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 collaborative 14NH3 IR spectroscopic analysis at 6000 cmâ¯1. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 280, 108076.	2.3	2
2	Anharmonicity and the IR Emission Spectrum of Neutral Interstellar PAH Molecules. Journal of Physical Chemistry A, 2022, 126, 3198-3209.	2.5	14
3	PDRs4All: A JWST Early Release Science Program on Radiative Feedback from Massive Stars. Publications of the Astronomical Society of the Pacific, 2022, 134, 054301.	3.1	26
4	Vibrational and Rovibrational Spectroscopy Applied to Astrochemistry. , 2022, , 235-295.		14
5	The unsolved issue with out-of-plane bending frequencies for C C multiply bonded systems. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119148.	3.9	12
6	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
7	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.	4.5	9
8	What It Takes to Compute Highly Accurate Rovibrational Line Lists for Use in Astrochemistry. Accounts of Chemical Research, 2021, 54, 1311-1321.	15.6	10
9	Modeling the infrared cascade spectra of small PAHs: the 11.2ÂÎ¼m band. Theoretical Chemistry Accounts, 2021, 140, 124.	1.4	8
10	PAH Spectroscopy from 1 to 5 Î¼m. Astrophysical Journal Letters, 2021, 917, L35.	8.3	8
11	Fundamental Vibrational Frequencies and Spectroscopic Constants of Substituted Cyclopropenylidene (c-C₃HX, X = F, Cl, CN). Journal of Physical Chemistry A, 2021, 125, 8860-8868.	2.5	8
12	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C₃H₂): the importance of numerical stability. Molecular Physics, 2020, 118, e1589007.	1.7	7
13	Highly Accurate Quartic Force Field and Rovibrational Spectroscopic Constants for the Azirinyl Cation (c-C₂NH₂⁺) and Its Isomers. Journal of Physical Chemistry A, 2020, 124, 362-370.	2.5	3
14	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.	2.8	8
15	Climate Metrics for C1â€“C4 Hydrofluorocarbons (HFCs). Journal of Physical Chemistry A, 2020, 124, 4793-4800.	2.5	5
16	Theoretical rovibrational characterization of the cis/trans-HCSH and H2SC isomers of the known interstellar molecule thioformaldehyde. Journal of Molecular Spectroscopy, 2020, 369, 111273.	1.2	11
17	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
18	Overcoming the out-of-plane bending issue in an aromatic hydrocarbon: the anharmonic vibrational frequencies of c-(CH)C₃H₂⁺. Physical Chemistry Chemical Physics, 2020, 22, 12951-12958.	2.8	11

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19	The Production and Potential Detection of Hexamethylenetetramine-Methanol in Space. Astrobiology, 2020, 20, 601-616.	3.0	15
20	Cation, Anion, and Radical Isomers of C4H4N: Computational Characterization and Implications for Astrophysical and Planetary Environments. Journal of Physical Chemistry A, 2020, 124, 2001-2013.	2.5	12
21	Exploring the limits of the Data-Model-Theory synergy: â€œHotâ€•MW transitions for rovibrational IR studies. Journal of Molecular Structure, 2020, 1217, 128260.	3.6	5
22	Computational vibrational spectroscopy for the detection of molecules in space. Annual Reports in Computational Chemistry, 2019, 15, 173-202.	1.7	59
23	The Calculated Infrared Spectra of Functionalized Hexamethylenetetramine (HMT) Molecules. Astrophysical Journal, 2019, 884, 64.	4.5	6
24	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.	2.3	15
25	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.	2.3	13
26	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
27	The possibility of :CNH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:msubsup><mml:mrow /><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:math> within Titanâ€™s atmosphere: Rovibrational analysis of :CNH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:msubsup><mml:mrow /><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:math> and :CCH2. Icarus, 2019, 321,	2.5	1
28	High Spectral Resolution SOFIA/EXES Observations of C₂H₂Âtoward Orion IRc2. Astrophysical Journal, 2018, 856, 9.	4.5	15
29	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
30	The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs. Physical Chemistry Chemical Physics, 2018, 20, 1189-1197.	2.8	46
31	Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. ACS Omega, 2018, 3, 16035-16039.	3.5	12
32	Fully anharmonic infrared cascade spectra of polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2018, 149, 134302.	3.0	37
33	Anharmonicity and the infrared emission spectrum of highly excited polycyclic aromatic hydrocarbons. Astronomy and Astrophysics, 2018, 618, A49.	5.1	14
34	Characterization of Azirine and Its Structural Isomers. Journal of Physical Chemistry A, 2018, 122, 8898-8904.	2.5	6
35	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
36	Rovibrational analysis of c-SiC2H2: Further evidence for out-of-plane bending issues in correlated methods. Journal of Chemical Physics, 2018, 149, 024303.	3.0	10

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37	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
38	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
39	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
40	Quantum Chemical Rovibrational Analysis of the HOSO Radical. Journal of Physical Chemistry A, 2017, 121, 8108-8114.	2.5	14
41	Mechanisms of the Formation of Adenine, Guanine, and Their Analogues in UV-Irradiated Mixed NH₃:H₂O Molecular Ices Containing Purine. Astrobiology, 2017, 17, 771-785.	3.0	25
42	Toward the laboratory identification of the not-so-simple NS2 neutral and anion isomers. Journal of Chemical Physics, 2017, 147, 074303.	3.0	5
43	Towards completing the cyclopropenylidene cycle: rovibrational analysis of cyclic N₃⁺, CNN, HCNN⁺, and CNC^{â^'}. Physical Chemistry Chemical Physics, 2017, 19, 22860-22869.	2.8	4
44	Communication: The failure of correlation to describe carbon=carbon bonding in out-of-plane bends. Journal of Chemical Physics, 2017, 147, 221101.	3.0	20
45	Mechanisms for the formation of thymine under astrophysical conditions and implications for the origin of life. Journal of Chemical Physics, 2016, 144, 144308.	3.0	21
46	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
47	Inclusion of 13C and D in protonated acetylene. Chemical Physics Letters, 2016, 650, 126-129.	2.6	13
48	Excited State Trends in Bidirectionally Expanded Closed-Shell PAH and PANH Anions. Journal of Physical Chemistry A, 2016, 120, 7327-7334.	2.5	8
49	Ames 32S16O18O line list for high-resolution experimental IR analysis. Journal of Molecular Spectroscopy, 2016, 330, 101-111.	1.2	13
50	Quantum Chemical Analysis of the COâ€“HNN⁺ Proton-Bound Complex. Journal of Physical Chemistry A, 2016, 120, 7745-7752.	2.5	12
51	INSIGHTS INTO HYDROCARBON CHAIN AND AROMATIC RING FORMATION IN THE INTERSTELLAR MEDIUM: COMPUTATIONAL STUDY OF THE ISOMERS OF AND AND THEIR FORMATION PATHWAYS. Astrophysical Journal, 2016, 830, 128.	4.5	11
52	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
53	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
54	Characterization of the Azirinyl Cation and Its Isomers. Journal of Physical Chemistry A, 2016, 120, 1275-1282.	2.5	13

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55	TOWARD THE ASTRONOMICAL DETECTION OF THE PROTON-BOUND COMPLEX NNâ€“HCO⁺: IMPLICATIONS FOR THE SPECTRA OF PROTOPLANETARY DISKS. Astrophysical Journal, 2016, 819, 141.	4.5	14
56	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
57	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS: THE REALM OF ANHARMONICITY. Astrophysical Journal, 2015, 814, 23.	4.5	51
58	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	3.0	42
59	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
60	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	2.5	81
61	Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. Journal of Physical Chemistry A, 2015, 119, 13048-13054.	2.5	13
62	Excited vibrational level rotational constants for SiC2: A sensitive molecular diagnostic for astrophysical conditions. Molecular Astrophysics, 2015, 1, 13-19.	1.6	60
63	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
64	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of C₄H₂⁺, C₆H₂⁺ and C₆H₄⁺ and their formation paths from acetylene and its fragments. Physical Chemistry Chemical Physics, 2015, 17, 1859-1869.	2.8	21
65	Rovibrational and energetic analysis of the hydroxyethynyl anion (CCOH^{â^'}). Molecular Physics, 2015, 113, 2012-2017.	1.7	9
66	Electronically excited states of PANH anions. Physical Chemistry Chemical Physics, 2015, 17, 14761-14772.	2.8	23
67	Linear transformation of anharmonic molecular force constants between normal and Cartesian coordinates. Journal of Chemical Physics, 2015, 142, 244107.	3.0	12
68	Photosynthesis and Photo-Stability of Nucleic Acids in Prebiotic Extraterrestrial Environments. Topics in Current Chemistry, 2014, 356, 123-164.	4.0	23
69	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
70	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OFc-C₃H^{â€“}. Astrophysical Journal, 2014, 796, 139.	4.5	17
71	Formation and Stability of C₆H₃⁺ Isomers. Journal of Physical Chemistry A, 2014, 118, 10109-10116.	2.5	8
72	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

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73	Fundamental Vibrational Frequencies and Spectroscopic Constants of cis- and trans-HOCS, HSCO, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry B, 2014, 118, 6498-6510.	2.6	16
74	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C₂H₃⁺, and Its Isotopologues. Journal of Physical Chemistry A, 2014, 118, 7034-7043.	2.5	75
75	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
76	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.	3.9	25
77	On the use of quartic force fields in variational calculations. Chemical Physics Letters, 2013, 574, 1-12.	2.6	66
78	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
79	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
80	Vibrational Frequencies and Spectroscopic Constants for 1 ³Aâ€² HNC and 1 ³Aâ€² HOC⁺ from High-Accuracy Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 11339-11345.	2.5	10
81	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
82	Association mechanisms of unsaturated C2 hydrocarbons with their cations: acetylene and ethylene. Physical Chemistry Chemical Physics, 2013, 15, 2012-2023.	2.8	21
83	The 1 ³Aâ€² HCN and 1 ³Aâ€² HCO⁺ Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 9324-9330.	2.5	23
84	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
85	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 1¹Aâ€²l-C₃H⁺: A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. Astrophysical Journal, 2013, 772, 39.	4.5	63
86	Protonated nitrous oxide, NNOH+: Fundamental vibrational frequencies and spectroscopic constants from quartic force fields. Journal of Chemical Physics, 2013, 139, 084313.	3.0	80
87	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.	3.0	11
88	ROVIBRATIONAL SPECTROSCOPIC CONSTANTS AND FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR ISOTOPOLOGUES OF CYCLIC AND BENT SINGLET HC₂N ISOMERS. Astrophysical Journal, 2013, 778, 160.	4.5	13
89	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.	3.0	8
90	THE POSSIBLE INTERSTELLAR ANION CH₂CN^{â€“}: SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. Astrophysical Journal, 2013, 762, 121.	4.5	38

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91	Quantum IR line list of NH3 and isotopologues for ISM and dwarf studies. Proceedings of the International Astronomical Union, 2012, 8, 248-248.	0.0	0
92	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
93	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
94	Photochemistry and Photophysics of n-Butanal, 3-Methylbutanal, and 3,3-Dimethylbutanal: Experimental and Theoretical Study. Journal of Physical Chemistry A, 2012, 116, 5830-5839.	2.5	17
95	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
96	A group increment scheme for infrared absorption intensities of greenhouse gases. Journal of Molecular Structure, 2012, 1009, 89-95.	3.6	6
97	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
98	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
99	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
100	SPECTROSCOPIC CONSTANTS FOR¹³C AND DEUTERIUM ISOTOPOLOGUES OF CYCLIC AND LINEAR C₃H₃⁺. Astrophysical Journal, 2011, 736, 33.	4.5	22
101	Initiating molecular growth in the interstellar medium via dimeric complexes of observed ions and molecules. Astronomy and Astrophysics, 2011, 535, A74.	5.1	18
102	The trans-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301.	3.0	116
103	Accurate ab initio quartic force fields of cyclic and bent HC2N isomers. Journal of Chemical Physics, 2011, 135, 244310.	3.0	33
104	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
105	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
106	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, 9049-9054.	7.1	18
107	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.	7.1	1
108	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

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109	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
110	Computational Interstellar Chemistry. Thirty Years of Astronomical Discovery With UKIRT, 2010, , 21-30.	0.3	0
111	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
112	An Approach to Include the Effects of Diffuse Functions in Potential Energy Surface Calculations. Journal of Physical Chemistry A, 2009, 113, 11954-11962.	2.5	7
113	Identifying the Molecular Origin of Global Warming. Journal of Physical Chemistry A, 2009, 113, 12694-12699.	2.5	44
114	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	27
115	Are isomers of the vinyl cyanide ion missing links for interstellar pyrimidine formation?. Journal of Chemical Physics, 2009, 131, 074303.	3.0	21
116	An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH3. Journal of Chemical Physics, 2008, 129, 214304.	3.0	70
117	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
118	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
119	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
120	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
121	Search for Stratospheric Bromine Reservoir Species:Â Theoretical Study of the Photostability of Mono-, Tri-, and Pentacoordinated Bromine Compounds. Journal of Physical Chemistry A, 2005, 109, 8133-8139.	2.5	5
122	Theoretical Study of Chlorine Nitrates: Implications for Stratospheric Chlorine Chemistry.. ChemInform, 2003, 34, no.	0.0	0
123	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
124	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
125	Theoretical Study of Chlorine Nitrates:Â Implications for Stratospheric Chlorine Chemistry. Journal of the American Chemical Society, 2003, 125, 10446-10458.	13.7	4
126	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

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127	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.	1.0	3
128	Theoretical study of infrared and Raman spectra of hydrated magnesium sulfate salts. Journal of Chemical Physics, 2002, 117, 2532-2537.	3.0	35
129	An accurate quartic force field, fundamental frequencies, and binding energy for the high energy density material TdN4. Chemical Physics Letters, 2002, 357, 319-325.	2.6	26
130	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
131	Towards the synthesis of the high energy density material TdN4: excited electronic states. Chemical Physics Letters, 2001, 345, 295-302.	2.6	22
132	Theoretical study of XONO2 (X=Br, OBr, O2Br): Implications for stratospheric bromine chemistry. Journal of Chemical Physics, 2000, 113, 145-152.	3.0	15
133	Accurate calculations on excited states: new theories applied to the â€“OX, â€“XO, and â€“XO2 (X=Cl and) Tj ETQq1 1 0.784314 rgBT / A: Molecular and Biomolecular Spectroscopy, 1999, 55, 561-574.	3.9	19
134	Accurate spectroscopic characterization of 12C14Nâ¯, 13C14Nâ¯, and 12C15Nâ¯. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 739-747.	3.9	16
135	Accurateab initioanharmonic force field and heat of formation for silane. Molecular Physics, 1999, 97, 945-953.	1.7	30
136	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. Molecular Physics, 1999, 96, 633-643.	1.7	25
137	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
138	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. Molecular Physics, 1999, 96, 633-643.	1.7	1
139	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.	3.0	20
140	A purely ab initio spectroscopic quality quartic force field for acetylene. Journal of Chemical Physics, 1998, 108, 676-691.	3.0	128
141	Adiabatic electron affinity and ionization potential for BrO radical. Journal of Chemical Physics, 1998, 109, 10818-10822.	3.0	18
142	Density functional and coupled-cluster study on the HNOâ†'HON transition state. Journal of Chemical Physics, 1997, 107, 8208-8209.	3.0	8
143	Ab initio quartic force fields for anions: A benchmark study on 16OHâ¯, 18OHâ¯, and 16ODâ¯. Journal of Chemical Physics, 1997, 107, 10373-10380.	3.0	14
144	Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. Journal of Chemical Physics, 1997, 107, 9980-9984.	3.0	31

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145	SINGLE REFERENCE COUPLED CLUSTER AND PERTURBATION THEORIES OF ELECTRONIC EXCITATION ENERGIES. Recent Advances in Computational, 1997, , 221-253.	0.8	15
146	A new spin-restricted triple excitation correction for coupled cluster theory. Journal of Chemical Physics, 1997, 107, 7943-7950.	3.0	27
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