Fock perturbation theory: Some considerations and comparisons. Journal of Chemical Physics, 1994, 100, 7400-7409.	3.0	92
49	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. Chemical Physics Letters, 1997, 275, 414-422.	2.6	92
50	An extensiveab initiostudy of the structures, vibrational spectra, quadratic force fields, and relative energetics of three isomers of Cl2O2. Journal of Chemical Physics, 1992, 97, 6593-6605.	3.0	89
51	Binding energies and bond distances of Ni(CO)x,x=1â€"4: An application of coupledâ€cluster theory. Journal of Chemical Physics, 1991, 95, 5898-5905.	3.0	84
52	Vibrational frequencies for Be3 and Be4. Journal of Chemical Physics, 1990, 92, 7050-7056.	3.0	82
53	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	2.5	81
54	Protonated nitrous oxide, NNOH+: Fundamental vibrational frequencies and spectroscopic constants from quartic force fields. Journal of Chemical Physics, 2013, 139, 084313.	3.0	80

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55	A parallel vectorized implementation of triple excitations in CCSD(T): application to the binding energies of the AlH3, AlH2F, AlHF2 and AlF3 dimers. Chemical Physics Letters, 1991, 178, 462-470.	2.6	78
56	An isotopic-independent highly accurate potential energy surface for CO2 isotopologues and an initial 12C16O2 infrared line list. Journal of Chemical Physics, 2012, 136, 124311.	3.0	78
57	Ab initio multireference study of the BN molecule. Journal of Chemical Physics, 1992, 97, 6549-6556.	3.0	77
58	ExoMol molecular line lists â€“ XIV. The rotationâ€“vibration spectrum of hot SO₂. Monthly Notices of the Royal Astronomical Society, 2016, 459, 3890-3899.	4.4	77
59	Accurate ab initio quartic force fields for the N2O and CO2 molecules. Chemical Physics Letters, 1993, 205, 535-542.	2.6	76
60	Extended line positions, intensities, empirical lower state energies and quantum assignments of NH3 from 6300 to 7000cmâ^'1. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1066-1083.	2.3	76
61	Ab Initio Characterization of Triatomic Bromine Molecules of Potential Interest in Stratospheric Chemistry. The Journal of Physical Chemistry, 1995, 99, 15074-15080.	2.9	75
62	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C₂H₃⁺, and Its Isotopologues. Journal of Physical Chemistry A, 2014, 118, 7034-7043.	2.5	75
63	Ames-2016 line lists for 13 isotopologues of CO2: Updates, consistency, and remaining issues. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 224-241.	2.3	74
64	Rovibrational spectra of ammonia. II. Detailed analysis, comparison, and prediction of spectroscopic assignments for 14NH3,15NH3, and 14ND3. Journal of Chemical Physics, 2011, 134, 044321.	3.0	73
65	A coupledâ€cluster study of XNO (X=H,F,Cl): An investigation of weak Xâ€“N single bonds. Journal of Chemical Physics, 1993, 99, 9783-9789.	3.0	72
66	Reliable infrared line lists for 13 CO2 isotopologues up to Eâ€²=18,000cmâ^'1 and 1500K, with line shape parameters. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 147, 134-144.	2.3	72
67	The anharmonic quartic force field infrared spectra of three polycyclic aromatic hydrocarbons: Naphthalene, anthracene, and tetracene. Journal of Chemical Physics, 2015, 143, 224314.	3.0	71
68	An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH3. Journal of Chemical Physics, 2008, 129, 214304.	3.0	70
69	Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS⁺, HSCO⁺, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry A, 2012, 116, 9582-9590.	2.5	70
70	Timeâ€dependent Density Functional Theory Calculations of Large Compact Polycyclic Aromatic Hydrocarbon Cations: Implications for the Diffuse Interstellar Bands. Astrophysical Journal, 2003, 587, 256-261.	4.5	69
71	An efficient formulation and implementation of the analytic energy gradient method to the single and double excitation coupledâ€cluster wave function: Application to Cl2O2. Journal of Chemical Physics, 1991, 94, 6219-6228.	3.0	68
72	Infrared spectrum of F.hivin..cntdot.H2O. Journal of the American Chemical Society, 1988, 110, 6327-6332.	13.7	67

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73	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. Chemical Physics Letters, 1993, 211, 94-100.	2.6	67
74	On the energy separation between the open and cyclic forms of ozone. Chemical Physics Letters, 1990, 169, 529-533.	2.6	66
75	On the use of quartic force fields in variational calculations. Chemical Physics Letters, 2013, 574, 1-12.	2.6	66
76	Semi-empirical 12C16O2 IR line lists for simulations up to 1500K and 20,000cmâ¯1. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 134-146.	2.3	65
77	Theoretical investigations of the structures and binding energies of Ben and Mgn(n=3â€“5) clusters. Journal of Chemical Physics, 1990, 92, 489-495.	3.0	63
78	Quantum chemistry on parallel computer architectures: coupled-cluster theory applied to the bending potential of fulminic acid. Chemical Physics Letters, 1992, 194, 84-94.	2.6	63
79	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 1¹Aâ€²l-C₃H^{â€“}: A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. Astrophysical Journal, 2013, 772, 39.	4.5	63
80	The polarizabilities of neon. Chemical Physics Letters, 1989, 163, 359-365.	2.6	62
81	Vibrational frequencies and spectroscopic constants from quartic force fields for cis-HOCO: The radical and the anion. Journal of Chemical Physics, 2011, 135, 214303.	3.0	62
82	Ab initio study of the molecular structure and vibrational spectrum of nitric acid and its protonated forms. The Journal of Physical Chemistry, 1992, 96, 650-657.	2.9	61
83	A global ab initio potential for HCN/HNC, exact vibrational energies, and comparison for experiment. Chemical Physics Letters, 1992, 198, 563-569.	2.6	60
84	Excited vibrational level rotational constants for SiC2: A sensitive molecular diagnostic for astrophysical conditions. Molecular Astrophysics, 2015, 1, 13-19.	1.6	60
85	Comparison between the s-cis and gauche conformers of 1,3-butadiene. Journal of the American Chemical Society, 1984, 106, 6250-6253.	13.7	59
86	[5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. Journal of the American Chemical Society, 1987, 109, 2902-2909.	13.7	59
87	Computational vibrational spectroscopy for the detection of molecules in space. Annual Reports in Computational Chemistry, 2019, 15, 173-202.	1.7	59
88	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
89	Accurate ab initio quartic force fields for borane and BeH2. Chemical Physics Letters, 1992, 200, 502-510.	2.6	57
90	Accurateab initioquartic force fields for the ions HCO+and HOC+. Journal of Chemical Physics, 1993, 99, 286-292.	3.0	56

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91	Comparison of one-particle basis set extrapolation to explicitly correlated methods for the calculation of accurate quartic force fields, vibrational frequencies, and spectroscopic constants: Application to H2O, N2H+, NO2+, and C2H2. Journal of Chemical Physics, 2010, 133, 244108.	3.0	55
92	Structures, Relative Stabilities, and Spectra of Isomers of HClO2. The Journal of Physical Chemistry, 1994, 98, 5644-5649.	2.9	54
93	SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES FOR l -C ₃ H ⁺ AND ISOTOPOLOGUES FROM HIGHLY ACCURATE QUARTIC FORCE FIELDS: THE DETECTION OF l -C ₃ H ⁺ IN THE HORSEHEAD NEBULA PDR QUESTIONED. Astrophysical Journal Letters, 2013, 768, L25.	8.3	54
94	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
95	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS: THE REALM OF ANHARMONICITY. Astrophysical Journal, 2015, 814, 23.	4.5	51
96	Triple and quadruple excitation contributions to the binding in Be clusters: Calibration calculations on Be3. Journal of Chemical Physics, 1990, 93, 8875-8880.	3.0	50
97	Comparison of the Brueckner and coupledâ€cluster approaches to electron correlation. Journal of Chemical Physics, 1992, 96, 8931-8937.	3.0	50
98	Accurate ab initio quartic force field and vibrational frequencies of the NH4+ ion and its deuterated forms. Chemical Physics Letters, 1996, 258, 129-135.	2.6	50
99	Highly-accurate quartic force fields for the prediction of anharmonic rotational constants and fundamental vibrational frequencies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119184.	3.9	50
100	The calculation of the vibrational frequencies of CuCO+, NiCO and CuCH3. Chemical Physics Letters, 1992, 189, 266-272.	2.6	49
101	A Comparative Coupled-Cluster Study of the XOCl and XClO (X = H, F, Cl) Isomers: An Investigation of Hypervalent Chlorine Compounds. The Journal of Physical Chemistry, 1994, 98, 3697-3700.	2.9	49
102	A Coupled-Cluster Study of the Molecular Structure, Vibrational Spectrum, and Heats of Formation of XONO2 (X = H, F, Cl). The Journal of Physical Chemistry, 1995, 99, 1943-1948.	2.9	48
103	Second-order perturbation theory and configuration interaction theory applied to medium-sized molecules: cyclopropane, ethylenimine, ethylene oxide, fluoroethane, and acetaldehyde. Journal of the American Chemical Society, 1988, 110, 1388-1393.	13.7	47
104	The energy separation between the classical and nonclassical isomers of protonated acetylene. An extensive study in oneâ€and nâ€particle space. Journal of Chemical Physics, 1991, 94, 8008-8014.	3.0	47
105	Thymine and Other Prebiotic Molecules Produced from the Ultraviolet Photo-Irradiation of Pyrimidine in Simple Astrophysical Ice Analogs. Astrobiology, 2013, 13, 948-962.	3.0	46
106	Highly accurate potential energy surface, dipole moment surface, rovibrational energy levels, and infrared line list for 32S16O2 up to 8000 cmâ¯1. Journal of Chemical Physics, 2014, 140, 114311.	3.0	46
107	The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs. Physical Chemistry Chemical Physics, 2018, 20, 1189-1197.	2.8	46
108	The form of spin orbitals for open-shell restricted Hartreeâ”Fock reference functions. Chemical Physics Letters, 1992, 199, 211-219.	2.6	44

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109	Ab Initio Calculations of Singlet and Triplet Excited States of Chlorine Nitrate and Nitric Acid. The Journal of Physical Chemistry, 1995, 99, 3493-3502.	2.9	44
110	Identifying the Molecular Origin of Global Warming. Journal of Physical Chemistry A, 2009, 113, 12694-12699.	2.5	44
111	Vibrations in small Mg clusters. Journal of Chemical Physics, 1990, 93, 6636-6641.	3.0	43
112	The structure of cis-butadiene. Chemical Physics Letters, 1989, 161, 277-284.	2.6	42
113	Proton affinity of methyl nitrate: less than proton affinity of nitric acid. Journal of the American Chemical Society, 1992, 114, 8247-8256.	13.7	42
114	Ab initio study of the chlorine nitrate protonation reaction: implications for loss of ClONO2 in the stratosphere. The Journal of Physical Chemistry, 1993, 97, 6637-6644.	2.9	42
115	Is there evidence for detection of cyclic C4 in IR spectra? An accurate ab initio computed quartic force field. Journal of Chemical Physics, 1996, 104, 4657-4663.	3.0	42
116	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	3.0	42
117	Ab initio characterization of nitryl chloride (ClNO2) and chlorine nitrites (cis-ClONO, and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5	2.9	41
118	Ordering of the Oâ€“O stretching vibrational frequencies in ozone. Journal of Chemical Physics, 1989, 90, 5635-5637.	3.0	40
119	The anharmonic quartic force field infrared spectra of five non-linear polycyclic aromatic hydrocarbons: Benz[a]anthracene, chrysene, phenanthrene, pyrene, and triphenylene. Journal of Chemical Physics, 2016, 145, 084313.	3.0	40
120	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
121	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
122	The molecular structure and vibrational spectrum of the cyclopropenyl cation, C3H+3, and its deuterated isotopomers. Journal of Chemical Physics, 1989, 90, 4330-4340.	3.0	39
123	Nearâ€Infrared Spectroscopy of Nitrogenated Polycyclic Aromatic Hydrocarbon Cations from 0.7 to 2.5 Î¼m. Astrophysical Journal, 2008, 680, 1243-1255.	4.5	39
124	Vibrational frequencies and infrared intensities for H2CN+, protonated HCN. Journal of Chemical Physics, 1984, 80, 2977-2978.	3.0	38
125	THE POSSIBLE INTERSTELLAR ANION CH₂CN^{â€“}: SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. Astrophysical Journal, 2013, 762, 121.	4.5	38
126	Accurate quartic force fields and vibrational frequencies for hydrogen cyanide and hydrogen isocyanide. The Journal of Physical Chemistry, 1993, 97, 8937-8943.	2.9	37

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127	Fully anharmonic infrared cascade spectra of polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2018, 149, 134302.	3.0	37
128	A Small Molecule with PAH Vibrational Properties and a Detectable Rotational Spectrum: c-(C)C₃H₂, Cyclopropenylidenyl Carbene. Astrophysical Journal, 2019, 871, 236.	4.5	37
129	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
130	The origin of differences between coupled cluster theory and quadratic configuration interaction for excited states. Chemical Physics Letters, 1994, 218, 139-146.	2.6	36
131	Empirical infrared line lists for five SO2 isotopologues: 32/33/34/36S16O2 and 32S18O2. Journal of Molecular Spectroscopy, 2015, 311, 19-24.	1.2	36
132	High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons in the 3â€‰Î¼m region: role of hydrogenation and alkylation. Astronomy and Astrophysics, 2018, 610, A65.	5.1	36
133	Ab initio characterization of peroxyhypochlorous acid: implications for atmospheric chemistry. The Journal of Physical Chemistry, 1993, 97, 6999-7002.	2.9	35
134	The [FHCl]â^'molecular anion: Structural aspects, global surface, and vibrational eigenspectrum. Journal of Chemical Physics, 1993, 99, 3865-3897.	3.0	35
135	Accurate ab Initio Quartic Force Fields, Vibrational Frequencies, and Heats of Formation for FCN, FNC, ClCN, and ClNC. The Journal of Physical Chemistry, 1995, 99, 15858-15863.	2.9	35
136	Electronic spectra and ionization potentials of a stable class of closed shell polycyclic aromatic hydrocarbon cations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 931-945.	3.9	35
137	Theoretical study of infrared and Raman spectra of hydrated magnesium sulfate salts. Journal of Chemical Physics, 2002, 117, 2532-2537.	3.0	35
138	The analytic gradient for the coupled pair functional method: Formula and application for HCl, H2CO, and the dimer H2COâ‹…â‹…â‹…HCl. Journal of Chemical Physics, 1988, 88, 7011-7023.	3.0	34
139	Connected triple excitations in coupled-cluster calculations of hyperpolarizabilities: neon. Chemical Physics Letters, 1992, 191, 23-28.	2.6	34
140	Electronic transitions in the IR: Matrix isolation spectroscopy and electronic structure theory calculations on polyacenes and dibenzopolyacenes. Physical Chemistry Chemical Physics, 2005, 7, 109.	2.8	34
141	Accurate ab initio quartic force fields of cyclic and bent HC2N isomers. Journal of Chemical Physics, 2011, 135, 244310.	3.0	33
142	Overcoming the Failure of Correlation for Out-of-Plane Motions in a Simple Aromatic: Rovibrational Quantum Chemical Analysis ofc-C₃H₂. Journal of Chemical Theory and Computation, 2018, 14, 2155-2164.	5.3	33
143	The varying nature of fluorine-oxygen bonds. Molecular Physics, 1996, 89, 1359-1372.	1.7	33
144	Evaluation of the contribution from triply excited intermediates to the fourth-order perturbation theory energy on Intel distributed memory supercomputers. Theoretica Chimica Acta, 1993, 84, 271-287.	0.8	32

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145	A diagnostic for the applicability of the CIS and CIS(D) excitation energy methods. Chemical Physics Letters, 1997, 279, 151-157.	2.6	32
146	LOW TEMPERATURE FORMATION OF NITROGEN-SUBSTITUTED POLYCYCLIC AROMATIC HYDROCARBONS (PANHs)â€"BARRIERLESS ROUTES TO DIHYDRO(iso)QUINOLINES. Astrophysical Journal, 2015, 815, 115.	4.5	32
147	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
148	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. Journal of Chemical Physics, 1997, 107, 9980-9984.	3.0	31
149	Ab initio geometry, quartic force field, and vibrational frequencies for P4. Journal of Chemical Physics, 1997, 107, 5051-5057.	3.0	31
150	A high-level ab initio study of the anionic hydrogen-bonded complexes FH.cntdot..cntdot..cntdot.CN-, FH.cntdot..cntdot..cntdot.NC-, H2O.cntdot..cntdot..cntdot.CN-, and H2O.cntdot..cntdot..cntdot.NC-. Journal of the American Chemical Society, 1989, 111, 7362-7371.	13.7	30
151	Accurateab initioanharmonic force field and heat of formation for silane. Molecular Physics, 1999, 97, 945-953.	1.7	30
152	Mechanism for the abiotic synthesis of uracil via UV-induced oxidation of pyrimidine in pure H2O ices under astrophysical conditions. Journal of Chemical Physics, 2010, 133, 104303.	3.0	30
153	Dipole Surface and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939.	2.5	30
154	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS IN THE 3 Î¼m REGION: ROLE OF PERIPHERY. Astrophysical Journal, 2016, 831, 58.	4.5	30
155	Evidence for the Formation of Pyrimidine Cations from the Sequential Reactions of Hydrogen Cyanide with the Acetylene Radical Cation. Journal of Physical Chemistry Letters, 2014, 5, 3392-3398.	4.6	29
156	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
157	FONO: A difficult case for theory and experiment. Journal of Chemical Physics, 1992, 97, 4223-4232.	3.0	28
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