Timothy J Lee

List of Publications by Year in Descending Order

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 collaborative 14NH3 IR spectroscopic analysis at 6000 cm−1. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2022**, 280, 108076	2.1	0
275	PDRs4All: A JWST Early Release Science Program on Radiative Feedback from Massive Stars. *Publications of the Astronomical Society of the Pacific*, **2022**, 134, 054301	5	2
274	Vibrational and Rovibrational Spectroscopy Applied to Astrochemistry **2022**, 235-295		1
273	Fundamental Vibrational Frequencies and Spectroscopic Constants of Substituted Cyclopropenylidene (c-CHX, X = F, Cl, CN). *Journal of Physical Chemistry A*, **2021**, 125, 8860-8868	2.8	0
272	The unsolved issue with out-of-plane bending frequencies for CC multiply bonded systems. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 248, 119148	4.4	5
271	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	4.4	17
270	The First Mid-infrared Detection of HNC in the Interstellar Medium: Probing the Extreme Environment toward the Orion Hot Core. *Astrophysical Journal*, **2021**, 907, 51	4.7	2
269	What It Takes to Compute Highly Accurate Rovibrational Line Lists for Use in Astrochemistry. *Accounts of Chemical Research*, **2021**, 54, 1311-1321	24.3	2
268	Modeling the infrared cascade spectra of small PAHs: the 11.2 μm band. *Theoretical Chemistry Accounts*, **2021**, 140, 124	1.9	0
267	PAH Spectroscopy from 1 to 5 μm. *Astrophysical Journal Letters*, **2021**, 917, L35	7.9	1
266	Climate Metrics for C1-C4 Hydrofluorocarbons (HFCs). *Journal of Physical Chemistry A*, **2020**, 124, 4793-4800	2.8	1
265	Theoretical rovibrational characterization of the cis/trans-HCSH and H2SC isomers of the known interstellar molecule thioformaldehyde. *Journal of Molecular Spectroscopy*, **2020**, 369, 111273	1.3	5
264	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
263	Overcoming the out-of-plane bending issue in an aromatic hydrocarbon: the anharmonic vibrational frequencies of c-(CH)CH. *Physical Chemistry Chemical Physics*, **2020**, 22, 12951-12958	3.6	6
262	The Production and Potential Detection of Hexamethylenetetramine-Methanol in Space. *Astrobiology*, **2020**, 20, 601-616	3.7	8
261	Cation, Anion, and Radical Isomers of CHN: Computational Characterization and Implications for Astrophysical and Planetary Environments. *Journal of Physical Chemistry A*, **2020**, 124, 2001-2013	2.8	6
260	Exploring the limits of the Data-Model-Theory synergy: Hot MW transitions for rovibrational IR studies. *Journal of Molecular Structure*, **2020**, 1217, 128260	3.4	2

259	Highly Accurate Quartic Force Field and Rovibrational Spectroscopic Constants for the Azirinyl Cation (c-CNH) and Its Isomers. *Journal of Physical Chemistry A*, **2020**, 124, 362-370	2.8	1
258	Molecular growth upon ionization of van der Waals clusters containing HCCH and HCN is a pathway to prebiotic molecules. *Physical Chemistry Chemical Physics*, **2020**, 22, 20337-20348	3.6	5
257	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C3H2): the importance of numerical stability. *Molecular Physics*, **2020**, 118, e1589007	1.7	4
256	The Calculated Infrared Spectra of Functionalized Hexamethylenetetramine (HMT) Molecules. *Astrophysical Journal*, **2019**, 884, 64	4.7	4
255	Quantitative validation of Ames IR intensity and new line lists for 32/33/34S16O2, 32S18O2 and 16O32S18O. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2019**, 225, 327-336	2.1	10
254	Isotopologue consistency of semi-empirically computed infrared line lists and further improvement for rare isotopologues: CO2 and SO2 case studies. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2019**, 230, 222-246	2.1	8
253	A Small Molecule with PAH Vibrational Properties and a Detectable Rotational Spectrum: c-(C)C3H2, Cyclopropenylidenyl Carbene. *Astrophysical Journal*, **2019**, 871, 236	4.7	22
252	Computational vibrational spectroscopy for the detection of molecules in space. *Annual Reports in Computational Chemistry*, **2019**, 15, 173-202	1.8	29
251	The possibility of :CNH2+ within Titan's atmosphere: Rovibrational analysis of :CNH2+ and :CCH2. *Icarus*, **2019**, 321, 260-265	3.8	1
250	High Spectral Resolution SOFIA/EXES Observations of C2H2toward Orion IRc2. *Astrophysical Journal*, **2018**, 856, 9	4.7	9
249	Overcoming the Failure of Correlation for Out-of-Plane Motions in a Simple Aromatic: Rovibrational Quantum Chemical Analysis of c-CH. *Journal of Chemical Theory and Computation*, **2018**, 14, 2155-2164	6.4	21
248	Rovibrational analysis of c-SiCH: Further evidence for out-of-plane bending issues in correlated methods. *Journal of Chemical Physics*, **2018**, 149, 024303	3.9	8
247	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	4.3	5
246	The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs. *Physical Chemistry Chemical Physics*, **2018**, 20, 1189-1197	3.6	33
245	Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. *ACS Omega*, **2018**, 3, 16035-16039	3.9	8
244	Fully anharmonic infrared cascade spectra of polycyclic aromatic hydrocarbons. *Journal of Chemical Physics*, **2018**, 149, 134302	3.9	21
243	Anharmonicity and the infrared emission spectrum of highly excited polycyclic aromatic hydrocarbons. *Astronomy and Astrophysics*, **2018**, 618, A49	5.1	7
242	Characterization of Azirine and Its Structural Isomers. *Journal of Physical Chemistry A*, **2018**, 122, 8898-8904	2.8	3

241	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
240	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
239	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
238	Quantum Chemical Rovibrational Analysis of the HOSO Radical. *Journal of Physical Chemistry A*, **2017**, 121, 8108-8114	2.8	14
237	Mechanisms of the Formation of Adenine, Guanine, and Their Analogues in UV-Irradiated Mixed NH:HO Molecular Ices Containing Purine. *Astrobiology*, **2017**, 17, 771-785	3.7	17
236	Toward the laboratory identification of the not-so-simple NS neutral and anion isomers. *Journal of Chemical Physics*, **2017**, 147, 074303	3.9	5
235	Towards completing the cyclopropenylidene cycle: rovibrational analysis of cyclic N, CNN, HCNN, and CNC. *Physical Chemistry Chemical Physics*, **2017**, 19, 22860-22869	3.6	3
234	Communication: The failure of correlation to describe carbon=carbon bonding in out-of-plane bends. *Journal of Chemical Physics*, **2017**, 147, 221101	3.9	16
233	Ames 32S16O18O line list for high-resolution experimental IR analysis. *Journal of Molecular Spectroscopy*, **2016**, 330, 101-111	1.3	12
232	Quantum Chemical Analysis of the CO-HNN Proton-Bound Complex. *Journal of Physical Chemistry A*, **2016**, 120, 7745-7752	2.8	11
231	INSIGHTS INTO HYDROCARBON CHAIN AND AROMATIC RING FORMATION IN THE INTERSTELLAR MEDIUM: COMPUTATIONAL STUDY OF THE ISOMERS OF ${{rm{C}}}_{4}{{{rm{H}}}_{3}}^{+}$ ${{rm{C}}}_{6}{{{rm{H}}}_{3}}^{+}$ AND ${{rm{C}}}_{6}{{{rm{H}}}_{5}}^{+}$ AND THEIR FORMATION PATHWAYS. *Astrophysical Journal*, **2016**, 830, 128	4.7	9
230	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS IN THE 3 μm REGION: ROLE OF PERIPHERY. *Astrophysical Journal*, **2016**, 831, 58	4.7	21
229	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
228	Characterization of the Azirinyl Cation and Its Isomers. *Journal of Physical Chemistry A*, **2016**, 120, 1275-82	2.8	11
227	TOWARD THE ASTRONOMICAL DETECTION OF THE PROTON-BOUND COMPLEX NNHCO+: IMPLICATIONS FOR THE SPECTRA OF PROTOPLANETARY DISKS. *Astrophysical Journal*, **2016**, 819, 141	4.7	13
226	Mechanisms for the formation of thymine under astrophysical conditions and implications for the origin of life. *Journal of Chemical Physics*, **2016**, 144, 144308	3.9	17
225	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
224	Inclusion of 13C and D in protonated acetylene. *Chemical Physics Letters*, **2016**, 650, 126-129	2.5	13

223	Excited State Trends in Bidirectionally Expanded Closed-Shell PAH and PANH Anions. *Journal of Physical Chemistry A*, **2016**, 120, 7327-34	2.8	6
222	Rovibrational and energetic analysis of the hydroxyethynyl anion (CCOH)1 *Molecular Physics*, **2015**, 113, 2012-2017	1.7	9
221	Electronically excited states of PANH anions. *Physical Chemistry Chemical Physics*, **2015**, 17, 14761-72	3.6	19
220	Linear transformation of anharmonic molecular force constants between normal and Cartesian coordinates. *Journal of Chemical Physics*, **2015**, 142, 244107	3.9	9
219	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
218	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS: THE REALM OF ANHARMONICITY. *Astrophysical Journal*, **2015**, 814, 23	4.7	40
217	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. *Journal of Chemical Physics*, **2015**, 143, 071102	3.9	39
216	LOW TEMPERATURE FORMATION OF NITROGEN-SUBSTITUTED POLYCYCLIC AROMATIC HYDROCARBONS (PANHs)BARRIERLESS ROUTES TO DIHYDRO(iso)QUINOLINES. *Astrophysical Journal*, **2015**, 815, 115	4.7	22
215	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN(+). *Journal of Physical Chemistry A*, **2015**, 119, 11623-31	2.8	64
214	Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. *Journal of Physical Chemistry A*, **2015**, 119, 13048-54	2.8	12
213	Excited vibrational level rotational constants for SiC2: A sensitive molecular diagnostic for astrophysical conditions. *Molecular Astrophysics*, **2015**, 1, 13-19	1.7	51
212	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
211	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of CH2, CH and CH and their formation paths from acetylene and its fragments. *Physical Chemistry Chemical Physics*, **2015**, 17, 1859-69	3.6	17
210	Photosynthesis and photo-stability of nucleic acids in prebiotic extraterrestrial environments. *Topics in Current Chemistry*, **2015**, 356, 123-64		17
209	Formation and stability of CH isomers. *Journal of Physical Chemistry A*, **2014**, 118, 10109-16	2.8	7
208	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, 3392-8	6.4	23
207	Fundamental vibrational frequencies and spectroscopic constants of cis- and trans-HOCS, HSCO, and isotopologues via quartic force fields. *Journal of Physical Chemistry B*, **2014**, 118, 6498-510	3.4	15
206	Quartic force field rovibrational analysis of protonated acetylene, C2H3(+), and its isotopologues. *Journal of Physical Chemistry A*, **2014**, 118, 7034-43	2.8	67

205	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
204	Limited rotational and rovibrational line lists computed with highly accurate quartic force fields and ab initio dipole surfaces. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 119, 76-83	4.4	21
203	Highly accurate potential energy surface, dipole moment surface, rovibrational energy levels, and infrared line list for S up to 8000 cm? *Journal of Chemical Physics*, **2014**, 140, 114311	3.9	32
202	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OFc-C3H *Astrophysical Journal*, **2014**, 796, 139	4.7	16
201	On the use of quartic force fields in variational calculations. *Chemical Physics Letters*, **2013**, 574, 1-12	2.5	59
200	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
199	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
198	Vibrational frequencies and spectroscopic constants for 1 3A' HNC and 1 3A' HOC+ from high-accuracy quartic force fields. *Journal of Physical Chemistry A*, **2013**, 117, 11339-45	2.8	10
197	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
196	Association mechanisms of unsaturated C2 hydrocarbons with their cations: acetylene and ethylene. *Physical Chemistry Chemical Physics*, **2013**, 15, 2012-23	3.6	19
195	The 1 3A' HCN and 1 3A' HCO+ vibrational frequencies and spectroscopic constants from quartic force fields. *Journal of Physical Chemistry A*, **2013**, 117, 9324-30	2.8	19
194	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
193	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
192	Protonated nitrous oxide, NNOH+: fundamental vibrational frequencies and spectroscopic constants from quartic force fields. *Journal of Chemical Physics*, **2013**, 139, 084313	3.9	72
191	Anharmonic rovibrational calculations of singlet cyclic C4 using a new ab initio potential and a quartic force field. *Journal of Chemical Physics*, **2013**, 139, 224302	3.9	8
190	ROVIBRATIONAL SPECTROSCOPIC CONSTANTS AND FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR ISOTOPOLOGUES OF CYCLIC AND BENT SINGLET HC2N ISOMERS. *Astrophysical Journal*, **2013**, 778, 160	4.7	8
189	Relative energies, structures, vibrational frequencies, and electronic spectra of pyrylium cation, an oxygen-containing carbocyclic ring isoelectronic with benzene, and its isomers. *Journal of Chemical Physics*, **2013**, 139, 174302	3.9	7
188	THE POSSIBLE INTERSTELLAR ANION CH2CN SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. *Astrophysical Journal*, **2013**, 762, 121	4.7	34

187	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
186	A group increment scheme for infrared absorption intensities of greenhouse gases. *Journal of Molecular Structure*, **2012**, 1009, 89-95	3.4	3
185	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
184	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
183	Photochemistry and photophysics of n-butanal, 3-methylbutanal, and 3,3-dimethylbutanal: experimental and theoretical study. *Journal of Physical Chemistry A*, **2012**, 116, 5830-9	2.8	14
182	Quantum IR line list of NH3 and isotopologues for ISM and dwarf studies. *Proceedings of the International Astronomical Union*, **2012**, 8, 248-248	0.1	
181	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
180	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
179	SPECTROSCOPIC CONSTANTS FOR13C AND DEUTERIUM ISOTOPOLOGUES OF CYCLIC AND LINEAR C3H3+. *Astrophysical Journal*, **2011**, 736, 33	4.7	19
178	Initiating molecular growth in the interstellar medium via dimeric complexes of observed ions and molecules. *Astronomy and Astrophysics*, **2011**, 535, A74	5.1	16
177	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
176	The trans-HOCO radical: quartic force fields, vibrational frequencies, and spectroscopic constants. *Journal of Chemical Physics*, **2011**, 135, 134301	3.9	105
175	Accurate ab initio quartic force fields of cyclic and bent HC2N isomers. *Journal of Chemical Physics*, **2011**, 135, 244310	3.9	30
174	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
173	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
172	Design strategies to minimize the radiative efficiency of global warming molecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9049-54	11.5	13
171	Reply to Wallington et al.: Differences in electronic structure of global warming molecules lead to different molecular properties. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, E180-E180	11.5	1
170	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

169	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
168	Computational Interstellar Chemistry. *Thirty Years of Astronomical Discovery With UKIRT*, **2010**, 21-30	0.3	
167	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
166	A diagnostic for determining the quality of single-reference electron correlation methods. *International Journal of Quantum Chemistry*, **2009**, 36, 199-207	2.1	663
165	An approach to include the effects of diffuse functions in potential energy surface calculations. *Journal of Physical Chemistry A*, **2009**, 113, 11954-62	2.8	6
164	Identifying the molecular origin of global warming. *Journal of Physical Chemistry A*, **2009**, 113, 12694-9	2.8	36
163	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
162	Are isomers of the vinyl cyanide ion missing links for interstellar pyrimidine formation?. *Journal of Chemical Physics*, **2009**, 131, 074303	3.9	19
161	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
160	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
159	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
158	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
157	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
156	Search for stratospheric bromine reservoir species: theoretical study of the photostability of mono-, tri-, and pentacoordinated bromine compounds. *Journal of Physical Chemistry A*, **2005**, 109, 8133-9	2.8	5
155	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
154	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
153	Theoretical study of chlorine nitrates: implications for stratospheric chlorine chemistry. *Journal of the American Chemical Society*, **2003**, 125, 10446-58	16.4	3
152	An Accurate Quartic Force Field and Fundamental Frequencies for the Ozonide Anion: A Rare Positive Anharmonicity for the Antisymmetric Stretch. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 189-201		3

151	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
150	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
149	Theoretical study of infrared and Raman spectra of hydrated magnesium sulfate salts. *Journal of Chemical Physics*, **2002**, 117, 2532-2537	3.9	31
148	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, 931-45	4.4	32
147	Towards the synthesis of the high energy density material TdN4: excited electronic states. *Chemical Physics Letters*, **2001**, 345, 295-302	2.5	20
146	Theoretical study of XONO2 (X=Br, OBr, O2Br): Implications for stratospheric bromine chemistry. *Journal of Chemical Physics*, **2000**, 113, 145-152	3.9	14
145	Accurate calculations on excited states: new theories applied to the □X, □O, and □O2 (X=Cl and Br) chromophores and implications for stratospheric bromine chemistry. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1999**, 55, 561-574	4.4	18
144	Accurate spectroscopic characterization of 12C14N□13C14N□and 12C15N□*Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1999**, 55, 739-747	4.4	15
143	Accurate ab initio anharmonic force field and heat of formation for silane. *Molecular Physics*, **1999**, 97, 945-953	1.7	29
142	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. *Molecular Physics*, **1999**, 96, 633-643	1.7	25
141	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
140	Ab initio investigation of the atmospheric molecule bromine nitrate: Equilibrium structure, vibrational spectrum, and heat of formation. *Journal of Chemical Physics*, **1998**, 109, 525-530	3.9	19
139	A purely ab initio spectroscopic quality quartic force field for acetylene. *Journal of Chemical Physics*, **1998**, 108, 676-691	3.9	115
138	Adiabatic electron affinity and ionization potential for BrO radical. *Journal of Chemical Physics*, **1998**, 109, 10818-10822	3.9	18
137	Density functional and coupled-cluster study on the HNO-HON transition state. *Journal of Chemical Physics*, **1997**, 107, 8208-8209	3.9	8
136	Ab initio quartic force fields for anions: A benchmark study on 16OH□18OH□and 16OD□*Journal of Chemical Physics*, **1997**, 107, 10373-10380	3.9	13
135	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. *Journal of Chemical Physics*, **1997**, 107, 9980-9984	3.9	31
134	SINGLE REFERENCE COUPLED CLUSTER AND PERTURBATION THEORIES OF ELECTRONIC EXCITATION ENERGIES. *Recent Advances in Computational*, **1997**, 221-253		15

133	A new spin-restricted triple excitation correction for coupled cluster theory. *Journal of Chemical Physics*, **1997**, 107, 7943-7950	3.9	23
132	Ab initio geometry, quartic force field, and vibrational frequencies for P4. *Journal of Chemical Physics*, **1997**, 107, 5051-5057	3.9	26
131	A challenge for density functional theory: the XONO and XNO2 (X=F, Cl, and Br) molecules. *Theoretical Chemistry Accounts*, **1997**, 97, 185-194	1.9	23
130	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
129	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. *Chemical Physics Letters*, **1997**, 275, 414-422	2.5	82
128	A diagnostic for the applicability of the CIS and CIS(D) excitation energy methods. *Chemical Physics Letters*, **1997**, 279, 151-157	2.5	29
127	Characterization of BrNO2, cis-BrONO, and trans-BrONO. Implications for Atmospheric Chemistry. *The Journal of Physical Chemistry*, **1996**, 100, 19847-19852		21
126	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
125	The varying nature of fluorine oxygen bonds. *Molecular Physics*, **1996**, 89, 1359-1372	1.7	4
124	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
123	The proton affinity of HOBr. *Chemical Physics Letters*, **1996**, 251, 400-404	2.5	10
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