Timothy J Lee

List of Publications by Citations

276 papers	14,902 citations	64 h-index	110 g-index
282 ext. papers	15,751 ext. citations	4.3 avg, IF	6.62 L-index

#	Paper	IF	Citations
276	A diagnostic for determining the quality of single-reference electron correlation methods. *International Journal of Quantum Chemistry*, **2009**, 36, 199-207	2.1	663
275	A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. *Chemical Physics Letters*, **1994**, 219, 21-29	2.5	553
274	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	3.9	358
273	The anharmonic force field of ethylene, C2H4, by means of accurate ab initio calculations. *Journal of Chemical Physics*, **1995**, 103, 2589-2602	3.9	338
272	Comparison of coupled-cluster methods which include the effects of connected triple excitations. *Journal of Chemical Physics*, **1990**, 93, 5851-5855	3.9	311
271	Systematic study of molecular anions within the self-consistent-field approximation: OH□CN□ C2H□NH□, and CH□. *Journal of Chemical Physics*, **1985**, 83, 1784-1794	3.9	305
270	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		298
269	The closed-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	3.9	291
268	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		288
267	Achieving Chemical Accuracy with Coupled-Cluster Theory **1995**, 47-108		231
266	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	3.9	228
265	Formulation and implementation of a relativistic unrestricted coupled-cluster method including noniterative connected triples. *Journal of Chemical Physics*, **1996**, 105, 8769-8776	3.9	210
264	An accurate ab initio quartic force field and vibrational frequencies for CH4 and isotopomers. *Journal of Chemical Physics*, **1995**, 102, 254-261	3.9	201
263	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	3.9	195
262	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	2.5	182
261	Coupled-cluster theory employing approximate integrals: An approach to avoid the input/output and storage bottlenecks. *Journal of Chemical Physics*, **1994**, 101, 400-408	3.9	171
260	The atomization energy and proton affinity of NH3. An ab initio calibration study. *Chemical Physics Letters*, **1996**, 258, 136-143	2.5	169

259	On the necessity of f basis functions for bending frequencies. *Journal of Chemical Physics*, **1988**, 88, 3187-3195	3.9	169
258	Ab initio calculation of a global potential, vibrational energies, and wave functions for HCN/HNC, and a simulation of the A X emission spectrum. *Journal of Chemical Physics*, **1993**, 99, 308-323	3.9	163
257	Analytic gradients for coupled-cluster energies that include noniterative connected triple excitations: Application to cis- and trans-HONO. *Journal of Chemical Physics*, **1991**, 94, 6229-6236	3.9	159
256	Open-shell coupled-cluster theory. *Journal of Chemical Physics*, **1993**, 98, 9734-9747	3.9	158
255	The vibrational frequencies of ozone. *Journal of Chemical Physics*, **1990**, 93, 489-494	3.9	149
254	An open-shell restricted Hartree Fock perturbation theory based on symmetric spin orbitals. *Chemical Physics Letters*, **1993**, 201, 1-10	2.5	136
253	Electronic Absorption Spectra of Neutral Perylene (C20H12), Terrylene (C30H16), and Quaterrylene (C40H20) and Their Positive and Negative Ions: Ne Matrix-Isolation Spectroscopy and Time-Dependent Density Functional Theory Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 3660-3669	2.8	134
252	A procedure for computing accurate ab initio quartic force fields: Application to HO2+ and H2O. *Journal of Chemical Physics*, **2008**, 129, 044312	3.9	131
251	Accelerating the convergence of the coupled-cluster approach. *Chemical Physics Letters*, **1986**, 130, 236-239	2.5	129
250	Theoretical characterization of tetrahedral N4. *Journal of Chemical Physics*, **1991**, 94, 1215-1221	3.9	121
249	Highly accurate quartic force fields, vibrational frequencies, and spectroscopic constants for cyclic and linear C3H3(+). *Journal of Physical Chemistry A*, **2011**, 115, 5005-16	2.8	119
248	An accurate ab initio quartic force field for ammonia. *Journal of Chemical Physics*, **1992**, 97, 8361-8371	3.9	118
247	An efficient closed-shell singles and doubles coupled-cluster method. *Chemical Physics Letters*, **1988**, 150, 406-415	2.5	117
246	A purely ab initio spectroscopic quality quartic force field for acetylene. *Journal of Chemical Physics*, **1998**, 108, 676-691	3.9	115
245	An Accurate ab Initio Quartic Force Field for Formaldehyde and Its Isotopomers. *Journal of Molecular Spectroscopy*, **1993**, 160, 105-116	1.3	112
244	Analytic second derivatives for Renner Teller potential energy surfaces. Examples of the five distinct cases. *Journal of Chemical Physics*, **1984**, 81, 356-361	3.9	109
243	The structure and energetics of the HCN -iHNC transition state. *Chemical Physics Letters*, **1991**, 177, 491-497	2.5	108
242	Accurate ab initio quartic force fields for NH2 and CCH and rovibrational spectroscopic constants for their isotopologs. *Journal of Chemical Physics*, **2009**, 131, 104301	3.9	107

241	The trans-HOCO radical: quartic force fields, vibrational frequencies, and spectroscopic constants. *Journal of Chemical Physics*, **2011**, 135, 134301	3.9	105
240	The determination of accurate dipole polarizabilities □and □for the noble gases. *Journal of Chemical Physics*, **1991**, 94, 4972-4979	3.9	104
239	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	16.4	103
238	The analytic evaluation of energy first derivatives for two-configuration self-consistent-field configuration interaction (TCSCF-CI) wave functions. Application to ozone and ethylene. *Journal of Chemical Physics*, **1987**, 87, 7062-7075	3.9	102
237	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, 5274-8	11.5	97
236	Toward the laboratory identification of cyclopropenylidene. *Journal of the American Chemical Society*, **1985**, 107, 137-142	16.4	97
235	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	2.1	94
234	Open-shell restricted Hartree□Fock perturbation theory: Some considerations and comparisons. *Journal of Chemical Physics*, **1994**, 100, 7400-7409	3.9	89
233	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	3.9	89
232	Rovibrational spectra of ammonia. I. Unprecedented accuracy of a potential energy surface used with nonadiabatic corrections. *Journal of Chemical Physics*, **2011**, 134, 044320	3.9	88
231	An extensive ab initio study of the structures, vibrational spectra, quadratic force fields, and relative energetics of three isomers of Cl2O2. *Journal of Chemical Physics*, **1992**, 97, 6593-6605	3.9	88
230	An accurate quartic force field and vibrational frequencies for HNO and DNO. *Journal of Chemical Physics*, **1994**, 101, 5853-5859	3.9	87
229	Kramers-restricted closed-shell CCSD theory. *International Journal of Quantum Chemistry*, **1995**, 56, 411-419	2.1	86
228	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. *Chemical Physics Letters*, **1997**, 275, 414-422	2.5	82
227	Vibrational frequencies for Be3 and Be4. *Journal of Chemical Physics*, **1990**, 92, 7050-7056	3.9	80
226	Binding energies and bond distances of Ni(CO)x, x=1□4: An application of coupled-cluster theory. *Journal of Chemical Physics*, **1991**, 95, 5898-5905	3.9	78
225	Ab initio multireference study of the BN molecule. *Journal of Chemical Physics*, **1992**, 97, 6549-6556	3.9	76
224	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	2.5	74

223	Protonated nitrous oxide, NNOH+: fundamental vibrational frequencies and spectroscopic constants from quartic force fields. *Journal of Chemical Physics*, **2013**, 139, 084313	3.9	72
222	Ab Initio Characterization of Triatomic Bromine Molecules of Potential Interest in Stratospheric Chemistry. *The Journal of Physical Chemistry*, **1995**, 99, 15074-15080		71
221	Accurate ab initio quartic force fields for the N2O and CO2 molecules. *Chemical Physics Letters*, **1993**, 205, 535-542	2.5	70
220	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	3.9	69
219	Quartic force field rovibrational analysis of protonated acetylene, C2H3(+), and its isotopologues. *Journal of Physical Chemistry A*, **2014**, 118, 7034-43	2.8	67
218	An efficient formulation and implementation of the analytic energy gradient method to the single and double excitation coupled-cluster wave function: Application to Cl2O2. *Journal of Chemical Physics*, **1991**, 94, 6219-6228	3.9	67
217	Extended line positions, intensities, empirical lower state energies and quantum assignments of NH3 from 6300 to 7000cm□1. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2012**, 113, 1066-1083	2.1	66
216	An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH(3). *Journal of Chemical Physics*, **2008**, 129, 214304	3.9	65
215	Infrared spectrum of F.hivin..cntdot.H2O. *Journal of the American Chemical Society*, **1988**, 110, 6327-6332	16.4	65
214	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN(+). *Journal of Physical Chemistry A*, **2015**, 119, 11623-31	2.8	64
213	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. *Chemical Physics Letters*, **1993**, 211, 94-100	2.5	64
212	Time-dependent Density Functional Theory Calculations of Large Compact Polycyclic Aromatic Hydrocarbon Cations: Implications for the Diffuse Interstellar Bands. *Astrophysical Journal*, **2003**, 587, 256-261	4.7	64
211	Fundamental vibrational frequencies and spectroscopic constants of HOCS+, HSCO+, and isotopologues via quartic force fields. *Journal of Physical Chemistry A*, **2012**, 116, 9582-90	2.8	63
210	On the energy separation between the open and cyclic forms of ozone. *Chemical Physics Letters*, **1990**, 169, 529-533	2.5	63
209	An isotopic-independent highly accurate potential energy surface for CO2 isotopologues and an initial (12)C(16)O2 infrared line list. *Journal of Chemical Physics*, **2012**, 136, 124311	3.9	61
208	Vibrational frequencies and spectroscopic constants from quartic force fields for cis-HOCO: the radical and the anion. *Journal of Chemical Physics*, **2011**, 135, 214303	3.9	61
207	A coupled-cluster study of XNO (X=H,F,Cl): An investigation of weak X□N single bonds. *Journal of Chemical Physics*, **1993**, 99, 9783-9789	3.9	61
206	The polarizabilities of neon. *Chemical Physics Letters*, **1989**, 163, 359-365	2.5	61

205	Quantum chemistry on parallel computer architectures: coupled-cluster theory applied to the bending potential of fulminic acid. *Chemical Physics Letters*, **1992**, 194, 84-94	2.5	60
204	Reliable infrared line lists for 13 CO2 isotopologues up to E?=18,000cm□ and 1500K, with line shape parameters. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2014**, 147, 134-144	2.1	59
203	On the use of quartic force fields in variational calculations. *Chemical Physics Letters*, **2013**, 574, 1-12	2.5	59
202	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		59
201	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 11A?l-C3H□A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. *Astrophysical Journal*, **2013**, 772, 39	4.7	58
200	Accurate ab initio quartic force fields for borane and BeH2. *Chemical Physics Letters*, **1992**, 200, 502-510	2.5	56
199	A global ab initio potential for HCN/HNC, exact vibrational energies, and comparison for experiment. *Chemical Physics Letters*, **1992**, 198, 563-569	2.5	56
198	Theoretical investigations of the structures and binding energies of Ben and Mgn(n=3□) clusters. *Journal of Chemical Physics*, **1990**, 92, 489-495	3.9	55
197	The anharmonic quartic force field infrared spectra of three polycyclic aromatic hydrocarbons: Naphthalene, anthracene, and tetracene. *Journal of Chemical Physics*, **2015**, 143, 224314	3.9	54
196	Comparison between the s-cis and gauche conformers of 1,3-butadiene. *Journal of the American Chemical Society*, **1984**, 106, 6250-6253	16.4	54
195	Semi-empirical 12C16O2 IR line lists for simulations up to 1500K and 20,000cm□. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2013**, 130, 134-146	2.1	53
194	Accurate ab initio quartic force fields for the ions HCO+ and HOC+. *Journal of Chemical Physics*, **1993**, 99, 286-292	3.9	53
193	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	3.9	53
192	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	2.1	52
191	Excited vibrational level rotational constants for SiC2: A sensitive molecular diagnostic for astrophysical conditions. *Molecular Astrophysics*, **2015**, 1, 13-19	1.7	51
190	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	7.9	50
189	Structures, Relative Stabilities, and Spectra of Isomers of HClO2. *The Journal of Physical Chemistry*, **1994**, 98, 5644-5649		50
188	Comparison of the Brueckner and coupled-cluster approaches to electron correlation. *Journal of Chemical Physics*, **1992**, 96, 8931-8937	3.9	49

187	[5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. *Journal of the American Chemical Society*, **1987**, 109, 2902-2909	16.4	49
186	Accurate ab initio quartic force field and vibrational frequencies of the NH4+ ion and its deuterated forms. *Chemical Physics Letters*, **1996**, 258, 129-135	2.5	48
185	Triple and quadruple excitation contributions to the binding in Be clusters: Calibration calculations on Be3. *Journal of Chemical Physics*, **1990**, 93, 8875-8880	3.9	48
184	Prebiotic Astrochemistry and the Formation of Molecules of Astrobiological Interest in Interstellar Clouds and Protostellar Disks. *Chemical Reviews*, **2020**, 120, 4616-4659	68.1	47
183	ExoMol molecular line lists □XIV. The rotation□vibration spectrum of hot SO2. *Monthly Notices of the Royal Astronomical Society*, **2016**, 459, 3890-3899	4.3	47
182	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		46
181	The efficient evaluation of configuration interaction analytic energy second derivatives: Application to hydrogen thioperoxide, HSOH. *Journal of Chemical Physics*, **1986**, 85, 3930-3938	3.9	46
180	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		45
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178	The energy separation between the classical and nonclassical isomers of protonated acetylene. An extensive study in one- and n-particle space. *Journal of Chemical Physics*, **1991**, 94, 8008-8014	3.9	44
177	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	16.4	43
176	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	3.9	42
175	Ab Initio Calculations of Singlet and Triplet Excited States of Chlorine Nitrate and Nitric Acid. *The Journal of Physical Chemistry*, **1995**, 99, 3493-3502		41
174	The form of spin orbitals for open-shell restricted Hartree□Fock reference functions. *Chemical Physics Letters*, **1992**, 199, 211-219	2.5	41
173	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS: THE REALM OF ANHARMONICITY. *Astrophysical Journal*, **2015**, 814, 23	4.7	40
172	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		40
171	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. *Journal of Chemical Physics*, **2015**, 143, 071102	3.9	39
170	Proton affinity of methyl nitrate: less than proton affinity of nitric acid. *Journal of the American Chemical Society*, **1992**, 114, 8247-8256	16.4	39

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168	Vibrations in small Mg clusters. *Journal of Chemical Physics*, **1990**, 93, 6636-6641	3.9	39
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166	Ordering of the OID stretching vibrational frequencies in ozone. *Journal of Chemical Physics*, **1989**, 90, 5635-5637	3.9	38
165	Analytic evaluation of infrared intensities and polarizabilities by two-configuration self-consistent field wave functions. *Theoretica Chimica Acta*, **1986**, 69, 337-352		38
164	Vibrational frequencies and infrared intensities for H2CN+, protonated HCN. *Journal of Chemical Physics*, **1984**, 80, 2977-2978	3.9	38
163	Accurate quartic force fields and vibrational frequencies for hydrogen cyanide and hydrogen isocyanide. *The Journal of Physical Chemistry*, **1993**, 97, 8937-8943		37
162	Ab initio characterization of nitryl chloride (ClNO2) and chlorine nitrites (cis-ClONO, and trans-ClONO). *The Journal of Physical Chemistry*, **1994**, 98, 111-115		37
161	Thymine and other prebiotic molecules produced from the ultraviolet photo-irradiation of pyrimidine in simple astrophysical ice analogs. *Astrobiology*, **2013**, 13, 948-62	3.7	36
160	Identifying the molecular origin of global warming. *Journal of Physical Chemistry A*, **2009**, 113, 12694-9	2.8	36
159	The origin of differences between coupled cluster theory and quadratic configuration interaction for excited states. *Chemical Physics Letters*, **1994**, 218, 139-146	2.5	36
158	The structure of cis-butadiene. *Chemical Physics Letters*, **1989**, 161, 277-284	2.5	36
157	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	3.9	36
156	THE POSSIBLE INTERSTELLAR ANION CH2CN−SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. *Astrophysical Journal*, **2013**, 762, 121	4.7	34
155	Near-Infrared Spectroscopy of Nitrogenated Polycyclic Aromatic Hydrocarbon Cations from 0.7 to 2.5 μm. *Astrophysical Journal*, **2008**, 680, 1243-1255	4.7	34
154	Connected triple excitations in coupled-cluster calculations of hyperpolarizabilities: neon. *Chemical Physics Letters*, **1992**, 191, 23-28	2.5	34
153	Empirical infrared line lists for five SO2 isotopologues: 32/33/34/36S16O2 and 32S18O2. *Journal of Molecular Spectroscopy*, **2015**, 311, 19-24	1.3	33
152	Accurate ab Initio Quartic Force Fields, Vibrational Frequencies, and Heats of Formation for FCN, FNC, ClCN, and ClNC. *The Journal of Physical Chemistry*, **1995**, 99, 15858-15863		33

151	Ab initio characterization of peroxyhypochlorous acid: implications for atmospheric chemistry. *The Journal of Physical Chemistry*, **1993**, 97, 6999-7002		33
150	The analytic gradient for the coupled pair functional method: Formula and application for HCl, H2CO, and the dimer H2CO???HCl. *Journal of Chemical Physics*, **1988**, 88, 7011-7023	3.9	33
149	The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs. *Physical Chemistry Chemical Physics*, **2018**, 20, 1189-1197	3.6	33
148	Highly accurate potential energy surface, dipole moment surface, rovibrational energy levels, and infrared line list for □S□O□ up to 8000 cm?□ *Journal of Chemical Physics*, **2014**, 140, 114311	3.9	32
147	Electronic transitions in the IR: Matrix isolation spectroscopy and electronic structure theory calculations on polyacenes and dibenzopolyacenes. *Physical Chemistry Chemical Physics*, **2005**, 7, 109	3.6	32
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145	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		32
144	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	3.9	32
143	The varying nature of fluorine-oxygen bonds. *Molecular Physics*, **1996**, 89, 1359-1372	1.7	32
142	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. *Journal of Chemical Physics*, **1997**, 107, 9980-9984	3.9	31
141	Theoretical study of infrared and Raman spectra of hydrated magnesium sulfate salts. *Journal of Chemical Physics*, **2002**, 117, 2532-2537	3.9	31
140	Accurate ab initio quartic force fields of cyclic and bent HC2N isomers. *Journal of Chemical Physics*, **2011**, 135, 244310	3.9	30
139	Computational vibrational spectroscopy for the detection of molecules in space. *Annual Reports in Computational Chemistry*, **2019**, 15, 173-202	1.8	29
138	A diagnostic for the applicability of the CIS and CIS(D) excitation energy methods. *Chemical Physics Letters*, **1997**, 279, 151-157	2.5	29
137	Accurate ab initio anharmonic force field and heat of formation for silane. *Molecular Physics*, **1999**, 97, 945-953	1.7	29
136	On the energy invariance of open-shell perturbation theory with respect to unitary transformations of molecular orbitals. *Journal of Chemical Physics*, **1996**, 105, 1060-1069	3.9	29
135	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	16.4	29
134	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	3.9	29

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132	Investigation of a diagnostic for perturbation theory. Comparison to the T1 diagnostic of coupled-cluster theory. *Chemical Physics Letters*, **1995**, 243, 402-408	2.5	28
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130	High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons in the 3 μm region: role of hydrogenation and alkylation. *Astronomy and Astrophysics*, **2018**, 610, A65	5.1	27
129	Dipole surface and infrared intensities for the cis- and trans-HOCO and DOCO radicals. *Journal of Physical Chemistry A*, **2013**, 117, 6932-9	2.8	26
128	Ab initio geometry, quartic force field, and vibrational frequencies for P4. *Journal of Chemical Physics*, **1997**, 107, 5051-5057	3.9	26
127	An accurate ab initio quartic force field and vibrational frequencies for cyclopropenylidene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1997**, 53, 1065-1077	4.4	26
126	The protonation of N2O reexamined: A case study on the reliability of various electron correlation methods for minima and transition states. *Journal of Chemical Physics*, **1993**, 98, 7951-7957	3.9	26
125	Bond distance and vibrational spectrum of the molecular cation NO+2. *Chemical Physics Letters*, **1992**, 188, 154-158	2.5	26
124	Mechanism for the abiotic synthesis of uracil via UV-induced oxidation of pyrimidine in pure H(2)O ices under astrophysical conditions. *Journal of Chemical Physics*, **2010**, 133, 104303	3.9	25
123	The effect of approximating some molecular integrals in coupled-cluster calculations: fundamental frequencies and rovibrational spectroscopic constants for isotopologues of cyclopropenylidene. *Molecular Physics*, **2009**, 107, 1139-1152	1.7	25
122	An accurate quartic force field, fundamental frequencies, and binding energy for the high energy density material TdN4. *Chemical Physics Letters*, **2002**, 357, 319-325	2.5	25
121	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. *Molecular Physics*, **1999**, 96, 633-643	1.7	25
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