Xinchuan Huang

List of Publications by Year
in descending order

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86 papers	5,192 citations	61984 43 h-index	85541 71 g-index
88 all docs	88 docs citations	88 times ranked	2456 citing authors

#	Article	IF	Citations
1	MULTIMODE: A code to calculate rovibrational energies of polyatomic molecules. International Reviews in Physical Chemistry, 2003, 22, 533-549.	2.3	413
2	Ab initio potential energy and dipole moment surfaces for H5O2+. Journal of Chemical Physics, 2005, 122, 044308.	3.0	257
3	Flexible, ab initio potential, and dipole moment surfaces for water. I. Tests and applications for clusters up to the 22-mer. Journal of Chemical Physics, 2011, 134, 094509.	3.0	238
4	The vibrational predissociation spectra of the H5O2+â^™RGn(RG=Ar,Ne) clusters: Correlation of the solvent perturbations in the free OH and shared proton transitions of the Zundel ion. Journal of Chemical Physics, 2005, 122, 244301.	3.0	228
5	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
6	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
7	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
8	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
9	The trans-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301.	3.0	116
10	Ab Initio Potential Energy and Dipole Moment Surfaces of (H2O)2â€. Journal of Physical Chemistry A, 2006, 110, 445-451.	2.5	115
11	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
12	New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2008, 128, 034312.	3.0	104
13	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
14	Full-dimensional vibrational calculations for H5O2+ using an ab initio potential energy surface. Journal of Chemical Physics, 2005, 122, 061101.	3.0	97
15	Quantum Deconstruction of the Infrared Spectrum of CH5+. Science, 2006, 311, 60-63.	12.6	97
16	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	4.6	97
17	The importance of an accurate CH4 vibrational partition function in full dimensionality calculations of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2001, 114, 9683-9684.	3.0	89
18	Ab Initio Diffusion Monte Carlo Calculations of the Quantum Behavior of CH5+ in Full Dimensionality. Journal of Physical Chemistry A, 2004, 108, 4991-4994.	2.5	87

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19	Quantum studies of the vibrations in H3O2â^' and D3O2â^'. Journal of Chemical Physics, 2005, 123, 064317.	3.0	83
20	Protonated nitrous oxide, NNOH+: Fundamental vibrational frequencies and spectroscopic constants from quartic force fields. Journal of Chemical Physics, 2013, 139, 084313.	3.0	80
21	A theoretical study of vibrational mode coupling in H5O2+. Journal of Chemical Physics, 2003, 119, 6571-6580.	3.0	79
22	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
23	Quantum Calculations of Vibrational Energies of H3O2-on an ab Initio Potential. Journal of the American Chemical Society, 2004, 126, 5042-5043.	13.7	77
24	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
25	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
26	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C₂H₃⁺, and Its Isotopologues. Journal of Physical Chemistry A, 2014, 118, 7034-7043.	2.5	75
27	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
28	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
29	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
30	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
31	An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH3. Journal of Chemical Physics, 2008, 129, 214304.	3.0	70
32	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
33	On the use of quartic force fields in variational calculations. Chemical Physics Letters, 2013, 574, 1-12.	2.6	66
34	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
35	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 1¹Aâ€²l-C₃H^{â€“}: A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. Astrophysical Journal, 2013, 772, 39.	4.5	63
36	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

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37	Ab initio potential energy surface and rovibrational energies of H3O+ and its isotopomers. Journal of Chemical Physics, 2003, 118, 5431-5441.	3.0	61
38	Vibrational Levels of Methanol Calculated by the Reaction Path Version of MULTIMODE, Using an ab initio, Full-Dimensional Potentialâ€. Journal of Physical Chemistry A, 2007, 111, 7317-7321.	2.5	61
39	Argon Predissociation Spectroscopy of the OH-Â·H2O and Cl-Â·H2O Complexes in the 1000â^'1900 cm-1Region:Â Intramolecular Bending Transitions and the Search for the Shared-Proton Fundamental in the Hydroxide Monohydrate. Journal of Physical Chemistry A, 2005, 109, 571-575.	2.5	56
40	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
41	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
42	HIGH-RESOLUTION IR ABSORPTION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS: THE REALM OF ANHARMONICITY. Astrophysical Journal, 2015, 814, 23.	4.5	51
43	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
44	The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs. Physical Chemistry Chemical Physics, 2018, 20, 1189-1197.	2.8	46
45	Full Dimensional Quantum Calculations of Vibrational Energies of H5O2+. Journal of Physical Chemistry A, 2003, 107, 7142-7151.	2.5	45
46	Deuteration Effects on the Structure and Infrared Spectrum of CH5+. Journal of the American Chemical Society, 2006, 128, 3478-3479.	13.7	45
47	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
48	Ab Initio Potential Energy Surface and Vibrational Energies of H3O+and Its Isotopomersâ€. Journal of Physical Chemistry B, 2002, 106, 8182-8188.	2.6	37
49	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
50	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
51	The determination of molecular properties from MULTIMODE with an application to the calculation of Franckâ€“Condon factors for photoionization of CF3to. Molecular Physics, 2006, 104, 33-45.	1.7	34
52	Tests of MULTIMODE calculations of rovibrational energies of CH4. Chemical Physics Letters, 2006, 426, 285-289.	2.6	34
53	Accurate ab initio quartic force fields of cyclic and bent HC2N isomers. Journal of Chemical Physics, 2011, 135, 244310.	3.0	33
54	Full dimensional calculations of vibrational energies of H3O+ and D3O+. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 839-848.	3.9	30

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55	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
56	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
57	Comparison of quantum, classical, and ring-polymer molecular dynamics infra-red spectra of Clâ¯(H2O) and H+(H2O)2. Chemical Physics Letters, 2008, 450, 253-257.	2.6	28
58	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
59	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
60	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
61	SPECTROSCOPIC CONSTANTS FOR¹³C AND DEUTERIUM ISOTOPOLOGUES OF CYCLIC AND LINEAR C₃H₃⁺. Astrophysical Journal, 2011, 736, 33.	4.5	22
62	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OFc-C₃H^{â“}. Astrophysical Journal, 2014, 796, 139.	4.5	17
63	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
64	High Spectral Resolution SOFIA/EXES Observations of C₂H₂Âtoward Orion IRc2. Astrophysical Journal, 2018, 856, 9.	4.5	15
65	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
66	ROVIBRATIONAL SPECTROSCOPIC CONSTANTS AND FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR ISOTOPOLOGUES OF CYCLIC AND BENT SINGLET HC₂N ISOMERS. Astrophysical Journal, 2013, 778, 160.	4.5	13
67	Ames 32S16O18O line list for high-resolution experimental IR analysis. Journal of Molecular Spectroscopy, 2016, 330, 101-111.	1.2	13
68	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
69	Linear transformation of anharmonic molecular force constants between normal and Cartesian coordinates. Journal of Chemical Physics, 2015, 142, 244107.	3.0	12
70	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
71	Comparison of classical, new corrected-classical, and semiclassical IR spectra of non-rotating H2O with quantum calculations. Chemical Physics Letters, 2004, 384, 80-85.	2.6	10
72	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

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73	Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy. Advances in Physical Chemistry, 2012, 2012, 1-4.	2.0	9
74	Comparison of independently calculated ab initio normal-mode displacements for the three Câ€“H stretching vibrations of methanol along the internal rotation path. Journal of Molecular Spectroscopy, 2014, 299, 11-16.	1.2	9
75	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
76	Comment on â€œNature of the Chemical Bond in Protonated Methaneâ€• Journal of Physical Chemistry A, 2007, 111, 2033-2034.	2.5	8
77	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
78	Communication: Prediction of the rate constant of bimolecular hydrogen exchange in the water dimer using an ab initio potential energy surface. Journal of Chemical Physics, 2010, 133, 111103.	3.0	7
79	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
80	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
81	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
82	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
83	A collaborative 14NH3 IR spectroscopic analysis at 6000 cmâ^’1. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 280, 108076.	2.3	2
84	Full Dimensional Quantum Calculations of Vibrational Energies of H5O+2.. ChemInform, 2003, 34, no.	0.0	0
85	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
86	SO₂ and CO₂ IR line lists for atmospheric modeling on Venus and Exoplanets. Proceedings of the International Astronomical Union, 2015, 11, .	0.0	0