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 HITRAN2016 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 3-69.	1.1	2,840
2	The HITRAN2020 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 277, 107949.	1.1	770
3	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	1.2	691
4	In pursuit of theab initiolimit for conformational energy prototypes. Journal of Chemical Physics, 1998, 108, 9751-9764.	1.2	659
5	Conformers of gaseous glycine. Journal of the American Chemical Society, 1992, 114, 9568-9575.	6.6	336
6	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
7	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	1.9	283
8	High-Accuracy ab Initio Rotation-Vibration Transitions for Water. Science, 2003, 299, 539-542.	6.0	281
9	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. Chemical Physics, 1990, 145, 427-466.	0.9	267
10	Capture of hydroxymethylene and its fast disappearance through tunnelling. Nature, 2008, 453, 906-909.	13.7	264
11	Recommended isolated-line profile for representing high-resolution spectroscopic transitions (IUPAC) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	225
12	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
13	MARVEL: measured active rotationalâ€“vibrational energy levels. Journal of Molecular Spectroscopy, 2007, 245, 115-125.	0.4	198
14	Definitive Ab Initio Studies of Model SN2 Reactions CH3X+F (X=F, Cl, CN, OH, SH, NH2, PH2). Chemistry - A European Journal, 2003, 9, 2173-2192.	1.7	196
15	The fourth age of quantum chemistry: molecules in motion. Physical Chemistry Chemical Physics, 2012, 14, 1085-1106.	1.3	196
16	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
17	Conformers of Gaseous Î±-Alanine. The Journal of Physical Chemistry, 1996, 100, 3541-3551.	2.9	183
18	Toward black-box-type full- and reduced-dimensional variational (ro)vibrational computations. Journal of Chemical Physics, 2009, 130, 134112.	1.2	180

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19	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
20	On the ab initio determination of higherâ€order force constants at nonstationary reference geometries. Journal of Chemical Physics, 1993, 98, 2983-3015.	1.2	164
21	On equilibrium structures of the water molecule. Journal of Chemical Physics, 2005, 122, 214305.	1.2	157
22	Ab initio characterization of building units in peptides and proteins. Progress in Biophysics and Molecular Biology, 1999, 71, 243-309.	1.4	152
23	On the structures of free glycine and Î±-alanine. Journal of Molecular Structure, 1995, 346, 141-152.	1.8	131
24	Conformers of Gaseous Cysteine. Journal of Chemical Theory and Computation, 2009, 5, 1511-1523.	2.3	126
25	Anatomy of relativistic energy corrections in light molecular systems. Molecular Physics, 2001, 99, 1769-1794.	0.8	123
26	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
27	CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. Journal of Chemical Physics, 2006, 125, 204307.	1.2	112
28	MARVEL: Measured active rotationalâ€“vibrational energy levels. II. Algorithmic improvements. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 929-935.	1.1	111
29	The puckering inversion barrier and vibrational spectrum of cyclopentene. A scaled quantum mechanical force field algorithm. Journal of the American Chemical Society, 1992, 114, 6834-6849.	6.6	109
30	Ab initio global potential, dipole, adiabatic, and relativistic correction surfaces for the HCNâ€“HNC system. Journal of Chemical Physics, 2001, 115, 3706-3718.	1.2	106
31	Conformers of Gaseous Proline. Chemistry - A European Journal, 2003, 9, 1008-1019.	1.7	106
32	Rotating full- and reduced-dimensional quantum chemical models of molecules. Journal of Chemical Physics, 2011, 134, 074105.	1.2	97
33	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
34	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
35	Ab Initio Anharmonic Vibrational Analyses of Non-Rigid Molecules. , 1993, , 343-373.		86
36	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	1.0	86

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37	The standard enthalpy of formation of CH2. Journal of Chemical Physics, 2003, 118, 10631-10642.	1.2	82
38	A new ab initio ground-state dipole moment surface for the water molecule. Journal of Chemical Physics, 2008, 128, 044304.	1.2	81
39	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
40	Molecular Structure of Proline. Chemistry - A European Journal, 2004, 10, 4512-4517.	1.7	76
41	A database of water transitions from experiment and theory (IUPAC Technical Report). Pure and Applied Chemistry, 2014, 86, 71-83.	0.9	76
42	The effect of 1s correlation on De, re, and Ï‰e of firstâ€row diatomics. Journal of Chemical Physics, 1996, 104, 2746-2748.	1.2	74
43	The barrier to linearity of water. Journal of Chemical Physics, 1999, 110, 11971-11981.	1.2	73
44	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
45	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
46	Calibration-quality adiabatic potential energy surfaces for ${m H}_3^+$H3+ and its isotopologues. Journal of Chemical Physics, 2012, 136, 184303.	1.2	72
47	Molecular structures of the two most stable conformers of free glycine. Journal of Computational Chemistry, 2007, 28, 1373-1383.	1.5	71
48	Spectroscopic networks. Journal of Molecular Spectroscopy, 2011, 266, 99-103.	0.4	70
49	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
50	MARVEL analysis of the measured high-resolution spectra of 14NH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 161, 117-130.	1.1	70
51	Anharmonic molecular force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 273-289.	6.2	69
52	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
53	Vibrational energy levels of water. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1101-1122.	2.0	66
54	Uncertainty estimates for theoretical atomic and molecular data. Journal Physics D: Applied Physics, 2016, 49, 363002.	1.3	66

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55	Variational vibrational calculations using high-order anharmonic force fields. Molecular Physics, 2004, 102, 2411-2423.	0.8	65
56	Scaled quantum mechanical (SQM) force field and theoretical vibrational spectrum for benzonitrile. Spectrochimica Acta Part A: Molecular Spectroscopy, 1989, 45, 845-854.	0.1	64
57	General derivative relations for anharmonic force fields. Molecular Physics, 1996, 89, 1213-1221.	0.8	62
58	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
59	Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. Journal of Chemical Physics, 2010, 133, 034113.	1.2	61
60	Interpretation of the vibrational spectra of matrix-isolated uracil from scaled ab initio quantum mechanical force fields. International Journal of Quantum Chemistry, 1986, 29, 799-815.	1.0	59
61	Equilibrium inversion barrier of NH3from extrapolated coupled-cluster pair energies. Journal of Computational Chemistry, 2001, 22, 1306-1314.	1.5	59
62	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
63	The Case of the Weak Nâ˜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
64	Relativistic correction to the potential energy surface and vibration-rotation levels of water. Chemical Physics Letters, 1998, 293, 317-323.	1.2	57
65	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â˜. Journal of Chemical Physics, 2000, 112, 4053-4063.	1.2	57
66	Equilibrium vs Ground-State Planarity of the CONH Linkage. Journal of Physical Chemistry A, 2007, 111, 2574-2586.	1.1	57
67	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
68	Millimeterâ€•and submillimeterâ€wave spectroscopy of dibridged Si2H2 isotopomers: Experimental and theoretical structure. Journal of Chemical Physics, 1994, 100, 8614-8624.	1.2	55
69	Toward resolution of the silicon dicarbide (SiC2) saga:Ab initioexcursions in the web of polytopism. Journal of Chemical Physics, 1997, 107, 1195-1211.	1.2	55
70	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
71	State-selective spectroscopy of water up to its first dissociation limit. Journal of Chemical Physics, 2009, 131, 221105.	1.2	54
72	Accurate empirical rovibrational energies and transitions of H₂¹⁶O. Physical Chemistry Chemical Physics, 2019, 21, 3473-3495.	1.3	54

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73	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
74	Dream or Reality: Complete Basis Set Full Configuration Interaction Potential Energy Hypersurfaces. , 2001, , 317-339.		51
75	Analysis of the Rotationalâ€“Vibrational States of the Molecular Ion H₃⁺. Journal of Chemical Theory and Computation, 2013, 9, 5471-5478.	2.3	51
76	Intermolecular bond lengths: extrapolation to the basis set limit on uncorrected and BSSE-corrected potential energy hypersurfaces. Journal of Computational Chemistry, 2001, 22, 196-207.	1.5	49
77	The second-order MÃ¸llerâ€“Plesset limit for the barrier to linearity of water. Journal of Chemical Physics, 2001, 114, 2875-2878.	1.2	49
78	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
79	Ab initiotorsional potential and transition frequencies of acetaldehyde. Journal of Chemical Physics, 2004, 120, 1203-1207.	1.2	48
80	MARVEL Analysis of the Measured High-resolution Rovibronic Spectra of ⁴⁸Ti¹⁶O. Astrophysical Journal, Supplement Series, 2017, 228, 15.	3.0	48
81	Domino Tunneling. Journal of the American Chemical Society, 2015, 137, 7828-7834.	6.6	46
82	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. ChemPhysChem, 2006, 7, 1664-1667.	1.0	45
83	Equilibrium CO bond lengths. Journal of Molecular Structure, 2012, 1023, 7-14.	1.8	45
84	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE ¹²C₂ MOLECULE. Astrophysical Journal, Supplement Series, 2016, 224, 44.	3.0	45
85	Anabinitiostudy of the structure and vibrational spectra of allyl and 1,4â€pentadienyl radicals. Journal of Chemical Physics, 1990, 93, 1246-1256.	1.2	44
86	Exact quantum mechanical vibrational kinetic energy operator of sequentially bonded molecules in valence internal coordinates. Journal of Chemical Physics, 1995, 102, 3962-3967.	1.2	44
87	Peptide models XX. Aromatic side-chainâ€“backbone interaction in phenylalanine-containing diamide model system. A systematic search for the identification of all the ab initio conformers of N-formyl-L-phenylalanine-amide. Canadian Journal of Chemistry, 1997, 75, 1120-1130.	0.6	43
88	Benchmark Thermochemistry of the Hydroperoxyl Radicalâ€. Journal of Physical Chemistry A, 2004, 108, 3195-3199.	1.1	43
89	Accurate ab initio determination of spectroscopic and thermochemical properties of mono- and dichlorocarbenes. Physical Chemistry Chemical Physics, 2005, 7, 2881.	1.3	43
90	Conformers of gaseous threonine. Molecular Physics, 2009, 107, 761-775.	0.8	43

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91	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	2.3	42
92	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
93	On one-dimensional discrete variable representations with general basis functions. Journal of Chemical Physics, 2003, 119, 10512-10518.	1.2	39
94	The role of intensities in determining characteristics of spectroscopic networks. Journal of Molecular Structure, 2012, 1009, 123-129.	1.8	39
95	The sodium superoxide radical: XÌƒ2A2 and Ãƒ 2B2 potential energy surfaces. Chemical Physics Letters, 1991, 186, 346-355.	1.2	38
96	Deformation of the benzene ring upon fluorination: equilibrium structures of all fluorobenzenes. Molecular Physics, 2013, 111, 1539-1562.	0.8	38
97	Theoretical prediction of vibrational spectra. Scaled quantum mechanical (SQM) force field for fluorobenzene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1067-1077.	0.1	37
98	Peptide models XXIII. Conformational model for polar side-chain containing amino acid residues: A comprehensive analysis of RHF, DFT, and MP2 properties of HCO-L-SER-NH2. Journal of Computational Chemistry, 2000, 21, 626-655.	1.5	37
99	Two-electron relativistic corrections to the potential energy surface and vibrationâ€“rotation levels of water. Chemical Physics Letters, 2001, 344, 413-420.	1.2	37
100	Symmetry analysis of internal rotation. Journal of Chemical Physics, 2002, 117, 6489-6492.	1.2	37
101	Definitive Ideal-Gas Thermochemical Functions of the H216O Molecule. Journal of Physical and Chemical Reference Data, 2016, 45, .	1.9	37
102	MARVEL analysis of the rotationalâ€“vibrational states of the molecular ions H2D+ and D2H+. Physical Chemistry Chemical Physics, 2013, 15, 10181.	1.3	36
103	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
104	Small Moleculesâ€”Big Data. Journal of Physical Chemistry A, 2016, 120, 8949-8969.	1.1	36
105	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
106	The [FHCl]â^'molecular anion: Structural aspects, global surface, and vibrational eigenspectrum. Journal of Chemical Physics, 1993, 99, 3865-3897.	1.2	35
107	Electronic states of ketene. Journal of Chemical Physics, 1996, 105, 1034-1045.	1.2	35
108	Spectroscopic-network-assisted precision spectroscopy and its application to water. Nature Communications, 2020, 11, 1708.	5.8	35

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109	Ab initio rovibrational spectroscopy of hydrogen sulfide. Journal of Chemical Physics, 2001, 115, 1229-1242.	1.2	34
110	Global spectroscopy of the water monomer. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2728-2748.	1.6	34
111	Simple molecules as complex systems. Scientific Reports, 2014, 4, 4654.	1.6	34
112	Anharmonic force field of carbon dioxide. The Journal of Physical Chemistry, 1992, 96, 7898-7904.	2.9	33
113	The Rotational Spectrum of Propene: Internal Rotation Analysis and ab Initio and Experimental Centrifugal Distortion Constants. Journal of Molecular Spectroscopy, 1994, 167, 239-247.	0.4	33
114	Enthalpy of Formation of 2Î3/2 SH. Journal of Physical Chemistry A, 2003, 107, 2061-2065.	1.1	33
115	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	1.0	33
116	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
117	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
118	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
119	Theoretical prediction of the vibrational spectrum geometry and scaled quantum mechanical force field for phenylacetylene. The Journal of Physical Chemistry, 1989, 93, 7644-7651.	2.9	32
120	The barrier to linearity of hydrogen sulphide. Chemical Physics Letters, 2000, 322, 119-128.	1.2	32
121	Hartreeâ€“Fock-limit energies and structures with a few dozen distributed Gaussians. Chemical Physics Letters, 2007, 438, 139-143.	1.2	32
122	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
123	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
124	The methylene saga continues: Stretching fundamentals and zero-point energy of CH2. Journal of Molecular Structure, 2006, 780-781, 283-294.	1.8	31
125	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
126	Anharmonic Force Field of N2O. The Journal of Physical Chemistry, 1994, 98, 8823-8826.	2.9	30

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127	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
128	Communication: Rigidity of the molecular ion ${m H}_5^+$H5+. Journal of Chemical Physics, 2014, 140, 051101.	1.2	30
129	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
130	First-principles rotationâ€“vibration spectrum of water above dissociation. Chemical Physics Letters, 2011, 507, 48-51.	1.2	29
131	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
132	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
133	Gas-phase molecular structure of (.eta.5-cyclopentadienyl)tris(tetrahydroborato)zirconium: electron-diffraction and EHMO study. Inorganic Chemistry, 1991, 30, 1371-1376.	1.9	28
134	Toward direct determination of conformations of protein building units from multidimensional NMR experiments I. A theoretical case study of For-Gly-NH2 and For-L-Ala-NH2. Journal of Computational Chemistry, 2000, 21, 882-900.	1.5	28
135	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
136	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
137	Controlling tunneling in ammonia isotopomers. Journal of Chemical Physics, 2019, 150, 014102.	1.2	28
138	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
139	Adiabatic approximations to internal rotation. Journal of Chemical Physics, 2006, 124, 224310.	1.2	26
140	Equilibrium Structure and Torsional Barrier of BH3NH3. Journal of Physical Chemistry A, 2008, 112, 4477-4482.	1.1	26
141	The enthalpy of formation of2II CH. Molecular Physics, 2002, 100, 3879-3883.	0.8	25
142	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
143	The rotational spectrum of benzonitrile: Experimental and theoretical determination of the quartic centrifugal distortion constants. Journal of Molecular Spectroscopy, 1989, 134, 297-304.	0.4	24
144	Rovibrational transitions of the methaneâ€“water dimer from intermolecular quantum dynamical computations. Physical Chemistry Chemical Physics, 2016, 18, 22816-22826.	1.3	24

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145	Marvel Analysis of the Measured High-resolution Rovibronic Spectra of ⁹⁰Zr¹⁶O. Astrophysical Journal, 2018, 867, 33.	1.6	24
146	Equilibrium geometries of uracil and its C- and N-methylated derivatives. Computational and Theoretical Chemistry, 1986, 137, 207-215.	1.5	23
147	On the form of the exact quantum mechanical vibrational kinetic energy operator for penta-atomic molecules in internal coordinates. Molecular Physics, 1995, 86, 959-979.	0.8	23
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	From a Network of Computed Reaction Enthalpies to Atomâ€Based Thermochemistry (NEAT). Chemistry - A European Journal, 2010, 16, 4826-4835.	1.7	23
150	Rovibrational quantum dynamical computations for deuterated isotopologues of the methaneâ€“water dimer. Physical Chemistry Chemical Physics, 2017, 19, 15335-15345.	1.3	23
151	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
152	Rovibrational energy levels of the F^{â^’}(H₂O) and F^{â^’}(D₂O) complexes. Physical Chemistry Chemical Physics, 2016, 18, 17678-17690.	1.3	22
153	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
154	Theoretical prediction of vibrational and rotational spectra. Formyl cyanide, HCOCN, and thioformyl cyanide, HCSCN. Chemical Physics Letters, 1989, 162, 361-368.	1.2	21
155	Low-lying quasibound rovibrational states of H₂ ¹⁶O^{**}. Molecular Physics, 2013, 111, 2131-2146.	0.8	21
156	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
157	An improved rovibrational linelist of formaldehyde, H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msubsup><mml:mrow /><mml:mn>2</mml:mn><mml:mrow><mml:mspace width="0.33em" /><mml:mn>12</mml:mn></mml:mrow></mml:msubsup></mml:math>C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msup><mml:mrow /><mml:mn>16</mml:mn></mml:msup></mml:math>O. Journal of Quantitative Spectroscopy and Radiative	1.1	21
158	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
159	On spectra of spectra. Journal of Mathematical Chemistry, 2016, 54, 806-822.	0.7	20
160	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
161	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
162	Vibrational spectra, scaled quantum-mechanical (SQM) force field and assignments for 4H-pyran-4-one. Spectrochimica Acta Part A: Molecular Spectroscopy, 1986, 42, 473-486.	0.1	19

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163	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
164	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
165	Complex rovibrational dynamics of the ArÂ·NO⁺ complex. Physical Chemistry Chemical Physics, 2017, 19, 8152-8160.	1.3	19
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