Attila G CsÃ¡szÃ¡r

List of Publications by Year
in descending order

254 papers	16,624 citations	22099 59 h-index	19136 118 g-index
268 all docs	268 docs citations	268 times ranked	8273 citing authors

#	Article	IF	Citations
1	The HITRAN2020 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 277, 107949.	1.1	770
2	MARVEL analysis of the high-resolution rovibrational spectra of H16O35Cl. Journal of Molecular Spectroscopy, 2022, 384, 111561.	0.4	1
3	A quantumâ€chemical perspective on the laserâ€induced alignment and orientation dynamics of the <scp>CH</scp>₃X (X = F, Cl, Br, I) molecules. Journal of Computational Chemistry, 2022, 43, 519-538.	1.5	7
4	Normal-Mode Vibrational Analysis of Weakly Bound Oligomers at Constrained Stationary Points of Arbitrary Order. Journal of Chemical Theory and Computation, 2022, 18, 1788-1798.	2.3	1
5	Ultraprecise relative energies in the (2 0 0) vibrational band of H₂¹⁶O. Molecular Physics, 2022, 120, .	0.8	8
6	Reduced-dimensional vibrational models of the water dimer. Journal of Chemical Physics, 2022, 156, 164304.	1.2	6
7	Partition sums for non-local thermodynamic equilibrium conditions for nine molecules of importance in planetary atmospheres. Icarus, 2022, 378, 114947.	1.1	9
8	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
9	Exactly solvable 1D model explains the low-energy vibrational level structure of protonated methane. Chemical Communications, 2021, 57, 4827-4830.	2.2	2
10	Exact Numerical Methods for Stationary-State-Based Quantum Dynamics of Complex Polyatomic Molecules. , 2021, , 43-78.		1
11	Comment on â€œWigner numbersâ€•[J. Chem. Phys. 151, 244122 (2019)]. Journal of Chemical Physics, 2021, 154, 087101.	1.2	0
12	Vibrational spectroscopy of H2He+ and D2He+. Journal of Molecular Spectroscopy, 2021, 377, 111423.	0.4	8
13	Understanding the structure of complex multidimensional wave functions. A case study of excited vibrational states of ammonia. Journal of Chemical Physics, 2021, 154, 144306.	1.2	1
14	On neglecting Coriolis and related couplings in first-principles rovibrational spectroscopy: Considerations of symmetry, accuracy, and simplicity. II. Case studies for H2O isotopologues, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si886.svg"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow><mml:mn>3</mml:mn><mml:mn>2</mml:mn></mml:msubsup><mml:mi>O</mml:mi></mml:mrow></mml:math>, and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msup><mml:mrow /><mml:mn>12</mml:mn></mml:msup><mml:mi>C</mml:mi><mml:msup><mml:mrow /><mml:mn>16</mml:mn></mml:msup><mml:mi>O</mml:mi></mml:math>. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 259, 107398.	2.0	9
15	Network-Based Design of Near-Infrared Lamb-Dip Experiments and the Determination of Pure Rotational Energies of H218O at kHz Accuracy. Journal of Physical and Chemical Reference Data, 2021, 50, 011102.	1.1	21
16	Network-Based Design of Near-Infrared Lamb-Dip Experiments and the Determination of Pure Rotational Energies of H218O at kHz Accuracy. Journal of Physical and Chemical Reference Data, 2021, 50, .	1.9	10
17	Selecting lines for spectroscopic (re)measurements to improve the accuracy of absolute energies of rovibronic quantum states. Journal of Cheminformatics, 2021, 13, 67.	2.8	4
18	autoECART: Automatic energy conservation analysis of rovibronic transitions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 272, 107756.	1.1	5

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19	The rovibrational Aharonovâ€“Bohm effect. Physical Chemistry Chemical Physics, 2021, 23, 24154-24164.	1.3	0
20	Quasistructural molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1432.	6.2	16
21	An update to the MARVEL data set and ExoMol line list for 12C2. Monthly Notices of the Royal Astronomical Society, 2020, 497, 1081-1097.	1.6	25
22	From bridges to cycles in spectroscopic networks. Scientific Reports, 2020, 10, 19489.	1.6	6
23	Rotationalâ€“vibrational resonance states. Physical Chemistry Chemical Physics, 2020, 22, 15081-15104.	1.3	10
24	Spectroscopic-network-assisted precision spectroscopy and its application to water. Nature Communications, 2020, 11, 1708.	5.8	35
25	On neglecting Coriolis and related couplings in first-principles rovibrational spectroscopy: considerations of symmetry, accuracy, and simplicity. Scientific Reports, 2020, 10, 4872.	1.6	8
26	W2020: A Database of Validated Rovibrational Experimental Transitions and Empirical Energy Levels of H216O. Journal of Physical and Chemical Reference Data, 2020, 49, .	1.9	23
27	Empirical rovibrational energy levels of ammonia up to 7500â€¯cm<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msup><mml:mrow /><mml:mrow><mml:mo>â^’</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:msup></mml:math>. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 251, 107027.	1.1	20
28	Spectroscopic signatures of HHe2+ and HHe3+. Physical Chemistry Chemical Physics, 2020, 22, 22885-22888.	1.3	15
29	The W2020 Database of Validated Rovibrational Experimental Transitions and Empirical Energy Levels of Water Isotopologues. II. H217O and H218O with an Update to H216O. Journal of Physical and Chemical Reference Data, 2020, 49, .	1.9	28
30	Light-Dressed Spectroscopy of Molecules. Topics in Applied Physics, 2020, , 77-100.	0.4	0
31	On the use of reduced-density matrices for the semi-automatic assignment of vibrational states. Molecular Physics, 2019, 117, 1682-1693.	0.8	7
32	Infrared Signatures of the HHe_n⁺ and DHe_n⁺ (n = 3â€“6) Complexes. Journal of Physical Chemistry Letters, 2019, 10, 5325-5330.	2.1	22
33	Rovibronic spectra of molecules dressed by light fields. Physical Review A, 2019, 100, .	1.0	11
34	Rovibrational quantum dynamics of the vinyl radical and its deuterated isotopologues. Physical Chemistry Chemical Physics, 2019, 21, 3453-3472.	1.3	13
35	Accurate empirical rovibrational energies and transitions of H₂¹⁶O. Physical Chemistry Chemical Physics, 2019, 21, 3473-3495.	1.3	54
36	Molecular dimers of methane clathrates: ab initio potential energy surfaces and variational vibrational states. Physical Chemistry Chemical Physics, 2019, 21, 13504-13525.	1.3	28

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37	Toward Automated Variational Computation of Rovibrational Resonances, Including a Case Study of the H₂ Dimer. Journal of Chemical Theory and Computation, 2019, 15, 4156-4169.	2.3	5
38	MARVEL analysis of the measured high-resolution spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si105.svg"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>14</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math>NH. Journal of Molecular Spectroscopy, 2019, 362, 69-76.	0.4	20
39	Fingerprints of microscopic superfluidity in HHen+ clusters. Molecular Physics, 2019, 117, 1559-1583.	0.8	15
40	MARVEL Analysis of the Measured High-Resolution Rovibronic Spectra and Definitive Ideal-Gas Thermochemistry of the 16O2 Molecule. Journal of Physical and Chemical Reference Data, 2019, 48, .	1.9	14
41	Heterocumulenic carbene nitric oxide radical OCCNOË™. Chemical Communications, 2019, 55, 13510-13513.	2.2	3
42	Controlling tunneling in ammonia isotopomers. Journal of Chemical Physics, 2019, 150, 014102.	1.2	28
43	Rovibrational Resonances in H₂He⁺. Journal of Chemical Theory and Computation, 2018, 14, 1523-1533.	2.3	14
44	The 1943 K emission spectrum of H216O between 6600 and 7050 cm<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:msup><mml:mrow /><mml:mrow><mml:mo>â^'</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:msup></mml:math>. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 206, 46-54.	1.1	7
45	Critical evaluation of measured rotationalâ€“vibrational transitions of four sulphur isotopologues of S16O2. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 208, 152-163.	1.1	32
46	MARVEL analysis of the measured high-resolution rovibrational spectra of C2H2. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 204, 42-55.	1.1	41
47	Definitive thermochemistry and kinetics of the interconversions among conformers of nâ€butane and nâ€pentane. Journal of Computational Chemistry, 2018, 39, 424-437.	1.5	2
48	Marvel Analysis of the Measured High-resolution Rovibronic Spectra of ⁹⁰Zr¹⁶O. Astrophysical Journal, 2018, 867, 33.	1.6	24
49	Conical Intersections Induced by Quantum Light: Field-Dressed Spectra from the Weak to the Ultrastrong Coupling Regimes. Journal of Physical Chemistry Letters, 2018, 9, 6215-6223.	2.1	59
50	Direct Signatures of Light-Induced Conical Intersections on the Field-Dressed Spectrum of Na₂. Journal of Physical Chemistry Letters, 2018, 9, 2739-2745.	2.1	28
51	Marvel analysis of the measured high-resolution rovibrational spectra of H232S. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 218, 178-186.	1.1	29
52	Vibrational quantum graphs and their application to the quantum dynamics of CH₅⁺. Physical Chemistry Chemical Physics, 2018, 20, 16913-16917.	1.3	13
53	Complex rovibrational dynamics of the ArÂ·NO⁺ complex. Physical Chemistry Chemical Physics, 2017, 19, 8152-8160.	1.3	19
54	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.	1.1	122

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55	MARVEL Analysis of the Measured High-resolution Rovibronic Spectra of ⁴⁸Ti¹⁶O. Astrophysical Journal, Supplement Series, 2017, 228, 15.	3.0	48
56	Four faces of the interaction between ions and aromatic rings. Journal of Computational Chemistry, 2017, 38, 1762-1773.	1.5	9
57	Recommended Ideal-Gas Thermochemical Functions for Heavy Water and its Substituent Isotopologues. Journal of Physical and Chemical Reference Data, 2017, 46, .	1.9	17
58	Rovibrational quantum dynamical computations for deuterated isotopologues of the methaneâ€“water dimer. Physical Chemistry Chemical Physics, 2017, 19, 15335-15345.	1.3	23
59	Cycle bases to the rescue. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 557-564.	1.1	17
60	Fourier Transform Microwave Spectrum of Propene-3-d₁ (CH₂â•CHCH₂D), Quadrupole Coupling Constants of Deuterium, and a Semiexperimental Equilibrium Structure of Propene. Journal of Physical Chemistry A, 2017, 121, 3155-3166.	1.1	9
61	On the use of nonrigid-molecular symmetry in nuclear motion computations employing a discrete variable representation: A case study of the bending energy levels of CH5+. Journal of Chemical Physics, 2017, 147, 134101.	1.2	36
62	High-accuracy calculations of the rotation-vibration spectrum of ${{m{H}}}_{3}^{+}$. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 232001.	0.6	15
63	A general variational approach for computing rovibrational resonances of polyatomic molecules. Application to the weakly bound H2He+ and H2â‹…CO systems. Journal of Chemical Physics, 2017, 147, 094106.	1.2	15
64	The HITRAN2016 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 3-69.	1.1	2,840
65	Interpretation of the vibrational energy level structure of the astructural molecular ion H5+ and all of its deuterated isotopomers. Journal of Chemical Physics, 2016, 144, 154309.	1.2	29
66	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE ¹²C₂ MOLECULE. Astrophysical Journal, Supplement Series, 2016, 224, 44.	3.0	45
67	The current status of the W@DIS information system. Proceedings of SPIE, 2016, , .	0.8	2
68	Definitive Ideal-Gas Thermochemical Functions of the H216O Molecule. Journal of Physical and Chemical Reference Data, 2016, 45, .	1.9	37
69	Small Moleculesâ€”Big Data. Journal of Physical Chemistry A, 2016, 120, 8949-8969.	1.1	36
70	Uncertainty estimates for theoretical atomic and molecular data. Journal Physics D: Applied Physics, 2016, 49, 363002.	1.3	66
71	Rovibrational energy levels of the F^{â˜}(H₂O) and F^{â˜}(D₂O) complexes. Physical Chemistry Chemical Physics, 2016, 18, 17678-17690.	1.3	22
72	Vibrational memory in quantum localized states. Physical Review A, 2016, 93, .	1.0	14

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73	Rovibrational transitions of the methaneâ€“water dimer from intermolecular quantum dynamical computations. Physical Chemistry Chemical Physics, 2016, 18, 22816-22826.	1.3	24
74	On spectra of spectra. Journal of Mathematical Chemistry, 2016, 54, 806-822.	0.7	20
75	Promoting and inhibiting tunneling via nuclear motions. Physical Chemistry Chemical Physics, 2016, 18, 1092-1104.	1.3	14
76	MARVEL analysis of the measured high-resolution spectra of 14NH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 161, 117-130.	1.1	70
77	Domino Tunneling. Journal of the American Chemical Society, 2015, 137, 7828-7834.	6.6	46
78	Modelling rotations, vibrations, and rovibrational couplings in astructural molecules â€“ a case study based on the H⁺₅ molecular ion. Molecular Physics, 2015, 113, 1873-1883.	0.8	15
79	Zero-Cost Estimation of Zero-Point Energies. Journal of Physical Chemistry A, 2015, 119, 10229-10240.	1.1	10
80	Toward accurate thermochemistry of the 24MgH, 25MgH, and 26MgH molecules at elevated temperatures: Corrections due to unbound states. Journal of Chemical Physics, 2015, 142, 014103.	1.2	21
81	Equilibrium Structures of Three-, Four-, Five-, Six-, and Seven-Membered Unsaturated N-Containing Heterocycles. Journal of Physical Chemistry A, 2015, 119, 1731-1746.	1.1	36
82	Recommended isolated-line profile for representing high-resolution spectroscopic transitions (IUPAC) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.9	225
83	Modelling non-adiabatic effects in H3+: Solution of the rovibrational SchrÃ¶dinger equation with motion-dependent masses and mass surfaces. Journal of Chemical Physics, 2014, 141, 154111.	1.2	19
84	A database of water transitions from experiment and theory (IUPAC Technical Report). Pure and Applied Chemistry, 2014, 86, 71-83.	0.9	76
85	Surprising Quenching of the Spinâ€“Orbit Interaction Significantly Diminishes H₂OÂ·Â·X [X = F, Cl, Br, I] Dissociation Energies. Journal of Physical Chemistry A, 2014, 118, 11956-11961.	1.1	6
86	Grid-Based Empirical Improvement of Molecular Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 6256-6265.	1.1	3
87	IUPAC critical evaluation of the rotationalâ€“vibrational spectra of water vapor. Part IV. Energy levels and transition wavenumbers for D216O, D217O, and D218O. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 142, 93-108.	1.1	80
88	A hybrid variationalâ€“perturbational nuclear motion algorithm. Molecular Physics, 2014, 112, 2462-2467.	0.8	11
89	Numerically constructed internal-coordinate Hamiltonian with Eckart embedding and its application for the inversion tunneling of ammonia. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 84-89.	2.0	49
90	Communication: Rigidity of the molecular ion ${m H}_5^+$H5+. Journal of Chemical Physics, 2014, 140, 051101.	1.2	30

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91	Simple molecules as complex systems. Scientific Reports, 2014, 4, 4654.	1.6	34
92	Analysis of the Rotationalâ€“Vibrational States of the Molecular Ion H₃⁺. Journal of Chemical Theory and Computation, 2013, 9, 5471-5478.	2.3	51
93	Accurate Determination of the Deformation of the Benzene Ring upon Substitution: Equilibrium Structures of Benzonitrile and Phenylacetylene. Journal of Physical Chemistry A, 2013, 117, 12969-12982.	1.1	33
94	Semiexperimental Equilibrium Structures for cis,cis- and trans,trans-1,4-Difluorobutadiene by the Mixed Estimation Method and Definitive Relative Energies of the Isomers. Journal of Physical Chemistry A, 2013, 117, 13166-13175.	1.1	1
95	Dynamics of the Fâ˙ + CH3Cl â†’ Clâ˙ + CH3F SN2 reaction on a chemically accurate potential energy surface. Chemical Science, 2013, 4, 4362.	3.7	70
96	MARVEL analysis of the rotationalâ€“vibrational states of the molecular ions H2D+ and D2H+. Physical Chemistry Chemical Physics, 2013, 15, 10181.	1.3	36
97	Reduced-Dimensional Quantum Computations for the Rotationalâ€“Vibrational Dynamics of F^{â€“}â€“CH₄ and F^{â€“}â€“CH₂D₂. Journal of Physical Chemistry A, 2013, 117, 6975-6983.	1.1	11
98	Deformation of the benzene ring upon fluorination: equilibrium structures of all fluorobenzenes. Molecular Physics, 2013, 111, 1539-1562.	0.8	38
99	Low-lying quasibound rovibrational states of H₂ ¹⁶O^{**}. Molecular Physics, 2013, 111, 2131-2146.	0.8	21
100	IUPAC critical evaluation of the rotationalâ€“vibrational spectra of water vapor, Part III: Energy levels and transition wavenumbers for H216O. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 117, 29-58.	1.1	215
101	The role of axis embedding on rigid rotor decomposition analysis of variational rovibrational wave functions. Journal of Chemical Physics, 2012, 136, 174112.	1.2	30
102	Global spectroscopy of the water monomer. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2728-2748.	1.6	34
103	Benchmarking Experimental and Computational Thermochemical Data: A Case Study of the Butane Conformers. Journal of Chemical Theory and Computation, 2012, 8, 479-486.	2.3	13
104	The fourth age of quantum chemistry: molecules in motion. Physical Chemistry Chemical Physics, 2012, 14, 1085-1106.	1.3	196
105	Spectroscopy of H ₃ ⁺ based on a new high-accuracy global potential energy surface. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 5014-5027.	1.6	33
106	Temperature-Dependent, Effective Structures of the ¹⁴NH₃ and ¹⁴ND₃ Molecules. Journal of Physical Chemistry A, 2012, 116, 4356-4362.	1.1	8
107	Equilibrium CO bond lengths. Journal of Molecular Structure, 2012, 1023, 7-14.	1.8	45
108	Precision Measurements and Computations of Transition Energies in Rotationally Cold Triatomic Hydrogen Ions up to the Midvisible Spectral Range. Physical Review Letters, 2012, 108, 023002.	2.9	88

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109	Calibration-quality adiabatic potential energy surfaces for ${m H}_3^+$H3+ and its isotopologues. Journal of Chemical Physics, 2012, 136, 184303.	1.2	72
110	Anharmonic molecular force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 273-289.	6.2	69
111	MARVEL: Measured active rotationalâ€“vibrational energy levels. II. Algorithmic improvements. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 929-935.	1.1	111
112	The role of intensities in determining characteristics of spectroscopic networks. Journal of Molecular Structure, 2012, 1009, 123-129.	1.8	39
113	A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements. Journal of Mathematical Chemistry, 2012, 50, 636-651.	0.7	12
114	Equilibrium Structures of Heterocyclic Molecules with Large Principal Axis Rotations upon Isotopic Substitution. Journal of Physical Chemistry A, 2011, 115, 14078-14091.	1.1	31
115	First-principles rotationâ€“vibration spectrum of water above dissociation. Chemical Physics Letters, 2011, 507, 48-51.	1.2	29
116	Spectroscopic networks. Journal of Molecular Spectroscopy, 2011, 266, 99-103.	0.4	70
117	Do the mercaptocarbene (Hâ€“Câ€“Sâ€“H) and selenocarbene (Hâ€“Câ€“Seâ€“H) congeners of hydroxycarbene (Hâ€“Câ€“Oâ€“H) undergo 1,2-H-tunneling?. Collection of Czechoslovak Chemical Communications, 2011, 76, 645-667.	1.0	14
118	Rotating full- and reduced-dimensional quantum chemical models of molecules. Journal of Chemical Physics, 2011, 134, 074105.	1.2	97
119	Variational quantum mechanical and active database approaches to the rotational-vibrational spectroscopy of ketene, H2CCO. Journal of Chemical Physics, 2011, 135, 094307.	1.2	57
120	From a Network of Computed Reaction Enthalpies to Atomâ€Based Thermochemistry (NEAT). Chemistry - A European Journal, 2010, 16, 4826-4835.	1.7	23
121	First-principles prediction and partial characterization of the vibrational states of water up to dissociation. Journal of Quantitative Spectroscopy and Radiative Transfer, 2010, 111, 1043-1064.	1.1	72
122	IUPAC critical evaluation of the rotationalâ€“vibrational spectra of water vapor. Part II. Journal of Quantitative Spectroscopy and Radiative Transfer, 2010, 111, 2160-2184.	1.1	178
123	Equilibrium structure in the presence of internal rotation: A case study of cis-methyl formate. Journal of Molecular Spectroscopy, 2010, 259, 70-79.	0.4	29
124	Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. Journal of Chemical Physics, 2010, 133, 034113.	1.2	61
125	Lowest-Lying Conformers of Alanine: Pushing Theory to Ascertain Precise Energetics and Semiexperimental R_e Structures. Journal of Chemical Theory and Computation, 2010, 6, 3066-3078.	2.3	73
126	On the efficiency of treating singularities in triatomic variational vibrational computations. The vibrational states of H+3 up to dissociation. Physical Chemistry Chemical Physics, 2010, 12, 8373.	1.3	33

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127	On the variational computation of a large number of vibrational energy levels and wave functions for medium-sized molecules. Journal of Chemical Physics, 2009, 131, 074106.	1.2	67
128	Adiabatic Jacobi corrections on the vibrational energy levels of H2+ isotopologues. Journal of Chemical Physics, 2009, 130, 134314.	1.2	14
129	Toward black-box-type full- and reduced-dimensional variational (ro)vibrational computations. Journal of Chemical Physics, 2009, 130, 134112.	1.2	180
130	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	1.0	33
131	IUPAC critical evaluation of the rotationalâ€“vibrational spectra of water vapor. Part Iâ€”Energy levels and transition wavenumbers for H217O and H218O. Journal of Quantitative Spectroscopy and Radiative Transfer, 2009, 110, 573-596.	1.1	188
132	Is the adiabatic approximation sufficient to account for the post-Bornâ€“Oppenheimer effects on molecular electric dipole moments?. Molecular Physics, 2009, 107, 1153-1159.	0.8	20
133	Conformers of Gaseous Cysteine. Journal of Chemical Theory and Computation, 2009, 5, 1511-1523.	2.3	126
134	Conformers of gaseous threonine. Molecular Physics, 2009, 107, 761-775.	0.8	43
135	Bridging Theory with Experiment: A Benchmark Study of Thermally Averaged Structural and Effective Spectroscopic Parameters of the Water Molecule. Journal of Physical Chemistry A, 2009, 113, 11665-11678.	1.1	52
136	Infrared signatures of the NCCO radical. Physical Chemistry Chemical Physics, 2009, 11, 10385.	1.3	13
137	State-selective spectroscopy of water up to its first dissociation limit. Journal of Chemical Physics, 2009, 131, 221105.	1.2	54
138	On employing , , , and lines as frequency standards in the 15â€“170cmâ^'1 window. Journal of Quantitative Spectroscopy and Radiative Transfer, 2008, 109, 1234-1251.	1.1	32
139	Capture of hydroxymethylene and its fast disappearance through tunnelling. Nature, 2008, 453, 906-909.	13.7	264
140	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	2.3	42
141	A new ab initio ground-state dipole moment surface for the water molecule. Journal of Chemical Physics, 2008, 128, 044304.	1.2	81
142	Equilibrium Structure and Torsional Barrier of BH3NH3. Journal of Physical Chemistry A, 2008, 112, 4477-4482.	1.1	26
143	Adiabatic Jacobi corrections for H2+-like systems. Journal of Chemical Physics, 2007, 126, 024102.	1.2	6
144	Vibrational energy levels with arbitrary potentials using the Eckart-Watson Hamiltonians and the discrete variable representation. Journal of Chemical Physics, 2007, 127, 084102.	1.2	90

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145	Equilibrium vs Ground-State Planarity of the CONH Linkage. Journal of Physical Chemistry A, 2007, 111, 2574-2586.	1.1	57
146	Secondary Structures of Peptides and Proteins via NMR Chemical-Shielding Anisotropy (CSA) Parameters. Journal of the American Chemical Society, 2007, 129, 1568-1577.	6.6	19
147	Influence of Intermolecular Interactions on the MÃ¶ssbauer Quadrupole Splitting of Organotin(IV) Compounds as Studied by DFT Calculations. Journal of Physical Chemistry A, 2007, 111, 13172-13181.	1.1	9
148	Electrostatic versus Nonelectrostatic Effects in DNA Sequence Discrimination by Divalent Ions Mg2+and Mn2+. Journal of Physical Chemistry B, 2007, 111, 6272-6279.	1.2	23
149	Use of a nondirect-product basis for treating singularities in triatomic rotationalâ€“vibrational calculations. Physical Chemistry Chemical Physics, 2007, 9, 3407.	1.3	8
150	Chapter 9 An Active Database Approach to Complete Rotationalâ€“Vibrational Spectra of Small Molecules. Annual Reports in Computational Chemistry, 2007, 3, 155-176.	0.9	54
151	Molecular structures of the two most stable conformers of free glycine. Journal of Computational Chemistry, 2007, 28, 1373-1383.	1.5	71
152	Hartreeâ€“Fock-limit energies and structures with a few dozen distributed Gaussians. Chemical Physics Letters, 2007, 438, 139-143.	1.2	32
153	MARVEL: measured active rotationalâ€“vibrational energy levels. Journal of Molecular Spectroscopy, 2007, 245, 115-125.	0.4	198
154	Empirical isotropic chemical shift surfaces. Journal of Biomolecular NMR, 2007, 38, 269-287.	1.6	7
155	The Case of the Weak Nâˆ™X Bond:â€‰ Ab Initio, Semi-Experimental, and Experimental Equilibrium Structures of XNO (X = H, F, Cl, OH) and FNO2. Journal of Physical Chemistry A, 2006, 110, 13609-13617.	1.1	58
156	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. Journal of Chemical Physics, 2006, 125, 064108.	1.2	312
157	The methylene saga continues: Stretching fundamentals and zero-point energy of CH2. Journal of Molecular Structure, 2006, 780-781, 283-294.	1.8	31
158	Spectroscopically determined potential energy surfaces of the H216O, H217O, and H218O isotopologues of water. Journal of Molecular Spectroscopy, 2006, 236, 216-223.	0.4	62
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