Guntram Rauhut

List of Publications by Year
in descending order

94 papers	6,149 citations	147566 31 h-index	69108 77 g-index
95 all docs	95 docs citations	95 times ranked	4206 citing authors

#	Article	IF	Citations
1	Quantum chemical rovibrational analysis of aminoborane and its isotopologues. Journal of Computational Chemistry, 2023, 44, 298-306.	1.5	4
2	Advances in vibrational configuration interaction theory â€•part 2: Fast screening of the correlation space. Journal of Computational Chemistry, 2022, 43, 6-18.	1.5	19
3	Efficient and automated quantum chemical calculation of rovibrational nonresonant Raman spectra. Journal of Chemical Physics, 2022, 156, 124102.	1.2	9
4	A combined computational and experimental study on the vibrational structure of ethynyl isothiocyanate, HCCNCS, a molecule with a Champagne bottle potential. Journal of Molecular Spectroscopy, 2022, , 111626.	0.4	0
5	Structure, energetics, and spectroscopy of the chromophores of HHe+n, H₂He+n, and He+n clusters and their deuterated isotopologues. Physical Chemistry Chemical Physics, 2022, , .	1.3	2
6	Comparison of body definitions for incremental vibrational configuration interaction theory (iVCI). Journal of Chemical Physics, 2022, 156, 174103.	1.2	2
7	Vibrational Configuration Interaction Theory. , 2022, , 1-40.		8
8	VCI Calculations Based on Canonical and Localized Normal Coordinates for Non-Abelian Molecules: Accurate Assignment of the Vibrational Overtones of Allene. Journal of Physical Chemistry A, 2021, 125, 990-998.	1.1	7
9	Vibrational spectrum and photochemistry of phosphaketene HPCO. Physical Chemistry Chemical Physics, 2021, 23, 19237-19243.	1.3	9
10	Incremental vibrational configuration interaction theory, iVCI: Implementation and benchmark calculations. Journal of Chemical Physics, 2021, 154, 124114.	1.2	10
11	Parity-violation effects in the vibrational spectra of CHFClBr and CDFClBr. Physical Review A, 2021, 103, .	1.0	6
12	The simplest alkynyl thiocyanate HCCSCN and its isomers. Chemical Communications, 2021, 57, 3343-3346.	2.2	1
13	Advances in vibrational configuration interaction theory â€•part 1: Efficient calculation of vibrational angular momentum terms. Journal of Computational Chemistry, 2021, 42, 2321-2333.	1.5	17
14	Modal optimisation within the time-independent eigenstate-free Raman wavefunction formalism. Molecular Physics, 2020, 118, .	0.8	0
15	The interplay of VSCF/VCI calculations and matrix-isolation IR spectroscopy â€“ Mid infrared spectrum of CH3CH2F and CD3CD2F. Journal of Molecular Spectroscopy, 2020, 367, 111224.	0.4	22
16	The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide. Angewandte Chemie - International Edition, 2020, 59, 21949-21953.	7.2	10
17	The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide. Angewandte Chemie, 2020, 132, 22133-22137.	1.6	1
18	Ab initio calculation of rovibrational states for non-degenerate double-well potentials: cisâ€“trans isomerization of HOPO. Journal of Chemical Physics, 2020, 152, 174306.	1.2	11

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19	Account of non-Condon effects in time-independent Raman wavefunction theory: Calculation of the S1 â†•S0 vibronic absorption spectrum of formaldehyde. Journal of Chemical Physics, 2020, 152, 114109.	1.2	0
20	Hydrogenâ€Atom Tunneling in Metaphosphorous Acid. Chemistry - A European Journal, 2020, 26, 8174-8174.	1.7	0
21	Assignment of vibrational states within configuration interaction calculations. Journal of Chemical Physics, 2020, 152, 194112.	1.2	11
22	Toward a fully automated calculation of rovibrational infrared intensities for semi-rigid polyatomic molecules. Journal of Chemical Physics, 2020, 152, 244104.	1.2	29
23	Hydrogenâ€Atom Tunneling in Metaphosphorous Acid. Chemistry - A European Journal, 2020, 26, 8205-8209.	1.7	10
24	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603
25	High-Level Rovibrational Calculations on Ketenimine. Frontiers in Chemistry, 2020, 8, 623641.	1.8	13
26	The Simplest, Isolable, Alkynyl Isocyanate HCâ‰¡CNCO: Synthesis and Characterization. Angewandte Chemie - International Edition, 2019, 58, 17277-17281.	7.2	9
27	Phosphorus Analogues of Methyl Nitrite and Nitromethane: CH₃OPO and CH₃PO₂. Angewandte Chemie - International Edition, 2019, 58, 12164-12169.	7.2	22
28	Localized Normal Coordinates in Accurate Vibrational Structure Calculations: Benchmarks for Small Molecules. Journal of Chemical Theory and Computation, 2019, 15, 4187-4196.	2.3	21
29	Toward fast and accurate ab initio calculation of magnetic exchange in polynuclear lanthanide complexes. Physical Chemistry Chemical Physics, 2019, 21, 9769-9778.	1.3	12
30	Accurate Vibrational Configuration Interaction Calculations on Diborane and Its Isotopologues. Journal of Physical Chemistry A, 2019, 123, 3367-3373.	1.1	15
31	Vibrational analysis of methyl cationâ€”Rare gas atom complexes: CH3+â€”Rg (Rg = He, Ne, Ar, Kr). Journal of Chemical Physics, 2019, 150, 084306.	1.2	11
32	Vibrational analysis of nitrosamine, a molecule with an almost constant potential along the inversion coordinate. Molecular Physics, 2019, 117, 1741-1745.	0.8	7
33	Refined analysis of the XÌƒâ€‰2A2â†XÌƒâ€‰1A1 photoelectron spectrum of furan. Journal of Chemical Physics, 2018, 148, 054306.	1.2	2
34	Exchange coupling and single molecule magnetism in redox-active tetraoxolene-bridged dilanthanide complexes. Chemical Science, 2018, 9, 1221-1230.	3.7	70
35	Rigorous use of symmetry within the construction of multidimensional potential energy surfaces. Journal of Chemical Physics, 2018, 149, 164110.	1.2	34
36	Crystal Field Splittings in Lanthanide Complexes: Inclusion of Correlation Effects beyond Second Order Perturbation Theory. Journal of Chemical Theory and Computation, 2018, 14, 3998-4009.	2.3	6

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37	A new efficient method for the calculation of interior eigenpairs and its application to vibrational structure problems. Journal of Chemical Physics, 2017, 146, 124101.	1.2	32
38	A General Approach for Calculating Strongly Anharmonic Vibronic Spectra with a High Density of States: The XÌƒ²B₁ â†•XÌƒ¹A₁ Photoelectron Spectrum of Difluoromethane. Journal of Chemical Theory and Computation, 2017, 13, 5515-5527.	2.3	15
39	Fast and reliable ab initio calculation of crystal field splittings in lanthanide complexes. Journal of Chemical Physics, 2017, 147, 164101.	1.2	24
40	Tensor decomposition in potential energy surface representations. Journal of Chemical Physics, 2016, 145, 104103.	1.2	11
41	Efficient generation of sum-of-products representations of high-dimensional potential energy surfaces based on multimode expansions. Journal of Chemical Physics, 2016, 144, 114114.	1.2	58
42	Truncated borrelidin analogues: synthesis by sequential cross metathesis/olefination for the southern fragment and biological evaluation. Organic and Biomolecular Chemistry, 2016, 14, 8261-8269.	1.5	3
43	Photolysis of Carbonyl Diisocyanate: Generation of Isocyanatocarbonyl Nitrene and Diazomethanone. Chemistry - an Asian Journal, 2016, 11, 2953-2959.	1.7	18
44	Time-independent eigenstate-free calculation of vibronic spectra beyond the harmonic approximation. Journal of Chemical Physics, 2015, 143, 234106.	1.2	8
45	Towards an automated and efficient calculation of resonating vibrational states based on state-averaged multiconfigurational approaches. Journal of Chemical Physics, 2015, 143, 244111.	1.2	4
46	Anharmonic Franckâ€“Condon Factors for the XÌƒ²B₁ â†• XÌƒ¹A₁ Photoionization of Ketene. Journal of Physical Chemistry A, 2015, 119, 10264-10271.	1.1	15
47	Semi-quartic force fields retrieved from multi-mode expansions: Accuracy, scaling behavior, and approximations. Journal of Chemical Physics, 2015, 142, 154118.	1.2	39
48	Comparison of methods for calculating Franckâ€“Condon factors beyond the harmonic approximation: how important are Duschinsky rotations?. Molecular Physics, 2015, 113, 3859-3873.	0.8	13
49	Transformation of potential energy surfaces for estimating isotopic shifts in anharmonic vibrational frequency calculations. Journal of Chemical Physics, 2014, 140, 184111.	1.2	18
50	Pushing the limits in accurate vibrational structure calculations: anharmonic frequencies of lithium fluoride clusters (LiF)_n, n = 2â€“10. Physical Chemistry Chemical Physics, 2014, 16, 16426.	1.3	20
51	Multi-reference vibration correlation methods. Journal of Chemical Physics, 2014, 140, 064110.	1.2	26
52	Towards black-box calculations of tunneling splittings obtained from vibrational structure methods based on normal coordinates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 100-106.	2.0	15
53	Modeling of high-order terms in potential energy surface expansions using the reference-geometry Harrisâ€“Foulkes method. Physical Chemistry Chemical Physics, 2013, 15, 10233.	1.3	12
54	Anharmonic zero point vibrational energies: Tipping the scales in accurate thermochemistry calculations?. Journal of Chemical Physics, 2013, 138, 044311.	1.2	52

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55	Azidoacetylene â€“ interpretation of gas phase infrared spectra based on high-level vibrational configuration interaction calculations. Physical Chemistry Chemical Physics, 2013, 15, 6719.	1.3	17
56	Efficient Calculation of Multi-dimensional Potential Energy Surfaces of Molecules and Molecular Clusters. , 2013, , 219-230.		2
57	Selected Aspects Concerning the Efficient Calculation of Vibrational Spectra beyond the Harmonic Approximation. Croatica Chemica Acta, 2012, 85, 379-390.	0.1	32
58	Explicitly correlated coupled cluster calculations for the propargyl cation (H2C3H+) and related species. Physical Chemistry Chemical Physics, 2011, 13, 7921.	1.3	25
59	Configuration selection within vibrational multiconfiguration self-consistent field theory: Application to bridged lithium compounds. Journal of Chemical Physics, 2011, 134, 204108.	1.2	20
60	Anharmonic Frequencies of CX₂Y₂ (X, Y = O, N, F, H, D) Isomers and Related Systems Obtained from Vibrational Multiconfiguration Self-Consistent Field Theory. Journal of Physical Chemistry A, 2011, 115, 11050-11056.	1.1	16
61	Convergence of vibrational angular momentum terms within the Watson Hamiltonian. Journal of Chemical Physics, 2011, 134, 064105.	1.2	61
62	Anharmonic frequencies of [F,C,N,X] isomers (X=O,S) obtained from explicitly correlated coupled-cluster calculations. Chemical Physics, 2011, 387, 1-4.	0.9	11
63	Accurate Vibrational Frequencies of Borane and Its Isotopologues. Journal of Chemical Theory and Computation, 2011, 7, 148-152.	2.3	27
64	Chemoenzymatic Synthesis of the C3â€“C11â€Fragment of Borrelidin. European Journal of Organic Chemistry, 2011, 2011, 4241-4249.	1.2	9
65	Towards automated multi-dimensional quantum dynamical investigations of double-minimum potentials: Principles and example applications. Chemical Physics, 2011, 380, 1-8.	0.9	5
66	Franckâ€“Condon profiles in photodetachment-photoelectron spectra of and based on vibrational configuration interaction wavefunctions. Molecular Physics, 2010, 108, 409-423.	0.8	11
67	Vibrational multiconfiguration self-consistent field theory: Implementation and test calculations. Journal of Chemical Physics, 2010, 132, 124102.	1.2	69
68	Relativistic coupled-cluster study of the parity-violation energy shift of CHFClBr. Physical Review A, 2010, 81, .	1.0	15
69	Toward large scale vibrational configuration interaction calculations. Journal of Chemical Physics, 2009, 131, 124129.	1.2	179
70	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 054105.	1.2	173
71	Modeling of high-order many-mode terms in the expansion of multidimensional potential energy surfaces: Application to vibrational spectra. Journal of Chemical Physics, 2009, 131, 014108.	1.2	32
72	A combined variational and perturbational study on the vibrational spectrum of P2F4. Chemical Physics, 2008, 346, 160-166.	0.9	78

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73	Configuration selection as a route towards efficient vibrational configuration interaction calculations. Journal of Chemical Physics, 2007, 127, 184109.	1.2	115
74	Vibrational spectra obtained from high quality potential energy surfaces spanned by low level normal coordinates: application to CHFClI and CDFClI. Molecular Physics, 2007, 105, 1385-1394.	0.8	15
75	Accurate calculation of anharmonic vibrational frequencies of medium sized molecules using local coupled cluster methods. Journal of Chemical Physics, 2007, 126, 134108.	1.2	81
76	Vibrational analyses for CHFClBr and CDFClBr based on high levelab initiocalculations. Journal of Chemical Physics, 2006, 125, 054308.	1.2	36
77	Impact of Local and Density Fitting Approximations on Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2006, 110, 2060-2064.	1.1	75
78	Energy-consistent pseudopotentials for group 11 and 12 atoms: adjustment to multi-configuration Diracâ€“Hartreeâ€“Fock data. Chemical Physics, 2005, 311, 227-244.	0.9	854
79	Multi-level vibrational SCF calculations and FTIR measurements on furazan. Theoretical Chemistry Accounts, 2005, 114, 327-332.	0.5	77
80	Towards accurate ab initio calculations on the vibrational modes of the alkaline earth metal hydrides. Physical Chemistry Chemical Physics, 2005, 7, 3123.	1.3	40
81	Efficient calculation of potential energy surfaces for the generation of vibrational wave functions. Journal of Chemical Physics, 2004, 121, 9313-9322.	1.2	267
82	Theoretische Chemie 2003. Nachrichten Aus Der Chemie, 2004, 52, 313-316.	0.0	0
83	Chemical Reactivity Controlled by Negative Hyperconjugation: A Theoretical Study. Chemistry - A European Journal, 2003, 9, 3143-3153.	1.7	31
84	Plateau Reactions:â€‰ Double Proton-Transfer Processes with Structureless Transition States. Journal of Physical Chemistry A, 2003, 107, 9668-9678.	1.1	34
85	FTIR measurements and quantum chemical calculations of ethylene adsorbed on CuNaY. Physical Chemistry Chemical Physics, 2002, 4, 3112-3121.	1.3	38
86	Computational Studies on 3-Aza-Cope Rearrangements: Protonation- Induced Switch of Mechanism in the Reaction of Vinylpropargylamine. Chemistry - A European Journal, 2002, 8, 641-649.	1.7	21
87	Analytical energy gradients for local coupled-cluster methodsElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b105126c/. Physical Chemistry Chemical Physics, 2001, 3, 4853-4862.	1.3	72
88	Theoretical Prediction of a Base-Catalyzed Bicyclic Boultonâ€'Katritzky Rearrangement. Journal of Organic Chemistry, 2001, 66, 5444-5448.	1.7	31
89	Quantum Chemical Studies on the Reactivity of Electron-Rich Heterocycles: Benzofuroxans. Science Progress, 1999, 82, 209-231.	1.0	12
90	Impact of local approximations on MP2 vibrational frequencies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 647-658.	2.0	72

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91	A Theoretical and Experimental Study of the Molecular Rearrangement of 5-Methyl-4-nitrobenzofuroxan. Journal of the American Chemical Society, 1999, 121, 6700-6711.	6.6	40
92	Analytical energy gradients for local second-order Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1998, 108, 5185-5193.	1.2	204
93	A Computational Study on the Reaction Mechanism of the Boultonâ€'Katritzky Rearrangement. Journal of the American Chemical Society, 1998, 120, 13478-13484.	6.6	48
94	Transferable Scaling Factors for Density Functional Derived Vibrational Force Fields. The Journal of Physical Chemistry, 1995, 99, 3093-3100.	2.9	1,789