

Sergei N Yurchenko

List of Publications by Year in descending order

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262
papers

12,344
citations

29994

54
h-index

33814

99
g-index

270
all docs

270
docs citations

270
times ranked

5262
citing authors

#	ARTICLE	IF	CITATIONS
1	The HITRAN2020 molecular spectroscopic database. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2022, 277, 107949.	1.1	770
2	From The Cover: Graphene nanostructures as tunable storage media for molecular hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 10439-10444.	3.3	573
3	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. <i>Journal of Molecular Spectroscopy</i> , 2016, 327, 73-94.	0.4	364
4	ExoMol: molecular line lists for exoplanet and other atmospheres. <i>Monthly Notices of the Royal Astronomical Society</i> , 2012, 425, 21-33.	1.6	354
5	ExoMol line lists – IV. The rotation–vibration spectrum of methane up to 1500 K. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 440, 1649-1661.	1.6	299
6	A variationally computed line list for hot NH ₃ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 413, 1828-1834.	1.6	286
7	ExoMol molecular line lists XXX: a complete high-accuracy line list for water. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 480, 2597-2608.	1.6	282
8	A chemical survey of exoplanets with ARIEL. <i>Experimental Astronomy</i> , 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. <i>Journal of Molecular Spectroscopy</i> , 2007, 245, 126-140.	0.4	248
10	A Population Study of Gaseous Exoplanets. <i>Astronomical Journal</i> , 2018, 155, 156.	1.9	219
11	Water vapour in the atmosphere of the habitable-zone eight-Earth-mass planet K2-18 b. <i>Nature Astronomy</i> , 2019, 3, 1086-1091.	4.2	204
12	DETECTION OF AN ATMOSPHERE AROUND THE SUPER-EARTH 55 CANCRI E. <i>Astrophysical Journal</i> , 2016, 820, 99.	1.6	202
13	TAU-REX I: A NEXT GENERATION RETRIEVAL CODE FOR EXOPLANETARY ATMOSPHERES. <i>Astrophysical Journal</i> , 2015, 802, 107.	1.6	198
14	ExoMol line lists – III. An improved hot rotation-vibration line list for HCN and HNC. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 437, 1828-1835.	1.6	164
15	A Variationally Computed $\langle i \rangle T \langle i \rangle = 300$ K Line List for NH ₃ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 11845-11855.	1.1	159
16	ExoMol molecular line lists – XXXIII. The spectrum of Titanium Oxide. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 488, 2836-2854.	1.6	149
17	Duo: A general program for calculating spectra of diatomic molecules. <i>Computer Physics Communications</i> , 2016, 202, 262-275.	3.0	134
18	The 2020 release of the ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 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 H ₂ S. 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 1500ÅK. 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 CH ₄ and 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 CH ₄ 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 SO ₂ . 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 <i>k</i> -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 the <i>X</i> ² Σ^+ 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 ¹⁴ NH ₃ . 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 NH ₃ 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 NH ₃ up to 20000cm ⁻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 CO ₂ . 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	The <i>ab initio</i> calculation 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, NO ₂ , and N ₂ O for the HITEMP database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2019, 232, 35-53.	1.1	59
57	ExoMol line lists – VIII. A variationally computed line list for hot formaldehyde. Monthly Notices of the Royal Astronomical Society, 2015, 448, 1704-1714.	1.6	56
58	Rotation-vibration motion of pyramidal XY ₃ molecules described in the Eckart frame: Theory and application to NH ₃ . Molecular Physics, 2005, 103, 359-378.	0.8	55
59	Re-analysis of ammonia spectra: Updating the HITRAN 14NH ₃ 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 PH ₃ obtained by simultaneous fitting of <i>ab initio</i> data and experimental vibrational band origins. Chemical Physics, 2003, 290, 59-67.	0.9	51
67	Optimized semiempirical potential energy surface for H ₂ 16O up to 26000 cm ⁻¹ . Optics and Spectroscopy (English Translation of Optika i Spektroskopiya), 2011, 110, 160-166.	0.2	51
68	ExoMol molecular line lists – 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 H ₂ ¹⁸ O and H ₂ ¹⁷ O. Monthly Notices of the Royal Astronomical Society, 2017, 466, 1363-1371.	1.6	49
70	A new “spectroscopic” 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	<i>Ab initio</i> dipole moment and theoretical rovibrational intensities in the electronic ground state of PH ₃ . Journal of Molecular Spectroscopy, 2006, 239, 71-87.	0.4	47

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73	A computed room temperature line list for phosphine. <i>Journal of Molecular Spectroscopy</i> , 2013, 288, 28-37.	0.4	45
74	ExoMol molecular line lists V: the ro-vibrational spectra of NaCl and KCl. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 442, 1821-1829.	1.6	45
75	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE $^{12}\text{C}^{2-}$ MOLECULE. <i>Astrophysical Journal, Supplement Series</i> , 2016, 224, 44.	3.0	45
76	ExoMol molecular line lists " XXVII. Spectra of C ₂ H ₄ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 478, 3220-3232.	1.6	45
77	Accurate <i>ab initio</i> vibrational energies of methyl chloride. <i>Journal of Chemical Physics</i> , 2015, 142, 244306.	1.2	44
78	ExoMol molecular line lists " XXIII. Spectra of PO and PS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017, 472, 3648-3658.	1.6	44
79	Dipole moment and rovibrational intensities in the electronic ground state of NH ₃ : Bridging the gap between <i>ab initio</i> theory and spectroscopic experiment. <i>Journal of Chemical Physics</i> , 2005, 122, 104317.	1.2	43
80	Study of the electronic and rovibronic structure of the $X^2\tilde{\Sigma}^+$, $A^2\tilde{\Pi}$, and $B^2\tilde{\Sigma}^+$ states of AlO. <i>Journal of Chemical Physics</i> , 2014, 141, 144312.	1.2	43
81	ExoMol line lists XXVIII: the rovibronic spectrum of AlH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 479, 1401-1411.	1.6	43
82	ExoMol molecular line lists " XIII. The spectrum of CaO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016, 456, 4524-4532.	1.6	42
83	ExoMol line lists XXIV: a new hot line list for silicon monohydride, SiH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 473, 5324-5333.	1.6	42
84	Molecular cross-sections for high-resolution spectroscopy of super-Earths, warm Neptunes, and hot Jupiters. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 495, 224-237.	1.6	42
85	Pressure-dependent water absorption cross sections for exoplanets and other atmospheres. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017, 187, 453-460.	1.1	41
86	MARVEL analysis of the measured high-resolution rovibrational spectra of C ₂ H ₂ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018, 204, 42-55.	1.1	41
87	Global Analytical Potential Energy Surface for the Electronic Ground State of NH ₃ from High Level <i>ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7502-7522.	1.1	39
88	Radiative lifetimes and cooling functions for astrophysically important molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016, 49, 044002.	0.6	39
89	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 6005-6013.	3.8	38
90	Terahertz spectroscopy of hydrogen sulfide. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2013, 130, 341-351.	1.1	38

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91	The calculated rovibronic spectrum of scandium hydride, ScH. <i>Molecular Physics</i> , 2015, 113, 1998-2011.	0.8	38
92	A highly accurate <i>ab initio</i> potential energy surface for methane. <i>Journal of Chemical Physics</i> , 2016, 145, 104305.	1.2	38
93	Rotation-Vibration Motion of Pyramidal XY ₃ Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to NH ₃ . <i>Advances in Quantum Chemistry</i> , 2005, 48, 209-238.	0.4	37
94	A theoretical room-temperature line list for 15NH ₃ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015, 152, 28-36.	1.1	37
95	ExoMol line lists XXXI: spectroscopy of lowest eight electronic states of C ₂ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 480, 3397-3411.	1.6	37
96	ExoMol molecular line lists X. The spectrum of sodium hydride. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 451, 634-638.	1.6	36
97	High-level <i>ab initio</i> potential energy surfaces and vibrational energies of H ₂ CS. <i>Journal of Chemical Physics</i> , 2011, 135, 074302.	1.2	35
98	Theoretical evidence for the formation of rotational energy level clusters in the vibrational ground state of PH ₃ . <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 573.	1.3	34
99	Global spectroscopy of the water monomer. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 2728-2748.	1.6	34
100	A theoretical study of the millimeterwave spectrum of CH ₅ ⁺ . <i>Journal of Molecular Structure</i> , 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. <i>Journal of Chemical Physics</i> , 2010, 132, 114305.	1.2	33
102	A variationally calculated room temperature line-list for H ₂ O ₂ . <i>Journal of Molecular Spectroscopy</i> , 2015, 318, 84-90.	0.4	33
103	Potential energy surface of HDO up to 25000cm ⁻¹ . <i>Journal of Chemical Physics</i> , 2008, 128, 044312.	1.2	32
104	An <i>ab initio</i> calculation of the vibrational energies and transition moments of HSOH. <i>Journal of Molecular Spectroscopy</i> , 2009, 257, 57-65.	0.4	32
105	Exomol molecular line lists VI. A high temperature line list for phosphorus nitride. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 445, 1383-1391.	1.6	32
106	ExoMol molecular line lists XVII. The rotation-vibration spectrum of hot SO ₃ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2016, 462, 4300-4313.	1.6	32
107	ExoMol molecular line lists XX. A comprehensive line list for H ₃ ⁺ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2017, 468, 1717-1725.	1.6	32
108	The EChO science case. <i>Experimental Astronomy</i> , 2015, 40, 329-391.	1.6	31

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109	A global potential energy surface and dipole moment surface for silane. <i>Journal of Chemical Physics</i> , 2015, 143, 244317.	1.2	30
110	Marvel analysis of the measured high-resolution rovibrational spectra of H ₂ S. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018, 218, 178-186.	1.1	29
111	Vibrational energies of PH ₃ calculated variationally at the complete basis set limit. <i>Journal of Chemical Physics</i> , 2008, 129, 044309.	1.2	28
112	ExoMol molecular line lists "XII. Line lists for eight isotopologues of CS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 454, 1931-1939.	1.6	28
113	The status of spectroscopic data for the exoplanet characterisation missions. <i>Experimental Astronomy</i> , 2015, 40, 563-575.	1.6	28
114	ExoMol line lists "XXII. The rotation-vibration spectrum of silane up to 1200 K. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017, 471, 5025-5032.	1.6	28
115	ExoMol molecular line lists XXXVI: χ^2_1 and $\chi^2_2 + \chi^2_3$ transitions of SH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 490, 1652-1665.	1.6	27
116	The ExoMol pressure broadening diet: H ₂ and He line-broadening parameters. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017, 203, 490-495.	1.1	26
117	Improved potential energy surface and spectral assignments for ammonia in the near-infrared region. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018, 219, 199-212.	1.1	25
118	Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment. <i>Astrophysical Journal</i> , 2020, 888, 21.	1.6	25
119	An update to the MARVEL data set and ExoMol line list for 12C ₂ . <i>Monthly Notices of the Royal Astronomical Society</i> , 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. <i>Journal of Molecular Spectroscopy</i> , 2016, 327, 21-30.	0.4	24
121	An ab initio variationally computed room-temperature line list for 32S16O ₃ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10118.	1.3	23
122	The dipole moment surface for hydrogen sulfide H ₂ S. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015, 161, 41-49.	1.1	23
123	ExoMol line lists "XV. A new hot line list for hydrogen peroxide. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016, 461, 1012-1022.	1.6	22
124	ExoMol line lists "XXXII. The rovibronic spectrum of MgO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 486, 2351-2365.	1.6	22
125	High-Resolution Spectroscopic Study of the (310) Local Mode Combination Band System of AsH ₃ . <i>Journal of Molecular Spectroscopy</i> , 1998, 187, 89-96.	0.4	21
126	PH ₃ revisited: Theoretical transition moments for the vibrational transitions below. <i>Journal of Molecular Spectroscopy</i> , 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	A near infrared line list of formaldehyde, H ₂ C=O. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 167, 126-134.	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 NH ₃ at high temperatures: 500â€“2100cm ⁻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 ⁻¹ . Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 251, 107027.	1.1	20
134	Analysis of high temperature ammonia spectra from 780 to 2100cm ⁻¹ . Journal of Molecular Spectroscopy, 2011, 269, 104-108.	0.4	19
135	<i>Ab initio</i> calculations 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 H ₂ O ₂ . Journal of Physical Chemistry A, 2013, 117, 7367-7377.	1.1	18
139	Rotational spectrum of SO ₃ 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 XY ₃ molecules: Excited vibrational states of BiH ₃ and SbH ₃ . 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. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 450, 3191-3200.	1.6	17
146	Predicted Landé g-factors for open shell diatomic molecules. <i>Journal of Molecular Spectroscopy</i> , 2016, 330, 57-62.	0.4	17
147	GPU Accelerated Einstein-MPI (GAIN-MPI): A new method of computing Einstein-A coefficients. <i>Computer Physics Communications</i> , 2017, 214, 216-224.	3.0	17
148	Climbing the Rotational Ladder to Chirality. <i>Physical Review Letters</i> , 2018, 121, 193201.	2.9	17
149	Synthetic spectra of BeH, BeD and BeT for emission modeling in JET plasmas. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2018, 51, 185701.	0.6	17
150	A method for calculating temperature-dependent photodissociation cross sections and rates. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16390-16400.	1.3	17
151	Observation of electric-quadrupole infrared transitions in water vapor. <i>Physical Review Research</i> , 2020, 2, .	1.3	17
152	A semi-empirical potential energy surface and line list for H ₂ O extending into the near-ultraviolet. <i>Atmospheric Chemistry and Physics</i> , 2020, 20, 10015-10027.	1.9	17
153	Hydrogen Physisorption on Carbon Foams upon Inclusion of Many-Body and Quantum Delocalization Effects. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19543-19553.	1.5	16
154	A hybrid variational-perturbation calculation of the ro-vibrational spectrum of nitric acid. <i>Journal of Chemical Physics</i> , 2015, 142, 094309.	1.2	16
155	Determination of glyphosate in surface water with high organic matter content. <i>Environmental Science and Pollution Research</i> , 2017, 24, 7880-7888.	2.7	16
156	ExoMol line lists XXV: a hot line list for silicon sulphide, SiS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 477, 1520-1527.	1.6	16
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