Edwin L Sibert Iii

List of Publications by Year
in descending order

107 papers	4,079 citations	117625 34 h-index	128289 60 g-index
107 all docs	107 docs citations	107 times ranked	1786 citing authors

#	Article	IF	Citations
1	Intramolecular vibrational relaxation and spectra of CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1115-1134.	3.0	330
2	Theoretical modeling of the OH stretch infrared spectrum of carboxylic acid dimers based on first-principles anharmonic couplings. Journal of Chemical Physics, 2003, 118, 1735-1746.	3.0	203
3	Classical dynamics of energy transfer between bonds in ABA triatomics. Journal of Chemical Physics, 1982, 77, 3583-3594.	3.0	202
4	Theoretical studies of vibrationally excited polyatomic molecules using canonical Van Vleck perturbation theory. Journal of Chemical Physics, 1988, 88, 4378-4390.	3.0	189
5	Classical dynamics of highly excited CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1135-1144.	3.0	170
6	Quantum mechanics of local mode ABA triatomic molecules. Journal of Chemical Physics, 1982, 77, 3595-3604.	3.0	143
7	A nine-dimensional perturbative treatment of the vibrations of methane and its isotopomers. Journal of Chemical Physics, 1999, 111, 4510-4522.	3.0	99
8	Intramolecular vibrational relaxation of CH overtones in benzene. Chemical Physics Letters, 1982, 92, 455-458.	2.6	92
9	Perturbative calculations of vibrational (J=0) energy levels of linear molecules in normal coordinate representations. Journal of Chemical Physics, 1991, 95, 3476-3487.	3.0	88
10	Variational and perturbative descriptions of highly vibrationally excited molecules. International Reviews in Physical Chemistry, 1990, 9, 1-27.	2.3	87
11	Rotationâ€“vibration interactions in highly excited states of SO2and H2CO. Journal of Chemical Physics, 1991, 95, 7449-7465.	3.0	87
12	The relative reactivity of CH3D molecules with excited symmetric and antisymmetric stretching vibrations. Journal of Chemical Physics, 2003, 119, 9568-9575.	3.0	87
13	An accurate quartic force field for formaldehyde. Journal of Chemical Physics, 1996, 104, 480-487.	3.0	69
14	Rotationally induced vibrational mixing in formaldehyde. Journal of Chemical Physics, 1989, 90, 2672-2683.	3.0	67
15	Quantum, semiclassical and classical dynamics of the bending modes of acetylene. Journal of Chemical Physics, 1996, 105, 469-478.	3.0	66
16	Anharmonic force field and vibrational frequencies of tetrafluoromethane (CF4) and tetrafluorosilane (SiF4). Journal of Chemical Physics, 2000, 112, 1353-1366.	3.0	64
17	Vibrational relaxation in liquid chloroform following ultrafast excitation of the CH stretch fundamental. Journal of Chemical Physics, 2002, 116, 237.	3.0	64
18	Quantum dynamics of energy transfer between bonds in coupled Morse oscillator systems. Journal of Chemical Physics, 1984, 81, 1314-1326.	3.0	63

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19	Complete active space selfâ€consistent field potential energy surfaces, dipole moment functions, and spectroscopic properties of O3, CF2, NOâ^'2, and NF+2. Journal of Chemical Physics, 1991, 94, 414-430.	3.0	57
20	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â^'. Journal of Chemical Physics, 2000, 112, 4053-4063.	3.0	57
21	Large anharmonic effects in the infrared spectra of the symmetrical CH3NO2â^'â‹…(H2O) and CH3CO2â^'â‹…(H2O) complexes. Journal of Chemical Physics, 2003, 119, 10138-10145.	3.0	57
22	VANVLK: An algebraic manipulation program for canonical Van Vleck perturbation theory. Computer Physics Communications, 1988, 51, 149-160.	7.5	54
23	The bending dynamics of acetylene. Journal of Chemical Physics, 1996, 105, 459-468.	3.0	54
24	Symmetric Double Proton Tunneling in Formic Acid Dimer:â€‰ A Diabatic Basis Approach. Journal of Physical Chemistry B, 2008, 112, 595-603.	2.6	53
25	Towards a first-principles model of Fermi resonance in the alkyl CH stretch region: Application to 1,2-diphenylethane and 2,2,2-paracyclophane. Journal of Chemical Physics, 2013, 138, 064308.	3.0	46
26	Calculation of infrared intensities of highly excited vibrational states of HCN using Van Vleck perturbation theory. Journal of Chemical Physics, 1991, 95, 3488-3493.	3.0	42
27	Isomer-Specific Spectroscopy of Benzeneâ€“(H₂O)_n, n = 6,7: Benzeneâ€™s Role in Reshaping Waterâ€™s Three-Dimensional Networks. Journal of Physical Chemistry Letters, 2015, 6, 1989-1995.	4.6	42
28	Fermi Resonance Effects in the Vibrational Spectroscopy of Methyl and Methoxy Groups. Journal of Physical Chemistry A, 2014, 118, 11272-11281.	2.5	41
29	Highly excited vibrational states of acetylene: A variational calculation. Journal of Chemical Physics, 1993, 99, 937-944.	3.0	40
30	Variable curvature coordinates for molecular vibrations. Journal of Chemical Physics, 1989, 91, 350-363.	3.0	38
31	Theoretical studies of the potential surface and vibrational spectroscopy of CH3OH and its deuterated analogs. Journal of Chemical Physics, 2005, 122, 194306.	3.0	38
32	Anharmonic modeling of the conformation-specific IR spectra of ethyl, n-propyl, and n-butylbenzene. Journal of Chemical Physics, 2016, 144, 224310.	3.0	37
33	Rotationâ€“vibration interactions between the two lowest frequency modes in formaldehyde. Journal of Chemical Physics, 1988, 89, 7201-7216.	3.0	35
34	Intensities of forbidden pure torsional bands inS1â€“S0spectra of toluenes. Journal of Chemical Physics, 1995, 102, 8718-8724.	3.0	35
35	A perturbative calculation of the rovibrational energy levels of methane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 863-872.	3.9	33
36	Full dimensional theoretical study of the torsion-vibration eigenstates and torsional splittings of CH3OH. Journal of Chemical Physics, 2003, 119, 11671-11681.	3.0	32

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37	Combined perturbative-variational investigation of the vibrations of CHBr3 and CDBr3. Journal of Chemical Physics, 2004, 120, 11011-11025.	3.0	32
38	Comparison of Perturbative and Variational Treatments of Molecular Vibrations:Â Application to the Vibrational Spectrum of HFCO up to 8000 cm-1â€. Journal of Physical Chemistry A, 2006, 110, 5420-5429.	2.5	31
39	The effects of asymmetric motions on the tunneling splittings in formic acid dimer. Journal of Chemical Physics, 2008, 129, 164317.	3.0	31
40	A First-Principles Model of Fermi Resonance in the Alkyl CH Stretch Region: Application to Hydronaphthalenes, Indanes, and Cyclohexane. Journal of Physical Chemistry B, 2014, 118, 8236-8245.	2.6	30
41	Infrared absorption of CH3O and CD3O radicals isolated in solid para-H2. Journal of Molecular Spectroscopy, 2015, 310, 57-67.	1.2	30
42	Local Mode Approach to OH Stretch Spectra of Benzeneâ€“(H₂O)_n Clusters, n = 2â€“7. Journal of Physical Chemistry A, 2015, 119, 9917-9930.	2.5	30
43	Modeling vibrational anharmonicity in infrared spectra of high frequency vibrations of polyatomic molecules. Journal of Chemical Physics, 2019, 150, 090901.	3.0	29
44	Coupled cluster anharmonic force fields, spectroscopic constants, and vibrational energies of AlF3 and SiF3+. Journal of Chemical Physics, 1997, 107, 1717-1724.	3.0	28
45	Ground State Conformational Preferences and CH Stretchâ€“Bend Coupling in a Model Alkoxy Chain: 1,2-Diphenoxyethane. Journal of Physical Chemistry A, 2013, 117, 2800-2811.	2.5	27
46	A nine-dimensional high order perturbative study of the vibration of silane and its isotopomers. Journal of Chemical Physics, 2000, 113, 5384.	3.0	26
47	Vibrational Energy Relaxation of the OH Stretch in Liquid Methanol. Journal of Physical Chemistry A, 2004, 108, 2389-2401.	2.5	26
48	Assignment and Extraction of Dynamics of a Small Molecule with a Complex Vibrational Spectrum:Â Thiophosgeneâ€. Journal of Physical Chemistry A, 2006, 110, 5317-5325.	2.5	26
49	An equilibrium focused approach to calculating the Raman spectrum of the symmetric OH stretch in formic acid dimer. Journal of Molecular Spectroscopy, 2008, 249, 78-85.	1.2	26
50	Theory of vibrationally mediated photodissociation of HOOH: Delocalized tails in a localized wave function. Journal of Chemical Physics, 1991, 94, 6519-6545.	3.0	25
51	A study of the vibrations of fluoroform with a sixth order nine-dimensional potential: a combined perturbative-variational approach. Molecular Physics, 2005, 103, 149-162.	1.7	25
52	Fluctuating Energy Level Landauâ^'Teller Theory:â€‰ Application to the Vibrational Energy Relaxation of Liquid Methanol. Journal of Physical Chemistry A, 2005, 109, 5777-5780.	2.5	25
53	Identifying the first folded alkylbenzene via ultraviolet, infrared, and Raman spectroscopy of pentylbenzene through decylbenzene. Chemical Science, 2017, 8, 5305-5318.	7.4	25
54	Local-Mode Approach to Modeling Multidimensional Infrared Spectra of Metal Carbonyls. Journal of Physical Chemistry A, 2011, 115, 5354-5363.	2.5	24

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55	Derivation of rotation-vibration Hamiltonians that satisfy the Casimir condition. Journal of Chemical Physics, 1997, 106, 6618-6621.	3.0	23
56	Dressed local mode Hamiltonians for CH stretch vibrations. Molecular Physics, 2013, 111, 2093-2099.	1.7	23
57	Determining potentialâ€energy surfaces from spectra: An iterative approach. Journal of Chemical Physics, 1992, 97, 2938-2947.	3.0	22
58	Fully and Partially Coherent Pathways in Multiply Enhanced Odd-Order Wave-Mixing Spectroscopy. Journal of Physical Chemistry A, 2010, 114, 817-832.	2.5	22
59	Investigating optimal coordinates for describing vibrational motion. Theoretica Chimica Acta, 1995, 92, 107-122.	0.8	21
60	The Effectiveness of Newton's Method for ImprovingAb InitioForce Fields with Applications to CO2and H2CO. Journal of Molecular Spectroscopy, 1998, 187, 167-178.	1.2	21
61	Fingerprints of inter- and intramolecular hydrogen bonding in saligeninâ€“water clusters revealed by mid- and far-infrared spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 20343-20356.	2.8	21
62	A threeâ€dimensional semiclassical quantization of H2O. Journal of Chemical Physics, 1985, 83, 5092-5104.	3.0	20
63	Trigonometric discrete variable representations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, L513-L516.	1.5	20
64	Infrared laser spectroscopy of the n-propyl and i-propyl radicals: Stretch-bend Fermi coupling in the alkyl CH stretch region. Journal of Chemical Physics, 2016, 145, 224304.	3.0	19
65	A random matrix approach to rotationâ€“vibration mixing in H2CO and D2CO. Journal of Chemical Physics, 1993, 98, 8419-8431.	3.0	18
66	Vibrational dynamics around the conical intersection: a study of methoxy vibrations on the X̃ƒ2E surface. Physical Chemistry Chemical Physics, 2010, 12, 8250.	2.8	18
67	Modeling the CH Stretch Vibrational Spectroscopy of M⁺[Cyclohexane] (M = Li, Na, and K) Ions. Journal of Physical Chemistry A, 2015, 119, 10293-10299.	2.5	18
68	Exact vibration-rotation kinetic energy operators in two sets of valence coordinates for centrally connected penta-atomic molecules. Molecular Physics, 2000, 98, 317-326.	1.7	17
69	Conformation-specific spectroscopy of alkyl benzyl radicals: Effects of a radical center on the CH stretch infrared spectrum of an alkyl chain. Journal of Chemical Physics, 2016, 145, 124314.	3.0	17
70	Infrared absorption spectra of partially deuterated methoxy radicals CH2DO and CHD2O isolated in solid para-hydrogen. Journal of Chemical Physics, 2017, 147, 154305.	3.0	16
71	Tunneling splittings in formic acid dimer: An adiabatic approximation to the Herring formula. Journal of Chemical Physics, 2015, 142, 084115.	3.0	15
72	Distributed Gaussian polynomials and associated Gaussian quadratures. Journal of Mathematical Physics, 1997, 38, 4815-4831.	1.1	14

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73	Vibrational energy relaxation of the OH(D) stretch fundamental of methanol in carbon tetrachloride. Journal of Chemical Physics, 2005, 123, 204508.	3.0	14
74	Combination of perturbative and variational methods for calculating molecular spectra: Calculation of the Ï…=3â€“5 CH stretch overtone spectrum of CHF3. Journal of Chemical Physics, 2006, 124, 114307.	3.0	14
75	Vibrational Relaxation of OH and CH Fundamentals of Polar and Nonpolar Molecules in the Condensed Phase. Journal of Physical Chemistry A, 2008, 112, 11291-11305.	2.5	14
76	Ground and excited state infrared spectroscopy of jet-cooled radicals: Exploring the photophysics of trihydronaphthyl and inden-2-ylmethyl. Journal of Chemical Physics, 2014, 140, 214302.	3.0	14
77	The Raman jet spectrum of trans-formic acid and its deuterated isotopologs: Combining theory and experiment to extend the vibrational database. Journal of Chemical Physics, 2021, 154, 064301.	3.0	14
78	A perturbative study of low-order resonances and chaos in the kinetically coupled two-degree-of-freedom morse system using lie transforms. Chemical Physics Letters, 1986, 128, 404-410.	2.6	13
79	An algebraic approach to calculating rotation-vibration spectra of polyatomic molecules. Molecular Physics, 1992, 77, 697-708.	1.7	13
80	A theoretical study of the vibrational spectrum of the CS2 molecule. Journal of Chemical Physics, 2002, 116, 7495-7508.	3.0	13
81	Infrared Spectra at a Conical Intersection: Vibrations of Methoxy. Journal of Physical Chemistry A, 2012, 116, 3846-3855.	2.5	13
82	Relaxation of the CH stretch in liquid CHBr3: Solvent effects and decay rates using classical nonequilibrium simulations. Journal of Chemical Physics, 2006, 125, 244513.	3.0	12
83	Time scales and pathways of vibrational energy relaxation in liquid CHBr3 and CDBr3. Journal of Chemical Physics, 2006, 125, 244512.	3.0	12
84	Cyclohexane Vibrations: High-Resolution Spectra and Anharmonic Local Mode Calculations. Journal of Physical Chemistry A, 2020, 124, 9991-10000.	2.5	12
85	Surface hopping simulation of vibrational predissociation of methanol dimer. Journal of Chemical Physics, 2012, 136, 224104.	3.0	11
86	Vibrational relaxation of the CH stretch fundamental in liquid CHBr3. Journal of Chemical Physics, 2006, 124, 234501.	3.0	10
87	Isobutane Infrared Bands: Partial Rotational Assignments, ab Initio Calculations, and Local Mode Analysis. Journal of Physical Chemistry A, 2019, 123, 6185-6193.	2.5	10
88	The missing NH stretch fundamental in S₁ methyl anthranilate: IR-UV double resonance experiments and local mode theory. Physical Chemistry Chemical Physics, 2020, 22, 14077-14087.	2.8	10
89	Elucidating energy disposal pathways following excitation of the symmetric OH stretching band in formic acid dimer. Chemical Physics Letters, 2008, 460, 42-45.	2.6	9
90	Spectroscopic Manifestations of Indirect Vibrational State Mixing: Novel Anharmonic Effects on a Prereactive H Atom Transfer Surface. Journal of Physical Chemistry A, 2021, 125, 7318-7330.	2.5	9

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91	How Do Hydrogen Bonds Break in Small Alcohol Oligomers?. Journal of Physical Chemistry A, 2009, 113, 7275-7285.	2.5	7
92	Simulation of laser excitation spectrum of CH3O and CD3O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 90-99.	3.9	7
93	Vibronic spectroscopy of methyl anthranilate and its water complex: hydrogen atom dislocation in the excited state. Physical Chemistry Chemical Physics, 2019, 21, 21355-21369.	2.8	7
94	The effect of nonadiabatic coupling on the calculation of N(E,J) for the methane association reaction. Journal of Chemical Physics, 1998, 109, 8897-8906.	3.0	5
95	Assigning the low lying vibronic states of CH3O and CD3O. Journal of Chemical Physics, 2017, 146, 174112.	3.0	5
96	Infrared-Enhanced Fluorescence-Gain Spectroscopy: Conformation-Specific Excited-State Infrared Spectra of Alkylbenzenes. Journal of Physical Chemistry Letters, 2017, 8, 5296-5300.	4.6	5
97	Neopentane Vibrations: High Resolution Spectra and Anharmonic Calculations. Journal of Physical Chemistry A, 2020, 124, 3438-3444.	2.5	5
98	Single-conformation spectroscopy of cold, protonated ^DPG-containing peptides: switching Î²-turn types and formation of a sequential type II/IIâ€² double Î²-turn. Physical Chemistry Chemical Physics, 2022, 24, 2095-2109.	2.8	5
99	Self-thermophoresis at the nanoscale using light induced solvation dynamics. Nanoscale, 2020, 12, 7557-7562.	5.6	4
100	A phase diagram for energy flow-limited reactivity. Journal of Chemical Physics, 2021, 154, 104301.	3.0	3
101	A perturbative treatment of classical vibrationalâ€“translational energy transfer in collinear collisions of an atom and a diatomic molecule. Chemical Physics Letters, 1999, 307, 437-444.	2.6	2
102	Investigating optimal coordinates for describing vibrational motion. Theoretica Chimica Acta, 1995, 92, 107.	0.8	2
103	A local mode study of ring puckering effects in the infrared spectra of cyclopentane. Journal of Chemical Physics, 0, , .	3.0	2
104	Vibrational relaxation of chloroiodomethane in cold argon. Journal of Chemical Physics, 2013, 139, 144312.	3.0	1
105	Local mode energy transfer: Ebb and flow. International Journal of Quantum Chemistry, 1982, 22, 375-383.	2.0	0
106	A perturbative description of non-adiabatic effects in methoxy vibrations. Molecular Physics, 2014, 112, 3138-3143.	1.7	0
107	Large-Scale, Team-Based Curriculum Transformation and Student Engagement in General Chemistry I and II. ACS Symposium Series, 2019, , 113-134.	0.5	0