Sergei N Yurchenko

List of Publications by Year
in descending order

262	12,344	30047	33869
papers	citations	54 h-index	99 g-index

270	270	270	5262
all docs	docs citations	times ranked	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	From The Cover: Graphene nanostructures as tunable storage media for molecular hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10439-10444.	3.3	573
3	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. Journal of Molecular Spectroscopy, 2016, 327, 73-94.	0.4	364
4	ExoMol: molecular line lists for exoplanet and other atmospheres. Monthly Notices of the Royal Astronomical Society, 2012, 425, 21-33.	1.6	354
5	ExoMol line lists â€“ IV. The rotationâ€“vibration spectrum of methane up to 1500ÂK. Monthly Notices of the Royal Astronomical Society, 2014, 440, 1649-1661.	1.6	299
6	A variationally computed line list for hot NH3. Monthly Notices of the Royal Astronomical Society, 2011, 413, 1828-1834.	1.6	286
7	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
8	A chemical survey of exoplanets with ARIEL. Experimental Astronomy, 2018, 46, 135-209.	1.6	249
9	Theoretical ROVibrational Energies (TROVE): A robust numerical approach to the calculation of rovibrational energies for polyatomic molecules. Journal of Molecular Spectroscopy, 2007, 245, 126-140.	0.4	248
10	A Population Study of Gaseous Exoplanets. Astronomical Journal, 2018, 155, 156.	1.9	219
11	Water vapour in the atmosphere of the habitable-zone eight-Earth-mass planet K2-18 b. Nature Astronomy, 2019, 3, 1086-1091.	4.2	204
12	DETECTION OF AN ATMOSPHERE AROUND THE SUPER-EARTH 55 CANCRI E. Astrophysical Journal, 2016, 820, 99.	1.6	202
13	TAU-REX I: A NEXT GENERATION RETRIEVAL CODE FOR EXOPLANETARY ATMOSPHERES. Astrophysical Journal, 2015, 802, 107.	1.6	198
14	ExoMol line lists â€“ III. An improved hot rotation-vibration line list for HCN and HNC. Monthly Notices of the Royal Astronomical Society, 2014, 437, 1828-1835.	1.6	164
15	A Variationally Computed T = 300 K Line List for NH₃. Journal of Physical Chemistry A, 2009, 113, 11845-11855.	1.1	159
16	ExoMol molecular line lists â€“ XXXIII. The spectrum of Titanium Oxide. Monthly Notices of the Royal Astronomical Society, 2019, 488, 2836-2854.	1.6	149
17	Duo: A general program for calculating spectra of diatomic molecules. Computer Physics Communications, 2016, 202, 262-275.	3.0	134
18	The 2020 release of the ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 255, 107228.	1.1	127

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19	ExoMol line lists â€“ XVIII. The high-temperature spectrum of VO. Monthly Notices of the Royal Astronomical Society, 2016, 463, 771-793.	1.6	126
20	${mathcal{T}}$-REx. II. RETRIEVAL OF EMISSION SPECTRA. Astrophysical Journal, 2015, 813, 13.	1.6	124
21	EXOCROSS: a general program for generating spectra from molecular line lists. Astronomy and Astrophysics, 2018, 614, A131.	2.1	123
22	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
23	Temperature-dependent molecular absorption cross sections for exoplanets and other atmospheres. Icarus, 2013, 226, 1673-1677.	1.1	112
24	Probing the extreme planetary atmosphere of WASP-12b. Icarus, 2013, 225, 432-445.	1.1	112
25	METHANE IN THE ATMOSPHERE OF THE TRANSITING HOT NEPTUNE GJ436B?. Astrophysical Journal, 2011, 731, 16.	1.6	110
26	The discovery of a very cool, very nearby brown dwarf in the Galactic plane. Monthly Notices of the Royal Astronomical Society: Letters, 2010, 408, L56-L60.	1.2	109
27	Structure-based sampling and self-correcting machine learning for accurate calculations of potential energy surfaces and vibrational levels. Journal of Chemical Physics, 2017, 146, 244108.	1.2	106
28	Laser-Induced Interference, Focusing, and Diffraction of Rescattering Molecular Photoelectrons. Physical Review Letters, 2004, 93, 223003.	2.9	102
29	Anab initiostudy of the CH3I photodissociation. I. Potential energy surfaces. Journal of Chemical Physics, 2007, 126, 234102.	1.2	102
30	ExoMol molecular line lists â€“ XVI. The rotationâ€“vibration spectrum of hot H₂S. Monthly Notices of the Royal Astronomical Society, 2016, 460, 4063-4074.	1.6	100
31	ExoMol line lists â€“ VII. The rotationâ€“vibration spectrum of phosphine up to 1500ÂK. Monthly Notices of the Royal Astronomical Society, 2015, 446, 2337-2347.	1.6	99
32	Five carbon- and nitrogen-bearing species in a hot giant planetâ€™s atmosphere. Nature, 2021, 592, 205-208.	13.7	99
33	EChO. Experimental Astronomy, 2012, 34, 311-353.	1.6	98
34	ExoMol line lists â€“ II. The ro-vibrational spectrum of SiO. Monthly Notices of the Royal Astronomical Society, 2013, 434, 1469-1475.	1.6	93
35	Spectrum of hot methane in astronomical objects using a comprehensive computed line list. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9379-9383.	3.3	93
36	A hybrid line list for CH₄and hot methane continuum. Astronomy and Astrophysics, 2017, 605, A95.	2.1	92

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37	ExoMol molecular line lists â€“ XXXV. A rotation-vibration line list for hot ammonia. Monthly Notices of the Royal Astronomical Society, 2019, 490, 4638-4647.	1.6	92
38	ExoMol molecular line lists â€“ IX. The spectrum of AlO. Monthly Notices of the Royal Astronomical Society, 2015, 449, 3613-3619.	1.6	90
39	Hot Exoplanet Atmospheres Resolved with Transit Spectroscopy (HEARTS). Astronomy and Astrophysics, 2020, 641, A123.	2.1	88
40	Vibrational transition moments of CH4 from first principles. Journal of Molecular Spectroscopy, 2013, 291, 69-76.	0.4	87
41	Towards efficient refinement of molecular potential energy surfaces: Ammonia as a case study. Journal of Molecular Spectroscopy, 2011, 268, 123-129.	0.4	77
42	ExoMol molecular line lists â€“ XIV. The rotationâ€“vibration spectrum of hot SO₂. Monthly Notices of the Royal Astronomical Society, 2016, 459, 3890-3899.	1.6	77
43	A high accuracy computed line list for the HDO molecule. Monthly Notices of the Royal Astronomical Society, 2010, 402, 492-496.	1.6	76
44	The ExoMolOP database: Cross sections and k-tables for molecules of interest in high-temperature exoplanet atmospheres. Astronomy and Astrophysics, 2021, 646, A21.	2.1	76
45	HELIOS-K 2.0 Opacity Calculator and Open-source Opacity Database for Exoplanetary Atmospheres. Astrophysical Journal, Supplement Series, 2021, 253, 30.	3.0	74
46	ExoMol line lists - I. The rovibrational spectrum of BeH, MgH and CaH in theXâ€‰²Î£⁺state. Monthly Notices of the Royal Astronomical Society, 2012, 425, 34-43.	1.6	73
47	MARVEL analysis of the measured high-resolution spectra of 14NH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 161, 117-130.	1.1	70
48	BLIND EXTRACTION OF AN EXOPLANETARY SPECTRUM THROUGH INDEPENDENT COMPONENT ANALYSIS. Astrophysical Journal, 2013, 766, 7.	1.6	69
49	Vibrational energies for NH3 based on high level ab initio potential energy surfaces. Journal of Chemical Physics, 2002, 117, 11265-11276.	1.2	68
50	Potential-energy surface for the electronic ground state of NH3 up to 20000cmâ¯1 above equilibrium. Journal of Chemical Physics, 2005, 123, 134308.	1.2	68
51	ExoMol line lists â€“ XXXIX. Ro-vibrational molecular line list for CO2. Monthly Notices of the Royal Astronomical Society, 2020, 496, 5282-5291.	1.6	67
52	Automatic differentiation method for numerical construction of the rotational-vibrational Hamiltonian as a power series in the curvilinear internal coordinates using the Eckart frame. Journal of Chemical Physics, 2015, 143, 014105.	1.2	66
53	ExoMol line list â€“ XXI. Nitric Oxide (NO). Monthly Notices of the Royal Astronomical Society, 2017, 470, 882-897.	1.6	66
54	Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets. Molecular Astrophysics, 2017, 8, 1-18.	1.7	65

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55	Theab initiocalculation of spectra of open shell diatomic molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 102001.	0.6	59
56	Spectroscopic line parameters of NO, NO2, and N2O for the HITEMP database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2019, 232, 35-53.	1.1	59
57	ExoMol line lists â€“ VIII. A variationally computed line list for hot formaldehyde. Monthly Notices of the Royal Astronomical Society, 2015, 448, 1704-1714.	1.6	56
58	Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378.	0.8	55
59	Re-analysis of ammonia spectra: Updating the HITRAN 14NH3 database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 260-272.	1.1	55
60	Methane and ammonia in the near-infrared spectra of late-T dwarfs. Monthly Notices of the Royal Astronomical Society, 2015, 450, 454-480.	1.6	55
61	Lightning chemistry on Earth-like exoplanets. Monthly Notices of the Royal Astronomical Society, 2017, 470, 187-196.	1.6	55
62	The ExoMol project: Software for computing large molecular line lists. International Journal of Quantum Chemistry, 2017, 117, 92-103.	1.0	54
63	Symmetry-Adapted Ro-vibrational Basis Functions for Variational Nuclear Motion Calculations: TROVE Approach. Journal of Chemical Theory and Computation, 2017, 13, 4368-4381.	2.3	53
64	Detecting Chirality in Molecules by Linearly Polarized Laser Fields. Physical Review Letters, 2016, 117, 033001.	2.9	52
65	The ExoMol Atlas of Molecular Opacities. Atoms, 2018, 6, 26.	0.7	52
66	Potential parameters of PH3 obtained by simultaneous fitting of ab initio data and experimental vibrational band origins. Chemical Physics, 2003, 290, 59-67.	0.9	51
67	Optimized semiempirical potential energy surface for H2 16O up to 26000 cmâ˜1. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2011, 110, 160-166.	0.2	51
68	ExoMol molecular line lists â€“ XXXVII. Spectra of acetylene. Monthly Notices of the Royal Astronomical Society, 2020, 493, 1531-1545.	1.6	51
69	ExoMol molecular line lists XIX: high-accuracy computed hot line lists for H₂¹⁸O and H₂¹⁷O. Monthly Notices of the Royal Astronomical Society, 2017, 466, 1363-1371.	1.6	49
70	A new â€œspectroscopicâ€•potential energy surface for formaldehyde in its ground electronic state. Journal of Chemical Physics, 2011, 134, 244307.	1.2	48
71	High temperature partition functions and thermodynamic data for ammonia and phosphine. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 142, 66-74.	1.1	48
72	Ab initio dipole moment and theoretical rovibrational intensities in the electronic ground state of PH3. Journal of Molecular Spectroscopy, 2006, 239, 71-87.	0.4	47

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73	A computed room temperature line list for phosphine. Journal of Molecular Spectroscopy, 2013, 288, 28-37.	0.4	45
74	ExoMol molecular line lists V: the ro-vibrational spectra of NaCl and KCl. Monthly Notices of the Royal Astronomical Society, 2014, 442, 1821-1829.	1.6	45
75	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE ¹²C₂ MOLECULE. Astrophysical Journal, Supplement Series, 2016, 224, 44.	3.0	45
76	ExoMol molecular line lists â€“ XXVII. Spectra of C2H4. Monthly Notices of the Royal Astronomical Society, 2018, 478, 3220-3232.	1.6	45
77	Accurate ab initio vibrational energies of methyl chloride. Journal of Chemical Physics, 2015, 142, 244306.	1.2	44
78	ExoMol molecular line lists â€“ XXIII. Spectra of PO and PS. Monthly Notices of the Royal Astronomical Society, 2017, 472, 3648-3658.	1.6	44
79	Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317.	1.2	43
80	Study of the electronic and rovibronic structure of the Xâ€˜2Î£+, Aâ€˜2Î, and Bâ€˜2Î£+ states of AlO. Journal of Chemical Physics, 2014, 141, 144312.	1.2	43
81	ExoMol linelists XXVIII: the rovibronic spectrum of AlH. Monthly Notices of the Royal Astronomical Society, 2018, 479, 1401-1411.	1.6	43
82	ExoMol molecular line lists â€“ XIII. The spectrum of CaO. Monthly Notices of the Royal Astronomical Society, 2016, 456, 4524-4532.	1.6	42
83	ExoMol line lists XXIV: a new hot line list for silicon monohydride, SiH. Monthly Notices of the Royal Astronomical Society, 2018, 473, 5324-5333.	1.6	42
84	Molecular cross-sections for high-resolution spectroscopy of super-Earths, warm Neptunes, and hot Jupiters. Monthly Notices of the Royal Astronomical Society, 2020, 495, 224-237.	1.6	42
85	Pressure-dependent water absorption cross sections for exoplanets and other atmospheres. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 187, 453-460.	1.1	41
86	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
87	Global Analytical Potential Energy Surface for the Electronic Ground State of NH₃ from High Level ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 7502-7522.	1.1	39
88	Radiative lifetimes and cooling functions for astrophysically important molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 044002.	0.6	39
89	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. International Journal of Hydrogen Energy, 2011, 36, 6005-6013.	3.8	38
90	Terahertz spectroscopy of hydrogen sulfide. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 341-351.	1.1	38

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91	The calculated rovibronic spectrum of scandium hydride, ScH. Molecular Physics, 2015, 113, 1998-2011.	0.8	38
92	A highly accurate ab initio potential energy surface for methane. Journal of Chemical Physics, 2016, 145, 104305.	1.2	38
93	Rotationâ€“Vibration Motion of Pyramidal XY3 Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to NH3. Advances in Quantum Chemistry, 2005, 48, 209-238.	0.4	37
94	A theoretical room-temperature line list for 15NH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 152, 28-36.	1.1	37
95	ExoMol line lists XXXI: spectroscopy of lowest eights electronic states of C2. Monthly Notices of the Royal Astronomical Society, 2018, 480, 3397-3411.	1.6	37
96	ExoMol molecular line lists â€“ X. The spectrum of sodium hydride. Monthly Notices of the Royal Astronomical Society, 2015, 451, 634-638.	1.6	36
97	High-level ab initio potential energy surfaces and vibrational energies of H2CS. Journal of Chemical Physics, 2011, 135, 074302.	1.2	35
98	Theoretical evidence for the formation of rotational energy level clusters in the vibrational ground state of PH3. Physical Chemistry Chemical Physics, 2005, 7, 573.	1.3	34
99	Global spectroscopy of the water monomer. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2728-2748.	1.6	34
100	A theoretical study of the millimeterwave spectrum of CH5+. Journal of Molecular Structure, 2004, 695-696, 253-261.	1.8	33
101	Thermal averaging of the indirect nuclear spin-spin coupling constants of ammonia: The importance of the large amplitude inversion mode. Journal of Chemical Physics, 2010, 132, 114305.	1.2	33
102	A variationally calculated room temperature line-list for H 2 O 2. Journal of Molecular Spectroscopy, 2015, 318, 84-90.	0.4	33
103	Potential energy surface of HDO up to 25000cmâ^'1. Journal of Chemical Physics, 2008, 128, 044312.	1.2	32
104	An ab initio calculation of the vibrational energies and transition moments of HSOH. Journal of Molecular Spectroscopy, 2009, 257, 57-65.	0.4	32
105	Exomol molecular line lists â€“ VI. A high temperature line list for phosphorus nitride. Monthly Notices of the Royal Astronomical Society, 2014, 445, 1383-1391.	1.6	32
106	ExoMol molecular line lists â€“ XVII. The rotationâ€“vibration spectrum of hot SO₃. Monthly Notices of the Royal Astronomical Society, 2016, 462, 4300-4313.	1.6	32
107	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
108	The EChO science case. Experimental Astronomy, 2015, 40, 329-391.	1.6	31

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109	A global potential energy surface and dipole moment surface for silane. Journal of Chemical Physics, 2015, 143, 244317.	1.2	30
110	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
111	Vibrational energies of PH3 calculated variationally at the complete basis set limit. Journal of Chemical Physics, 2008, 129, 044309.	1.2	28
112	ExoMol molecular line lists â€“ XII. Line lists for eight isotopologues of CS. Monthly Notices of the Royal Astronomical Society, 2015, 454, 1931-1939.	1.6	28
113	The status of spectroscopic data for the exoplanet characterisation missions. Experimental Astronomy, 2015, 40, 563-575.	1.6	28
114	ExoMol line lists â€“ XXII. The rotation-vibration spectrum of silane up to 1200â€‰K. Monthly Notices of the Royal Astronomical Society, 2017, 471, 5025-5032.	1.6	28
115	ExoMol molecular line lists XXXVI: XÂ2Î â€“ XÂ2Î and AÂ2Î£+ â€“ XÂ2Î transitions of SH. Monthly Notices of the Royal Astronomical Society, 2019, 490, 1652-1665.	1.6	27
116	The ExoMol pressure broadening diet: H2 and He line-broadening parameters. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 490-495.	1.1	26
117	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
118	Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment. Astrophysical Journal, 2020, 888, 21.	1.6	25
119	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
120	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
121	An ab initio variationally computed room-temperature line list for 32S16O3. Physical Chemistry Chemical Physics, 2013, 15, 10118.	1.3	23
122	The dipole moment surface for hydrogen sulfide H2S. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 161, 41-49.	1.1	23
123	ExoMol line lists â€“ XV. A new hot line list for hydrogen peroxide. Monthly Notices of the Royal Astronomical Society, 2016, 461, 1012-1022.	1.6	22
124	ExoMol line lists â€“ XXXII. The rovibronic spectrum of MgO. Monthly Notices of the Royal Astronomical Society, 2019, 486, 2351-2365.	1.6	22
125	High-Resolution Spectroscopic Study of the (310) Local Mode Combination Band System of AsH3. Journal of Molecular Spectroscopy, 1998, 187, 89-96.	0.4	21
126	PH3 revisited: Theoretical transition moments for the vibrational transitions below. Journal of Molecular Spectroscopy, 2008, 252, 121-128.	0.4	21

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127	ExoMol molecular line lists â€“ XI. The spectrum of nitric acid. Monthly Notices of the Royal Astronomical Society, 2015, 452, 1702-1706.	1.6	21
128	A near infrared line list for NH 3 : Analysis of a Kitt Peak spectrum after 35 years. Journal of Molecular Spectroscopy, 2016, 325, 7-12.	0.4	21
129	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 Radiati	1.1	21
130	Data structures for ExoMol: Molecular line lists for exoplanet and other atmospheres. AIP Conference Proceedings, 2013, , .	0.3	20
131	Hybrid variationalâ€“perturbation method for calculating ro-vibrational energy levels of polyatomic molecules. Molecular Physics, 2015, 113, 1559-1575.	0.8	20
132	High-resolution absorption measurements of NH3 at high temperatures: 500â€“2100cmâ^'1. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 167, 126-134.	1.1	20
133	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
134	Analysis of high temperature ammonia spectra from 780 to 2100cmâ^'1. Journal of Molecular Spectroscopy, 2011, 269, 104-108.	0.4	19
135	Ab initiocalculations to support accurate modelling of the rovibronic spectroscopy calculations of vanadium monoxide (VO). Molecular Physics, 2016, 114, 3232-3248.	0.8	19
136	ExoMol molecular line lists â€“ XXVI: spectra of SH and NS. Monthly Notices of the Royal Astronomical Society, 2018, 478, 270-282.	1.6	19
137	Spectroscopy of YO from first principles. Physical Chemistry Chemical Physics, 2019, 21, 22794-22810.	1.3	19
138	Variational Calculation of Highly Excited Rovibrational Energy Levels of H₂O₂. Journal of Physical Chemistry A, 2013, 117, 7367-7377.	1.1	18
139	Rotational spectrum of SO3 and theoretical evidence for the formation of sixfold rotational energy-level clusters in its vibrational ground state. Journal of Chemical Physics, 2014, 140, 244316.	1.2	18
140	Treating linear molecule HCCH in calculations of rotation-vibration spectra. Journal of Chemical Physics, 2018, 149, 014101.	1.2	18
141	Empirical Line Lists in the ExoMol Database. Atoms, 2020, 8, 7.	0.7	18
142	A high-resolution line list for AlO. Monthly Notices of the Royal Astronomical Society, 2021, 508, 3181-3193.	1.6	18
143	ExoMol line lists â€“ XLIV. Infrared and ultraviolet line list for silicon monoxide (28Si16O). Monthly Notices of the Royal Astronomical Society, 2021, 510, 903-919.	1.6	18
144	Rotational energy cluster formation in XY3 molecules: Excited vibrational states of BiH3 and SbH3. Journal of Molecular Spectroscopy, 2006, 240, 174-187.	0.4	17

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145	Accurate prediction of the ammonia probes of a variable proton-to-electron mass ratio. Monthly Notices of the Royal Astronomical Society, 2015, 450, 3191-3200.	1.6	17
146	Predicted LandÃ© g-factors for open shell diatomic molecules. Journal of Molecular Spectroscopy, 2016, 330, 57-62.	0.4	17
147	G PU A ccelerated IN tensities MPI (GAIN-MPI): A new method of computing Einstein-A coefficients. Computer Physics Communications, 2017, 214, 216-224.	3.0	17
148	Climbing the Rotational Ladder to Chirality. Physical Review Letters, 2018, 121, 193201.	2.9	17
149	Synthetic spectra of BeH, BeD and BeT for emission modeling in JET plasmas. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 185701.	0.6	17
150	A method for calculating temperature-dependent photodissociation cross sections and rates. Physical Chemistry Chemical Physics, 2021, 23, 16390-16400.	1.3	17
151	Observation of electric-quadrupole infrared transitions in water vapor. Physical Review Research, 2020, 2, .	1.3	17
152	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
153	Hydrogen Physisorption on Carbon Foams upon Inclusion of Many-Body and Quantum Delocalization Effects. Journal of Physical Chemistry C, 2012, 116, 19543-19553.	1.5	16
154	A hybrid variational-perturbation calculation of the ro-vibrational spectrum of nitric acid. Journal of Chemical Physics, 2015, 142, 094309.	1.2	16
155	Determination of glyphosate in surface water with high organic matter content. Environmental Science and Pollution Research, 2017, 24, 7880-7888.	2.7	16
156	ExoMol line lists XXV: a hot line list for silicon sulphide, SiS. Monthly Notices of the Royal Astronomical Society, 2018, 477, 1520-1527.	1.6	16
157	Ions in the Thermosphere of Exoplanets: Observable Constraints Revealed by Innovative Laboratory Experiments. Astrophysical Journal, 2020, 895, 77.	1.6	16
158	A weak spectral signature of water vapour in the atmosphere of HD 179949 b at high spectral resolution in the L band. Monthly Notices of the Royal Astronomical Society, 2020, 494, 108-119.	1.6	16
159	Quantum and classical equilibrium properties for exactly solvable models of weakly interacting systems. Physical Chemistry Chemical Physics, 2004, 6, 4152.	1.3	15
160	Theoretical rotation-torsion energies of HSOH. Journal of Chemical Physics, 2008, 129, 154314.	1.2	15
161	Communication: Tunnelling splitting in the phosphine molecule. Journal of Chemical Physics, 2016, 145, 091102.	1.2	15
162	A global ab initio dipole moment surface for methyl chloride. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 184, 100-110.	1.1	15

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163	The high-temperature rotation-vibration spectrum and rotational clustering of silylene (SiH2). Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 246, 106929.	1.1	15
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