Tucker Carrington

List of Publications by Year
in descending order

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232 papers	11,081 citations	24978 57 h-index	38300 95 g-index
245 all docs	245 docs citations	245 times ranked	3189 citing authors

#	Article	IF	Citations
1	Computational study of the rovibrational spectrum of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e9065" altimg="si22.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>O-HF. Journal of Molecular Spectroscopy, 2022, 384, 111587.	0.4	6
2	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	1.0	69
3	Neural Network Potential Energy Surfaces for Small Molecules and Reactions. Chemical Reviews, 2021, 121, 10187-10217.	23.0	163
4	Using collocation to study the vibrational dynamics of molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119158.	2.0	10
5	Using nondirect product Wigner D basis functions and the symmetry-adapted Lanczos algorithm to compute the ro-vibrational spectrum of CH4â€“H2O. Journal of Chemical Physics, 2021, 154, 124112.	1.2	7
6	A rectangular collocation multi-configuration time-dependent Hartree (MCTDH) approach with time-independent points for calculations on general potential energy surfaces. Journal of Chemical Physics, 2021, 154, 114107.	1.2	10
7	Using collocation and solutions for a sum-of-product potential to compute vibrational energy levels for general potentials. Chemical Physics Letters, 2021, 781, 138967.	1.2	3
8	Computing vibrational energy levels by solving linear equations using a tensor method with an imposed rank. Journal of Chemical Physics, 2021, 155, 234105.	1.2	4
9	Efficiently Transforming from Values of a Function on a Sparse Grid to Basis Coefficients. Lecture Notes in Computational Science and Engineering, 2021, , 229-244.	0.1	3
10	Computational study of the rovibrational spectrum of CO2â€“N2. Physical Chemistry Chemical Physics, 2020, 22, 22674-22683.	1.3	12
11	A variational calculation of vibrational levels of vinyl radical. Journal of Chemical Physics, 2020, 152, 204311.	1.2	6
12	A collocation-based multi-configuration time-dependent Hartree method using mode combination and improved relaxation. Journal of Chemical Physics, 2020, 152, 164117.	1.2	10
13	Machine Learning Optimization of the Collocation Point Set for Solving the Kohnâ€“Sham Equation. Journal of Physical Chemistry A, 2019, 123, 10631-10642.	1.1	12
14	Computational Study of the Rovibrational Spectra of CH₂D⁺ and CHD₂⁺. Journal of Physical Chemistry A, 2019, 123, 10281-10289.	1.1	5
15	Using quadrature and an iterative eigensolver to compute fine-structure ro-vibrational levels of Van der Waals complexes: NH(Î£â¾3)â€“He, O2(Î£gâ¾3)â€“Ar, and O2(Î£gâ¾3)â€“He. Journal of Chemical Physics, 2019, 151, 054101.	1.2	2
16	Computational study of the ro-vibrational spectrum of COâ€“CO2. Journal of Chemical Physics, 2019, 151, 084307.	1.2	19
17	Using collocation and a hierarchical basis to solve the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2019, 150, 204108.	1.2	8
18	A pruned collocation-based multiconfiguration time-dependent Hartree approach using a Smolyak grid for solving the SchrÃ¶dinger equation with a general potential energy surface. Journal of Chemical Physics, 2019, 150, 154108.	1.2	21

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19	A Comparison of Methods for Determining the Time Step When Propagating with the Lanczos Algorithm. Mathematics, 2019, 7, 1109.	1.1	1
20	Computing vibrationâ€“rotation-tunnelling levels of HOD dimer. Physical Chemistry Chemical Physics, 2019, 21, 3527-3536.	1.3	2
21	Using monomer vibrational wavefunctions to compute numerically exact (12D) rovibrational levels of water dimer. Journal of Chemical Physics, 2018, 148, 074108.	1.2	51
22	Computing energy levels of CH4, CHD3, CH3D, and CH3F with a direct product basis and coordinates based on the methyl subsystem. Journal of Chemical Physics, 2018, 148, 074113.	1.2	7
23	Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces. Journal of Chemical Physics, 2018, 148, 102321.	1.2	40
24	Ab initio study of the COâ€“N2 complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum. Physical Chemistry Chemical Physics, 2018, 20, 12624-12636.	1.3	14
25	The He2-OCS complex: Comparison between theory and experiment. Chemical Physics Letters, 2018, 694, 35-39.	1.2	0
26	A new collocation-based multi-configuration time-dependent Hartree (MCTDH) approach for solving the SchrÃ¶dinger equation with a general potential energy surface. Journal of Chemical Physics, 2018, 148, 044115.	1.2	23
27	A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra. Chemical Physics, 2018, 509, 139-144.	0.9	25
28	Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy. Journal of Chemical Physics, 2018, 148, 241702.	1.2	157
29	Iterative Methods for Computing Vibrational Spectra. Mathematics, 2018, 6, 13.	1.1	3
30	Using rectangular collocation with finite difference derivatives to solve electronic SchrÃ¶dinger equation. Journal of Chemical Physics, 2018, 149, 204105.	1.2	11
31	Redundant coordinates in quantum mechanics. Chemical Physics, 2018, 515, 336-341.	0.9	0
32	Infrared spectrum and intermolecular potential energy surface of the COâ€“O₂ dimer. Physical Chemistry Chemical Physics, 2018, 20, 14431-14440.	1.3	13
33	Using an iterative eigensolver and intertwined rank reduction to compute vibrational spectra of molecules with more than a dozen atoms: Uracil and naphthalene. Journal of Chemical Physics, 2018, 149, 064108.	1.2	28
34	Comparing Nested Sequences of Leja and PseudoGauss Points to Interpolate in 1D and Solve the Schroedinger Equation in 9D. Lecture Notes in Computational Science and Engineering, 2018, , 1-17.	0.1	3
35	Comparison of different eigensolvers for calculating vibrational spectra using low-rank, sum-of-product basis functions. Molecular Physics, 2017, 115, 1740-1749.	0.8	10
36	An intertwined method for making low-rank, sum-of-product basis functions that makes it possible to compute vibrational spectra of molecules with more than 10 atoms. Journal of Chemical Physics, 2017, 146, 204110.	1.2	26

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37	Perspective: Computing (ro-)vibrational spectra of molecules with more than four atoms. Journal of Chemical Physics, 2017, 146, 120902.	1.2	83
38	Using monomer vibrational wavefunctions as contracted basis functions to compute rovibrational levels of an H2O-atom complex in full dimensionality. Journal of Chemical Physics, 2017, 146, 104105.	1.2	28
39	Applying a Smolyak collocation method to Cl₂CO. Molecular Physics, 2017, 115, 1775-1785.	0.8	16
40	Systematically expanding nondirect product bases within the pruned multi-configuration time-dependent Hartree (MCTDH) method: A comparison with multi-layer MCTDH. Journal of Chemical Physics, 2017, 146, 194105.	1.2	26
41	Computing vibrational energy levels of CH4 with a Smolyak collocation method. Journal of Chemical Physics, 2017, 147, 144102.	1.2	19
42	Reducing the cost of using collocation to compute vibrational energy levels: Results for CH2NH. Journal of Chemical Physics, 2017, 147, 064103.	1.2	19
43	Pruned bases that are compatible with iterative eigensolvers and general potentials: New results for CH3CN. Chemical Physics, 2017, 482, 3-8.	0.9	23
44	Using a pruned, nondirect product basis in conjunction with the multi-configuration time-dependent Hartree (MCTDH) method. Journal of Chemical Physics, 2016, 145, 044110.	1.2	29
45	Computational study of the rovibrational spectra of CO2â€“C2H2 and CO2â€“C2D2. Journal of Molecular Spectroscopy, 2016, 330, 170-178.	0.4	23
46	Using an expanding nondirect product harmonic basis with an iterative eigensolver to compute vibrational energy levels with as many as seven atoms. Journal of Chemical Physics, 2016, 145, 144104.	1.2	36
47	Calculated vibrational states of ozone up to dissociation. Journal of Chemical Physics, 2016, 144, 074302.	1.2	39
48	Using an internal coordinate Gaussian basis and a space-fixed Cartesian coordinate kinetic energy operator to compute a vibrational spectrum with rectangular collocation. Journal of Chemical Physics, 2016, 145, 224110.	1.2	32
49	Calculated rotation-bending energy levels of CH5+ and a comparison with experiment. Journal of Chemical Physics, 2016, 144, 204304.	1.2	33
50	Methods for Computing Ro-vibrational Energy Levels. , 2016, , 135-149.		2
51	Computational study of the rovibrational spectrum of (CO2)2. Journal of Molecular Spectroscopy, 2016, 330, 179-187.	0.4	27
52	Assessing the utility of phase-space-localized basis functions: Exploiting direct product structure and a new basis function selection procedure. Journal of Chemical Physics, 2016, 144, 244115.	1.2	21
53	Intermolecular vibrations of the CO2â€“CS2 complex: Experiment and theory agree, but understanding remains challenging. Journal of Molecular Spectroscopy, 2016, 330, 188-193.	0.4	3
54	Using symmetry-adapted optimized sum-of-products basis functions to calculate vibrational spectra. Chemical Physics Letters, 2016, 644, 183-188.	1.2	18

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55	Using multi-dimensional Smolyak interpolation to make a sum-of-products potential. Journal of Chemical Physics, 2015, 143, 044106.	1.2	23
56	Using an iterative eigensolver to compute vibrational energies with phase-spaced localized basis functions. Journal of Chemical Physics, 2015, 143, 044104.	1.2	23
57	A multi-dimensional Smolyak collocation method in curvilinear coordinates for computing vibrational spectra. Journal of Chemical Physics, 2015, 143, 214108.	1.2	33
58	Computing vibrational and ro-vibrational spectra of CH5+. AIP Conference Proceedings, 2015, , .	0.3	2
59	Using Nested Contractions and a Hierarchical Tensor Format To Compute Vibrational Spectra of Molecules with Seven Atoms. Journal of Physical Chemistry A, 2015, 119, 13074-13091.	1.1	49
60	Explicitly correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations. Molecular Physics, 2015, 113, 1823-1833.	0.8	63
61	Comment on â€œPhase-Space Approach to Solving the Time-Independent SchrÃ¶dinger Equationâ€. Physical Review Letters, 2015, 114, 058901.	2.9	8
62	The vibration-rotation-tunneling levels of N2â€“H2O and N2â€“D2O. Journal of Chemical Physics, 2015, 143, 024303.	1.2	10
63	Computing the Anharmonic Vibrational Spectrum of UF₆ in 15 Dimensions with an Optimized Basis Set and Rectangular Collocation. Journal of Physical Chemistry A, 2015, 119, 9557-9567.	1.1	30
64	Neural networkâ€based approaches for building high dimensional and quantum dynamicsâ€friendly potential energy surfaces. International Journal of Quantum Chemistry, 2015, 115, 1012-1020.	1.0	170
65	Calculating vibrational spectra with sum of product basis functions without storing full-dimensional vectors or matrices. Journal of Chemical Physics, 2014, 140, 174111.	1.2	70
66	Computational study of the rovibrational spectrum of CO2â€“CS2. Journal of Chemical Physics, 2014, 140, 114303.	1.2	30
67	Using experimental data and a contracted basis Lanczos method to determine an accurate methane potential energy surface from a least squares optimization. Journal of Chemical Physics, 2014, 141, 154106.	1.2	52
68	Rovibrational levels and wavefunctions of Clâ¯H2O. Journal of Chemical Physics, 2014, 140, 204306.	1.2	24
69	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	1.1	32
70	Vibrational energy levels of difluorodioxirane computed with variational and perturbative methods from a hybrid force field. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 107-112.	2.0	1
71	CO Dimer: New Potential Energy Surface and Rovibrational Calculations. Journal of Physical Chemistry A, 2013, 117, 7612-7630.	1.1	61
72	Tribute to Joel M. Bowman. Journal of Physical Chemistry A, 2013, 117, 6905-6906.	1.1	0

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73	Methane line parameters in the HITRAN2012 database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 201-219.	1.1	121
74	Computing rovibrational levels of polyatomic molecules with polyspherical coordinates and a contracted basis built with a K-independent vibrational primitive basis. Molecular Physics, 2013, 111, 2320-2333.	0.8	7
75	Calculating and assigning rovibrational energy levels of (15N2O)2, (15N14NO)2, 14N2Oâ€“15N2O and 15N14NOâ€“15N2O. Physical Chemistry Chemical Physics, 2013, 15, 19159.	1.3	3
76	Anharmonic vibrations of the carboxyl group in acetic acid on TiO2: implications for adsorption mode assignment in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 10028.	1.3	24
77	Computing rovibrational levels of methane with curvilinear internal vibrational coordinates and an Eckart frame. Journal of Chemical Physics, 2013, 138, 104106.	1.2	73
78	Using a Nondirect Product Basis to Compute J > 0 Rovibrational States of H₃⁺. Journal of Physical Chemistry A, 2013, 117, 9493-9500.	1.1	19
79	Analysis of the rovibrational spectrum of 13CH4 in the Octad range. Journal of Molecular Spectroscopy, 2013, 291, 33-47.	0.4	48
80	Solving the Schroedinger equation using Smolyak interpolants. Journal of Chemical Physics, 2013, 139, 134114.	1.2	46
81	Communication: Favorable dimensionality scaling of rectangular collocation with adaptable basis functions up to 7 dimensions. Journal of Chemical Physics, 2013, 139, 051101.	1.2	18
82	Computational study of the rovibrational spectrum of (OCS)2. Journal of Chemical Physics, 2012, 136, 134306.	1.2	55
83	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. Materials Research Society Symposia Proceedings, 2012, 1484, 1.	0.1	11
84	Solving the vibrational SchrÃ¶dinger equation using bases pruned to include strongly coupled functions and compatible quadratures. Journal of Chemical Physics, 2012, 137, 174108.	1.2	62
85	K-independent vibrational bases for systems with large amplitude motion. Molecular Physics, 2012, 110, 825-835.	0.8	14
86	Rovibrational spectra of molecules in small helium clusters. , 2012, , .		1
87	Representing potential energy surfaces with neural networks and high dimensional model representations. , 2012, , .		0
88	Using pruned basis sets to compute vibrational spectra. , 2012, , .		1
89	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. Journal of Chemical Theory and Computation, 2012, 8, 2053-2061.	2.3	21
90	Computing polarizabilities without a Hamiltonian matrix. Chemical Physics Letters, 2012, 524, 96-99.	1.2	1

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91	Nonspectral Methods for Solving the SchrÃ¶dinger Equation for Electronic and Vibrational Problems. Journal of Physical Chemistry Letters, 2011, 2, 2193-2199.	2.1	11
92	Using a pruned basis, a non-product quadrature grid, and the exact Watson normal-coordinate kinetic energy operator to solve the vibrational SchrÃ¶dinger equation for C2H4. Journal of Chemical Physics, 2011, 135, 064101.	1.2	115
93	Using nonproduct quadrature grids to solve the vibrational SchrÃ¶dinger equation in 12D. Journal of Chemical Physics, 2011, 134, 054126.	1.2	108
94	The vibrationâ€“rotationâ€“tunneling spectrum of the polar and T-shaped-N-in isomers of (NNO)2. Journal of Molecular Spectroscopy, 2011, 268, 53-65.	0.4	38
95	On the advantages of a rectangular matrix collocation equation for computing vibrational spectra from small basis sets. Chemical Physics Letters, 2011, 511, 434-439.	1.2	29
96	Computing roâ€vibrational spectra of van der Waals molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 952-963.	6.2	32
97	Calculating anharmonic vibrational frequencies of molecules adsorbed on surfaces directly from ab initio energies with a molecule-independent method: H2O on Pt(111). Surface Science, 2011, 605, 616-622.	0.8	23
98	Theoretical study of the rovibrational spectrum of H2Oâ€“H2. Journal of Chemical Physics, 2011, 134, 044313.	1.2	55
99	Extracting Functional Dependence from Sparse Data Using Dimensionality Reduction: Application to Potential Energy Surface Construction. Lecture Notes in Computational Science and Engineering, 2011, , 133-149.	0.1	5
100	Nonproduct Quadrature Grids: Solving the Vibrational SchrÃ¶dinger Equation in 12d. , 2011, , 1-12.		0
101	A new approach for determining the time step when propagating with the Lanczos algorithm. Computer Physics Communications, 2010, 181, 1859-1861.	3.0	7
102	Parallel methods for high-dimensional quantum dynamics. Computer Physics Communications, 2010, 181, 455-461.	3.0	11
103	Solving the time-dependent Schroedinger equation by discarding high-energy basis functions. Chemical Physics Letters, 2010, 501, 130-133.	1.2	7
104	Nitrous oxide dimer: A new potential energy surface and rovibrational spectrum of the nonpolar isomer. Journal of Chemical Physics, 2010, 133, 134304.	1.2	94
105	Theoretical study of the rovibrational spectrum of He₂â€“OCS. Canadian Journal of Chemistry, 2010, 88, 779-786.	0.6	7
106	A Parallel Algorithm for Computing the Spectrum of CH $_5^+$. Lecture Notes in Computer Science, 2010, , 109-116.	1.0	0
107	Nonproduct quadrature grids for solving the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2009, 131, 174103.	1.2	99
108	Computing vibrational energy levels by using mappings to fully exploit the structure of a pruned product basis. Journal of Chemical Physics, 2009, 130, 214110.	1.2	30

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109	Fitting sparse multidimensional data with low-dimensional terms. Computer Physics Communications, 2009, 180, 2002-2012.	3.0	50
110	Theoretical and Experimental Study of the Rovibrational Spectrum of He₂â^'CO. Journal of Physical Chemistry A, 2009, 113, 13331-13341.	1.1	22
111	Theoretical and experimental study of infrared spectra of He₂-CO₂This article is part of a Special Issue on Spectroscopy at the University of New Brunswick in honour of Colan Linton and Ron Lees.. Canadian Journal of Physics, 2009, 87, 417-423.	0.4	18
112	A discrete variable representation method for studying the rovibrational quantum dynamics of molecules with more than three atoms. Journal of Chemical Physics, 2009, 130, 094101.	1.2	29
113	Using a neural network based method to solve the vibrational SchrÃ¶dinger equation for H2O. Chemical Physics Letters, 2009, 474, 217-221.	1.2	27
114	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	0.8	402
115	Using neural networks, optimized coordinates, and high-dimensional model representations to obtain a vinyl bromide potential surface. Journal of Chemical Physics, 2008, 129, 224104.	1.2	100
116	Vibrational energy levels of CH5+. Journal of Chemical Physics, 2008, 129, 234102.	1.2	140
117	Using a nondirect product discrete variable representation for angular coordinates to compute vibrational levels of polyatomic molecules. Journal of Chemical Physics, 2008, 128, 194109.	1.2	11
118	Using redundant coordinates to represent potential energy surfaces with lower-dimensional functions. Journal of Chemical Physics, 2007, 127, 014103.	1.2	93
119	Vibrational Levels of Ar4:Â New Odd-Parity Bosonic Statesâ€. Journal of Physical Chemistry A, 2007, 111, 10220-10225.	1.1	17
120	Discrete-Variable Representations and their Utilization. Advances in Chemical Physics, 2007, , 263-310.	0.3	496
121	Using neural networks to represent potential surfaces as sums of products. Journal of Chemical Physics, 2006, 125, 194105.	1.2	156
122	A Nested Molecule-Independent Neural Network Approach for High-Quality Potential Fitsâ€. Journal of Physical Chemistry A, 2006, 110, 5295-5304.	1.1	166
123	A random-sampling high dimensional model representation neural network for building potential energy surfaces. Journal of Chemical Physics, 2006, 125, 084109.	1.2	211
124	Vibronic coupling in square planar complexes of palladium(II) and platinum(II). Chemical Physics, 2006, 329, 90-98.	0.9	9
125	Using simultaneous diagonalization and trace minimization to make an efficient and simple multidimensional basis for solving the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2006, 124, 054102.	1.2	31
126	Calculating vibrational energies and wave functions of vinylidene using a contracted basis with a locally reorthogonalized coupled two-term Lanczos eigensolver. Journal of Chemical Physics, 2006, 125, 094311.	1.2	85

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127	Computing resonance energies, widths, and wave functions using a Lanczos method in real arithmetic. Journal of Chemical Physics, 2005, 122, 244107.	1.2	15
128	Calculating intensities using effective Hamiltonians in terms of Coriolis-adapted normal modes. Journal of Chemical Physics, 2005, 122, 034106.	1.2	2
129	Improving the calculation of rovibrational spectra of five-atom molecules with three identical atoms by using a C3Ì…(G6) symmetry-adapted grid: Applied to CH3D and CHD3. Journal of Chemical Physics, 2005, 123, 154303.	1.2	33
130	How to choose one-dimensional basis functions so that a very efficient multidimensional basis may be extracted from a direct product of the one-dimensional functions: Energy levels of coupled systems with as many as 16 coordinates. Journal of Chemical Physics, 2005, 122, 134101.	1.2	80
131	Theoretical and experimental studies of the infrared rovibrational spectrum of He2â€“N2O. Journal of Chemical Physics, 2005, 123, 034301.	1.2	71
132	Contracted basis Lanczos methods for computing numerically exact rovibrational levels of methane. Journal of Chemical Physics, 2004, 121, 2937-2954.	1.2	117
133	A multidimensional discrete variable representation basis obtained by simultaneous diagonalization. Journal of Chemical Physics, 2004, 121, 726-736.	1.2	46
134	Using preconditioned adaptive step size Runge-Kutta methods for solving the time-dependent SchrÃ¶dinger equation. Journal of Chemical Physics, 2004, 121, 11535-11541.	1.2	44
135	Using simply contracted basis functions with the Lanczos algorithm to calculate vibrational spectra. International Journal of Quantum Chemistry, 2004, 99, 556-566.	1.0	4
136	Methods for calculating vibrational energy levels. Canadian Journal of Chemistry, 2004, 82, 900-914.	0.6	31
137	USING LEBEDEV GRIDS, SINE SPHERICAL HARMONICS, AND MONOMER CONTRACTED BASIS FUNCTIONS TO CALCULATE BENDING ENERGY LEVELS OF HF TRIMER. Journal of Theoretical and Computational Chemistry, 2003, 02, 599-608.	1.8	20
138	A finite basis representation Lanczos calculation of the bend energy levels of methane. Journal of Chemical Physics, 2003, 118, 6946-6956.	1.2	85
139	Deficiencies of the bend symmetry coordinates used for methane. Journal of Chemical Physics, 2003, 118, 6260-6263.	1.2	23
140	A contracted basis-Lanczos calculation of vibrational levels of methane: Solving the SchrÃ¶dinger equation in nine dimensions. Journal of Chemical Physics, 2003, 119, 101-117.	1.2	177
141	Semiclassically optimized complex absorbing potentials of polynomial form. II. Complex case. Journal of Chemical Physics, 2003, 119, 77-89.	1.2	35
142	Semiclassically optimized complex absorbing potentials of polynomial form. I. Pure imaginary case. Journal of Chemical Physics, 2003, 118, 17-28.	1.2	57
143	Using C3v symmetry with polyspherical coordinates for methane. Journal of Chemical Physics, 2003, 119, 94-100.	1.2	23
144	A general framework for discrete variable representation basis sets. Journal of Chemical Physics, 2002, 116, 8691-8703.	1.2	129

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145	Comment on â€œSpectral filters in quantum mechanics: A measurement theory perspectiveâ€• Physical Review E, 2002, 65, 028701.	0.8	11
146	A preconditioned inexact spectral transform method for calculating resonance energies and widths, as applied to HCO. Journal of Chemical Physics, 2002, 116, 1215-1227.	1.2	74
147	New ideas for using contracted basis functions with a Lanczos eigensolver for computing vibrational spectra of molecules with four or more atoms. Journal of Chemical Physics, 2002, 117, 6923-6934.	1.2	129
148	State-to-state and total rotational energy transfer rate constants for CN(Bâ€Š2Î£+,v=0,N)+H2, CN(Xâ€Š2Î£+,v=2,N)+H2, D2, and CN(Xâ€Š2Î£+,v=3,N)+NO. Journal of Chemical Physics, 2002, 116, 3617-3625.	1.2	16
149	Energy disposal in CN(Xâ€‰2Î£+) produced in the 157 nm photodissociation of acrylonitrile. Journal of Chemical Physics, 2001, 115, 8411-8417.	1.2	4
150	The Utility of Constraining Basis Function Indices When Using the Lanczos Algorithm to Calculate Vibrational Energy Levelsâ€. Journal of Physical Chemistry A, 2001, 105, 2575-2581.	1.1	61
151	Calculating interior eigenvalues and eigenvectors with an implicitly restarted and a filter diagonalization method. Applied Numerical Mathematics, 2001, 37, 307-317.	1.2	2
152	A simple equation including anharmonic effects for the vibrational polarisability of a diatomic molecule. Chemical Physics Letters, 2001, 348, 317-320.	1.2	0
153	A symmetry-adapted Lanczos method for calculating energy levels with different symmetries from a single set of iterations. Journal of Chemical Physics, 2001, 114, 1473-1477.	1.2	99
154	V3: Structure and vibrations from density functional theory, Franckâ€“Condon factors, and the pulsed-field ionization zero-electron-kinetic energy spectrum. Journal of Chemical Physics, 2001, 114, 4036-4044.	1.2	53
155	Accelerating the calculation of energy levels and wave functions using an efficient preconditioner with the inexact spectral transform method. Journal of Chemical Physics, 2001, 114, 9254-9264.	1.2	78
156	Using the symmetric quasiminimal residuals method to accelerate an inexact spectral transform calculation of energy levels and wave functions. Journal of Chemical Physics, 2001, 114, 6485-6486.	1.2	5
157	Six-dimensional variational calculation of the bending energy levels of HF trimer and DF trimer. Journal of Chemical Physics, 2001, 115, 9781-9796.	1.2	82
158	Ro-vibrational levels for HF2+: The effect of rotation on vibrational splittings for proton transfer. Journal of Chemical Physics, 2000, 113, 7273-7275.	1.2	0
159	The advantage of writing kinetic energy operators in polyspherical curvilinear coordinates in terms of zi=cosâ€Šîti. Journal of Chemical Physics, 2000, 112, 4413-4414.	1.2	12
160	Photodissociation of HCN at 157â€‚nm: Energy disposal in the CN(Aâ€Š2Î) fragment. Journal of Chemical Physics, 2000, 112, 8904-8909.	1.2	15
161	A simple method for deriving kinetic energy operators. Journal of Chemical Physics, 2000, 113, 7097-7101.	1.2	46
162	A new iterative method for calculating energy levels and wave functions. Journal of Chemical Physics, 2000, 112, 8765-8771.	1.2	88

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163	Effect of rotation and vibration on nuclear magnetic resonance chemical shifts: Density functional theory calculations. Journal of Chemical Physics, 1999, 110, 7153-7159.	1.2	26
164	Calculating rovibrational energy levels of a triatomic molecule with a simple Lanczos method. Journal of Chemical Physics, 1999, 110, 10269-10274.	1.2	57
165	A direct-operation time-dependent method for calculating absorption spectra involving multiple electronic states and its application to trans-OsO2(oxalate)22â^. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 575-583.	2.0	14
166	A comparison of filter diagonalisation methods with the Lanczos method for calculating vibrational energy levels. Chemical Physics Letters, 1999, 312, 311-318.	1.2	63
167	An exact Eckart-embedded kinetic energy operator in Radau coordinates for triatomic molecules. Chemical Physics Letters, 1998, 287, 289-300.	1.2	53
168	Vibrational polarizabilities of Na3 computed from density functional theory property surfaces and a variational vibrational calculation. Chemical Physics Letters, 1998, 287, 307-314.	1.2	4
169	Rate constants in quantum mechanical systems: A rigorous and practical path-integral formulation for computer simulations. Chemical Physics Letters, 1998, 293, 209-220.	1.2	18
170	Explicit expressions for triatomic Eckart frames in Jacobi, Radau, and bond coordinates. Journal of Chemical Physics, 1997, 107, 2813-2818.	1.2	49
171	The triatomic Eckart-frame kinetic energy operator in bond coordinates. Journal of Chemical Physics, 1997, 107, 9493-9501.	1.2	46
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