Oleg L Polyansky

List of Publications by Year
in descending order

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83	4,812	94381	91828
papers	citations	37 h-index	69 g-index

86	86	86	2529
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. Journal of Molecular Spectroscopy, 2016, 327, 73-94.	0.4	364
2	ExoMol molecular line lists XXX: a complete high-accuracy line list for water. Monthly Notices of the Royal Astronomical Society, 2018, 480, 2597-2608.	1.6	282
3	High-Accuracy ab Initio Rotation-Vibration Transitions for Water. Science, 2003, 299, 539-542.	6.0	281
4	DVR3D: a program suite for the calculation of rotationâ€“vibration spectra of triatomic molecules. Computer Physics Communications, 2004, 163, 85-116.	3.0	232
5	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
6	The potential energy surface of H2â€‰16O. Journal of Chemical Physics, 1996, 105, 6490-6497.	1.2	161
7	A global, high accuracy ab initio dipole moment surface for the electronic ground state of the water molecule. Journal of Chemical Physics, 2011, 135, 034113.	1.2	147
8	Ab initio calculation of the rotationâ€“vibration energy levels of H3+ and its isotopomers to spectroscopic accuracy. Journal of Chemical Physics, 1999, 110, 5056-5064.	1.2	135
9	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
10	A spectroscopically determined potential energy surface for the ground state of H216O: A new level of accuracy. Journal of Chemical Physics, 1994, 101, 7651-7657.	1.2	118
11	The near infrared, visible, and near ultraviolet overtone spectrum of water. Journal of Chemical Physics, 1999, 111, 2444-2450.	1.2	115
12	High-Temperature Rotational Transitions of Water in Sunspot and Laboratory Spectra. Journal of Molecular Spectroscopy, 1997, 186, 422-447.	0.4	111
13	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
14	High-Accuracy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Line Intensities Determined from Theory and Experiment. Physical Review Letters, 2015, 114, 243001.	2.9	103
15	Vibration-rotation levels of water beyond the Born-Oppenheimer approximation. Chemical Physics Letters, 1996, 260, 381-387.	1.2	96
16	Spectroscopically determined potential energy surface of H216O up to 25â€Š000 cmâ¯1. Journal of Chemical Physics, 2003, 118, 2124-2129.	1.2	94
17	A room temperature CO2 line list with ab initio computed intensities. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 177, 31-42.	1.1	91
18	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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19	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	1.0	86
20	A new ab initio ground-state dipole moment surface for the water molecule. Journal of Chemical Physics, 2008, 128, 044304.	1.2	81
21	Monodromy in the water molecule. Chemical Physics Letters, 2005, 414, 193-197.	1.2	76
22	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
23	Calibration-quality adiabatic potential energy surfaces for ${m H}_3^+$H3+ and its isotopologues. Journal of Chemical Physics, 2012, 136, 184303.	1.2	72
24	Calculation of Rotationâ€“Vibration Energy Levels of the Water Molecule with Near-Experimental Accuracy Based on an ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 9633-9643.	1.1	70
25	Accurate bond dissociation energy of water determined by triple-resonance vibrational spectroscopy and ab initio calculations. Chemical Physics Letters, 2013, 568-569, 14-20.	1.2	60
26	[ITAL]K[/ITAL]-Band Spectrum of Water in Sunspots. Astrophysical Journal, 1997, 489, L205-L208.	1.6	59
27	Water line lists close to experimental accuracy using a spectroscopically determined potential energy surface for H2O16, H2O17, and H2O18. Journal of Chemical Physics, 2008, 128, 224306.	1.2	59
28	Relativistic correction to the potential energy surface and vibration-rotation levels of water. Chemical Physics Letters, 1998, 293, 317-323.	1.2	57
29	The Emission Spectrum of Hot Water in the Region between 370 and 930 cmâ^'1. Journal of Molecular Spectroscopy, 1996, 176, 305-315.	0.4	55
30	State-selective spectroscopy of water up to its first dissociation limit. Journal of Chemical Physics, 2009, 131, 221105.	1.2	54
31	Room temperature line lists for CO2 symmetric isotopologues with ab initio computed intensities. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 189, 267-280.	1.1	49
32	Opacity Data for HCN and HNC from a New Ab Initio Line List. Astrophysical Journal, 2002, 578, 657-663.	1.6	46
33	A global potential energy surface for the H3+ molecule. Chemical Physics Letters, 1997, 273, 107-114.	1.2	44
34	An accurate, global,ab initiopotential energy surface for the H⁺₃molecule. Molecular Physics, 2000, 98, 261-273.	0.8	44
35	New Assignments for the Infrared Spectrum of H3+. Journal of Molecular Spectroscopy, 1997, 181, 142-150.	0.4	41
36	Approaching the full set of energy levels of water. Journal of Chemical Physics, 2007, 126, 241101.	1.2	39

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37	Vibrationally and rotationally nonadiabatic calculations on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math>using coordinate-dependent vibrational and rotational masses. Physical Review A, 2013, 88, .	1.0	39
38	Spectroscopically determined Bornâ€“Oppenheimer and adiabatic surfaces for H3+, H2D+, D2H+, and D3+. Journal of Chemical Physics, 1995, 103, 10433-10438.	1.2	38
39	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
40	Ab initio rovibrational spectroscopy of hydrogen sulfide. Journal of Chemical Physics, 2001, 115, 1229-1242.	1.2	34
41	Ab initio rotationâ€“vibration energy levels of triatomics to spectroscopic accuracy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 663-672.	2.0	34
42	Global spectroscopy of the water monomer. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2728-2748.	1.6	34
43	Accurate line intensities for water transitions in the infrared: Comparison of theory and experiment. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 88-102.	1.1	34
44	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
45	ExoMol molecular line lists â€“ XX. A comprehensive line list for H3+. Monthly Notices of the Royal Astronomical Society, 2017, 468, 1717-1725.	1.6	32
46	Room temperature linelists for CO2 asymmetric isotopologues with ab initio computed intensities. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 265-281.	1.1	31
47	Asymmetric adiabatic correction to the rotationâ€“vibration levels of H2D+and D2H+. Journal of Chemical Physics, 1995, 102, 9322-9326.	1.2	30
48	Ab initio rotationâ€“vibration spectra of HCN and HNC. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 673-690.	2.0	30
49	First-principles rotationâ€“vibration spectrum of water above dissociation. Chemical Physics Letters, 2011, 507, 48-51.	1.2	29
50	High-accuracy water potential energy surface for the calculation of infrared spectra. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170149.	1.6	29
51	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
52	Collisionally Assisted Spectroscopy of Water from 27â€‰000 to 34â€‰000 cmâ¯1. Journal of Physical Chemistry A, 2008, 112, 10539-10545.	1.1	27
53	Absolute 13C/12C isotope amount ratio for Vienna PeeDee Belemnite from infrared absorption spectroscopy. Nature Physics, 2021, 17, 889-893.	6.5	27
54	Improved potential energy surface and spectral assignments for ammonia in the near-infrared region. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 219, 199-212.	1.1	25

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55	Calculation of rotation-vibration energy levels of the ammonia molecule based on an ab initio potential energy surface. Journal of Molecular Spectroscopy, 2016, 327, 21-30.	0.4	24
56	Calculated line lists for H216O and H218O with extensive comparisons to theoretical and experimental sources including the HITRAN2016 database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 241, 106711.	1.1	23
57	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
58	A highly accurate ab initio dipole moment surface for the ground electronic state of water vapour for spectra extending into the ultraviolet. Journal of Chemical Physics, 2018, 149, 084307.	1.2	22
59	QED correction for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow><mml:mo>+</mml:mo></mml:msup></mml:m Physical Review A, 2014, 89, .	1.0	19
60	Variational Calculation of Highly Excited Rovibrational Energy Levels of H₂O₂. Journal of Physical Chemistry A, 2013, 117, 7367-7377.	1.1	18
61	A global potential energy surface for H₃⁺. Molecular Physics, 2019, 117, 1663-1672.	0.8	18
62	A semi-empirical potential energy surface and line list for H₂¹⁶O extending into the near-ultraviolet. Atmospheric Chemistry and Physics, 2020, 20, 10015-10027.	1.9	17
63	Communication: Visible line intensities of the triatomic hydrogen ion from experiment and theory. Journal of Chemical Physics, 2014, 141, 241104.	1.2	16
64	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
65	High Accuracy ab Initio Calculations of Rotationalâ€“Vibrational Levels of the HCN/HNC System. Journal of Physical Chemistry A, 2018, 122, 1326-1343.	1.1	15
66	Potential energy surface, dipole moment surface and the intensity calculations for the 10 Âµm, 5 Âµm and 3 Âµm bands of ozone. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 210, 127-135.	1.1	14
67	Calculations of rotationâ€“vibration states with thezaxis perpendicular to the plane: High accuracy results for H3+. Journal of Chemical Physics, 2002, 116, 7564-7573.	1.2	13
68	Absorption spectra of ammonia near 1 Î¼m. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 392-397.	1.1	11
69	A new spectroscopically-determined potential energy surface and ab initio dipole moment surface for high accuracy HCN intensity calculations. Journal of Molecular Spectroscopy, 2018, 353, 40-53.	0.4	10
70	On the determination of potential energy surfaces of spectroscopic accuracy. Computational and Theoretical Chemistry, 1995, 341, 133-140.	1.5	9
71	Analysis of the red and green optical absorption spectrum of gas phase ammonia. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 209, 224-231.	1.1	9
72	Use of the complete basis set limit for computing highly accurate ab initio dipole moments. Journal of Chemical Physics, 2020, 152, 024105.	1.2	9

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73	Saddle point localization of molecular wavefunctions. Scientific Reports, 2016, 6, 33068.	1.6	6
74	An experimentally-accurate and complete room-temperature infrared HCN line-list for the HITRAN database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 270, 107666.	1.1	5
75	Ab initio calculation of the ro-vibrational spectrum of H2F+. Journal of Molecular Spectroscopy, 2015, 316, 38-44.	0.4	4
76	Synthesis of ab initio and effective Hamiltonian line lists for ozone. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 269, 107651.	1.1	4
77	Highly accurate HF dimer ab initio potential energy surface. Journal of Chemical Physics, 2022, 156, 164305.	1.2	3
78	Sub-percent accuracy for the intensity of a near-infrared water line at 10,670â€‰cm^{â^'1}: experiment and analysis. Molecular Physics, 2022, 120, .	0.8	3
79	Variational analysis of HF dimer tunneling rotational spectra using an ab initio potential energy surface. Journal of Molecular Spectroscopy, 2021, 379, 111481.	0.4	2
80	Determination of quantum labels based on projections of the total angular momentum on the molecule-fixed axis. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 270, 107716.	1.1	2
81	The spectrum of ammonia near 0.793Â<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si32.svg"><mml:mrow><mml:mi mathvariant="normal">Î¼</mml:mi></mml:mrow></mml:math>m. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 273, 107838.	1.1	2
82	Detection of OH and H<inf>2</inf>O in an atmospheric flame by near-infrared optical frequency comb spectroscopy. , 2017, , .		0
83	Reducing Uncertainties of Molecular Line Intensities Via Cavity Ring-Down Spectroscopy Measurements and Ab Initio Calculations. , 2018, , .		0