

# Guntram Rauhut

## List of Publications by Year in descending order

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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	Transferable Scaling Factors for Density Functional Derived Vibrational Force Fields. <i>The Journal of Physical Chemistry</i> , 1995, 99, 3093-3100.	2.9	1,789
2	Energy-consistent pseudopotentials for group 11 and 12 atoms: adjustment to multi-configuration Dirac-Hartree-Fock data. <i>Chemical Physics</i> , 2005, 311, 227-244.	0.9	854
3	The Molpro quantum chemistry package. <i>Journal of Chemical Physics</i> , 2020, 152, 144107.	1.2	603
4	Efficient calculation of potential energy surfaces for the generation of vibrational wave functions. <i>Journal of Chemical Physics</i> , 2004, 121, 9313-9322.	1.2	267
5	Analytical energy gradients for local second-order Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 1998, 108, 5185-5193.	1.2	204
6	Toward large scale vibrational configuration interaction calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 124129.	1.2	179
7	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2009, 130, 054105.	1.2	173
8	Configuration selection as a route towards efficient vibrational configuration interaction calculations. <i>Journal of Chemical Physics</i> , 2007, 127, 184109.	1.2	115
9	Accurate calculation of anharmonic vibrational frequencies of medium sized molecules using local coupled cluster methods. <i>Journal of Chemical Physics</i> , 2007, 126, 134108.	1.2	81
10	A combined variational and perturbational study on the vibrational spectrum of P2F4. <i>Chemical Physics</i> , 2008, 346, 160-166.	0.9	78
11	Multi-level vibrational SCF calculations and FTIR measurements on furazan. <i>Theoretical Chemistry Accounts</i> , 2005, 114, 327-332.	0.5	77
12	Impact of Local and Density Fitting Approximations on Harmonic Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2060-2064.	1.1	75
13	Impact of local approximations on MP2 vibrational frequencies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 647-658.	2.0	72
14	Analytical energy gradients for local coupled-cluster methods Electronic Supplementary Information available. See <a href="http://www.rsc.org/suppdata/cp/b1/b105126c/">http://www.rsc.org/suppdata/cp/b1/b105126c/</a> . <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4853-4862.	1.3	72
15	Exchange coupling and single molecule magnetism in redox-active tetraoxolene-bridged dlanthanide complexes. <i>Chemical Science</i> , 2018, 9, 1221-1230.	3.7	70
16	Vibrational multiconfiguration self-consistent field theory: Implementation and test calculations. <i>Journal of Chemical Physics</i> , 2010, 132, 124102.	1.2	69
17	Convergence of vibrational angular momentum terms within the Watson Hamiltonian. <i>Journal of Chemical Physics</i> , 2011, 134, 064105.	1.2	61
18	Efficient generation of sum-of-products representations of high-dimensional potential energy surfaces based on multimode expansions. <i>Journal of Chemical Physics</i> , 2016, 144, 114114.	1.2	58

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19	Anharmonic zero point vibrational energies: Tipping the scales in accurate thermochemistry calculations?. <i>Journal of Chemical Physics</i> , 2013, 138, 044311.	1.2	52
20	A Computational Study on the Reaction Mechanism of the Boultonâˆ™Katritzky Rearrangement. <i>Journal of the American Chemical Society</i> , 1998, 120, 13478-13484.	6.6	48
21	A Theoretical and Experimental Study of the Molecular Rearrangement of 5-Methyl-4-nitrobenzofuroxan. <i>Journal of the American Chemical Society</i> , 1999, 121, 6700-6711.	6.6	40
22	Towards accurate ab initio calculations on the vibrational modes of the alkaline earth metal hydrides. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3123.	1.3	40
23	Semi-quartic force fields retrieved from multi-mode expansions: Accuracy, scaling behavior, and approximations. <i>Journal of Chemical Physics</i> , 2015, 142, 154118.	1.2	39
24	FTIR measurements and quantum chemical calculations of ethylene adsorbed on CuNaY. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3112-3121.	1.3	38
25	Vibrational analyses for CHFClBr and CDFClBr based on high level ab initio calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 054308.	1.2	36
26	Plateau Reactions:â€‰ Double Proton-Transfer Processes with Structureless Transition States. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9668-9678.	1.1	34
27	Rigorous use of symmetry within the construction of multidimensional potential energy surfaces. <i>Journal of Chemical Physics</i> , 2018, 149, 164110.	1.2	34
28	Modeling of high-order many-mode terms in the expansion of multidimensional potential energy surfaces: Application to vibrational spectra. <i>Journal of Chemical Physics</i> , 2009, 131, 014108.	1.2	32
29	Selected Aspects Concerning the Efficient Calculation of Vibrational Spectra beyond the Harmonic Approximation. <i>Croatica Chemica Acta</i> , 2012, 85, 379-390.	0.1	32
30	A new efficient method for the calculation of interior eigenpairs and its application to vibrational structure problems. <i>Journal of Chemical Physics</i> , 2017, 146, 124101.	1.2	32
31	Theoretical Prediction of a Base-Catalyzed Bicyclic Boultonâˆ™Katritzky Rearrangement. <i>Journal of Organic Chemistry</i> , 2001, 66, 5444-5448.	1.7	31
32	Chemical Reactivity Controlled by Negative Hyperconjugation: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2003, 9, 3143-3153.	1.7	31
33	Toward a fully automated calculation of rovibrational infrared intensities for semi-rigid polyatomic molecules. <i>Journal of Chemical Physics</i> , 2020, 152, 244104.	1.2	29
34	Accurate Vibrational Frequencies of Borane and Its Isotopologues. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 148-152.	2.3	27
35	Multi-reference vibration correlation methods. <i>Journal of Chemical Physics</i> , 2014, 140, 064110.	1.2	26
36	Explicitly correlated coupled cluster calculations for the propargyl cation (H <sub>2</sub> C <sub>3</sub> H <sup>+</sup> ) and related species. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7921.	1.3	25

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37	Fast and reliable <i>ab initio</i> calculation of crystal field splittings in lanthanide complexes. <i>Journal of Chemical Physics</i> , 2017, 147, 164101.	1.2	24
38	Phosphorus Analogues of Methyl Nitrite and Nitromethane: CH <sub>3</sub> OPO and CH <sub>3</sub> PO <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12164-12169.	7.2	22
39	The interplay of VSCF/VCI calculations and matrix-isolation IR spectroscopy – Mid infrared spectrum of CH <sub>3</sub> CH <sub>2</sub> F and CD <sub>3</sub> CD <sub>2</sub> F. <i>Journal of Molecular Spectroscopy</i> , 2020, 367, 111224.	0.4	22
40	Computational Studies on 3-Aza-Cope Rearrangements: Protonation- Induced Switch of Mechanism in the Reaction of Vinylpropargylamine. <i>Chemistry - A European Journal</i> , 2002, 8, 641-649.	1.7	21
41	Localized Normal Coordinates in Accurate Vibrational Structure Calculations: Benchmarks for Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4187-4196.	2.3	21
42	Configuration selection within vibrational multiconfiguration self-consistent field theory: Application to bridged lithium compounds. <i>Journal of Chemical Physics</i> , 2011, 134, 204108.	1.2	20
43	Pushing the limits in accurate vibrational structure calculations: anharmonic frequencies of lithium fluoride clusters (LiF) <sub>n</sub> , n = 2–10. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16426.	1.3	20
44	Advances in vibrational configuration interaction theory – part 2: Fast screening of the correlation space. <i>Journal of Computational Chemistry</i> , 2022, 43, 6-18.	1.5	19
45	Transformation of potential energy surfaces for estimating isotopic shifts in anharmonic vibrational frequency calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 184111.	1.2	18
46	Photolysis of Carbonyl Diisocyanate: Generation of Isocyanatocarbonyl Nitrene and Diazomethanone. <i>Chemistry - an Asian Journal</i> , 2016, 11, 2953-2959.	1.7	18
47	Azidoacetylene – interpretation of gas phase infrared spectra based on high-level vibrational configuration interaction calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6719.	1.3	17
48	Advances in vibrational configuration interaction theory – part 1: Efficient calculation of vibrational angular momentum terms. <i>Journal of Computational Chemistry</i> , 2021, 42, 2321-2333.	1.5	17
49	Anharmonic Frequencies of CX <sub>2</sub> Y <sub>2</sub> (X, Y = O, N, F, H, D) Isomers and Related Systems Obtained from Vibrational Multiconfiguration Self-Consistent Field Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11050-11056.	1.1	16
50	Vibrational spectra obtained from high quality potential energy surfaces spanned by low level normal coordinates: application to CHFCl and CDFCl. <i>Molecular Physics</i> , 2007, 105, 1385-1394.	0.8	15
51	Relativistic coupled-cluster study of the parity-violation energy shift of CHFClBr. <i>Physical Review A</i> , 2010, 81, .	1.0	15
52	Towards black-box calculations of tunneling splittings obtained from vibrational structure methods based on normal coordinates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 119, 100-106.	2.0	15
53	Anharmonic Franck-Condon Factors for the $X^1\Sigma^+_{g^{-}}B_{1g}$ – $X^1\Sigma^+_{g^{-}}A_{1g}$ Photoionization of Ketene. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10264-10271.	1.1	15
54	A General Approach for Calculating Strongly Anharmonic Vibronic Spectra with a High Density of States: The $X^1\Sigma^+_{g^{-}}B_{1g}$ – $X^1\Sigma^+_{g^{-}}A_{1g}$ Photoelectron Spectrum of Difluoromethane. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5515-5527.	2.3	15

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55	Accurate Vibrational Configuration Interaction Calculations on Diborane and Its Isotopologues. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3367-3373.	1.1	15
56	Comparison of methods for calculating Franck-Condon factors beyond the harmonic approximation: how important are Duschinsky rotations?. <i>Molecular Physics</i> , 2015, 113, 3859-3873.	0.8	13
57	High-Level Rovibrational Calculations on Ketenimine. <i>Frontiers in Chemistry</i> , 2020, 8, 623641.	1.8	13
58	Quantum Chemical Studies on the Reactivity of Electron-Rich Heterocycles: Benzofuroxans. <i>Science Progress</i> , 1999, 82, 209-231.	1.0	12
59	Modeling of high-order terms in potential energy surface expansions using the reference-geometry Harris-Foulkes method. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10233.	1.3	12
60	Toward fast and accurate <i>ab initio</i> calculation of magnetic exchange in polynuclear lanthanide complexes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9769-9778.	1.3	12
61	Franck-Condon profiles in photodetachment-photoelectron spectra of and based on vibrational configuration interaction wavefunctions. <i>Molecular Physics</i> , 2010, 108, 409-423.	0.8	11
62	Anharmonic frequencies of [F,C,N,X] isomers (X=O,S) obtained from explicitly correlated coupled-cluster calculations. <i>Chemical Physics</i> , 2011, 387, 1-4.	0.9	11
63	Tensor decomposition in potential energy surface representations. <i>Journal of Chemical Physics</i> , 2016, 145, 104103.	1.2	11
64	Vibrational analysis of methyl cation-Rare gas atom complexes: CH <sub>3</sub> +Rg (Rg = He, Ne, Ar, Kr). <i>Journal of Chemical Physics</i> , 2019, 150, 084306.	1.2	11
65	<i>Ab initio</i> calculation of rovibrational states for non-degenerate double-well potentials: <i>cis-trans</i> isomerization of HOPO. <i>Journal of Chemical Physics</i> , 2020, 152, 174306.	1.2	11
66	Assignment of vibrational states within configuration interaction calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 194112.	1.2	11
67	The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21949-21953.	7.2	10
68	Hydrogen-Atom Tunneling in Metaphosphorous Acid. <i>Chemistry - A European Journal</i> , 2020, 26, 8205-8209.	1.7	10
69	Incremental vibrational configuration interaction theory, iVCI: Implementation and benchmark calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 124114.	1.2	10
70	Chemoenzymatic Synthesis of the C <sub>3</sub> -C <sub>11</sub> Fragment of Borrelidin. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 4241-4249.	1.2	9
71	The Simplest, Isolable, Alkynyl Isocyanate HC≡NCNO: Synthesis and Characterization. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17277-17281.	7.2	9
72	Vibrational spectrum and photochemistry of phosphaketene HPCO. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19237-19243.	1.3	9

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73	Efficient and automated quantum chemical calculation of rovibrational nonresonant Raman spectra. Journal of Chemical Physics, 2022, 156, 124102.	1.2	9
74	Time-independent eigenstate-free calculation of vibronic spectra beyond the harmonic approximation. Journal of Chemical Physics, 2015, 143, 234106.	1.2	8
75	Vibrational Configuration Interaction Theory. , 2022, , 1-40.		8
76	Vibrational analysis of nitrosamine, a molecule with an almost constant potential along the inversion coordinate. Molecular Physics, 2019, 117, 1741-1745.	0.8	7
77	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
78	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
79	Parity-violation effects in the vibrational spectra of CHFClBr and CDFClBr. Physical Review A, 2021, 103, .	1.0	6
80	Towards automated multi-dimensional quantum dynamical investigations of double-minimum potentials: Principles and example applications. Chemical Physics, 2011, 380, 1-8.	0.9	5
81	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
82	Quantum chemical rovibrational analysis of aminoborane and its isotopologues. Journal of Computational Chemistry, 2023, 44, 298-306.	1.5	4
83	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
84	Efficient Calculation of Multi-dimensional Potential Energy Surfaces of Molecules and Molecular Clusters. , 2013, , 219-230.		2
85	Refined analysis of the $\lambda_{1/2}^{\text{He}}$ photoelectron spectrum of furan. Journal of Chemical Physics, 2018, 148, 054306.	1.2	2
86	Structure, energetics, and spectroscopy of the chromophores of $\text{HHe}_n$ , $\text{H}_2\text{He}_n$ , and $\text{He}_n$ clusters and their deuterated isotopologues. Physical Chemistry Chemical Physics, 2022, , .	1.3	2
87	Comparison of body definitions for incremental vibrational configuration interaction theory (iVCI). Journal of Chemical Physics, 2022, 156, 174103.	1.2	2
88	The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide. Angewandte Chemie, 2020, 132, 22133-22137.	1.6	1
89	The simplest alkynyl thiocyanate HCCSCN and its isomers. Chemical Communications, 2021, 57, 3343-3346.	2.2	1
90	Theoretische Chemie 2003. Nachrichten Aus Der Chemie, 2004, 52, 313-316.	0.0	0

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91	Modal optimisation within the time-independent eigenstate-free Raman wavefunction formalism. <i>Molecular Physics</i> , 2020, 118, .	0.8	0
92	Account of non-Condon effects in time-independent Raman wavefunction theory: Calculation of the S1 $\hat{\leftarrow}$ S0 vibronic absorption spectrum of formaldehyde. <i>Journal of Chemical Physics</i> , 2020, 152, 114109.	1.2	0
93	Hydrogen-Atom Tunneling in Metaphosphorous Acid. <i>Chemistry - A European Journal</i> , 2020, 26, 8174-8174.	1.7	0
94	A combined computational and experimental study on the vibrational structure of ethynyl isothiocyanate, HCCNCS, a molecule with a Champagne bottle potential. <i>Journal of Molecular Spectroscopy</i> , 2022, , 111626.	0.4	0