

Sergei N Yurchenko

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

249
papers

8,709
citations

48
h-index

82
g-index

270
ext. papers

10,502
ext. citations

3.5
avg, IF

6.65
L-index

#	Paper	IF	Citations
249	A Method for the Variational Calculation of Hyperfine-Resolved Rovibronic Spectra of Diatomic Molecules.. <i>Journal of Chemical Theory and Computation</i> , 2022 ,	6.4	2
248	Non-local thermal equilibrium spectra of atmospheric molecules for exoplanets. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022 , 512, 2911-2924	4.3	0
247	VIB5 database with accurate ab initio quantum chemical molecular potential energy surfaces.. <i>Scientific Data</i> , 2022 , 9, 84	8.2	1
246	Partition sums for non-local thermodynamic equilibrium conditions for nine molecules of importance in planetary atmospheres. <i>Icarus</i> , 2022 , 378, 114947	3.8	1
245	Cross-sections for heavy atmospheres: H ₂ O self-broadening. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2022 , 283, 108146	2.1	0
244	New physical insights: Formamide discharge decomposition and the role of fragments in the formation of large biomolecules.. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022 , 278, 121322	4.4	
243	Detectable Abundance of Cyanoacetylene (HC ₃ N) Predicted on Reduced Nitrogen-rich Super-Earth Atmospheres. <i>Astrophysical Journal Letters</i> , 2021 , 921, L28	7.9	0
242	Cross-sections for heavy atmospheres: H ₂ O continuum. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 278, 108013	2.1	2
241	ExoMol at 10. <i>Astronomy and Geophysics</i> , 2021 , 62, 6.16-6.21	0.2	0
240	Calculation of electric quadrupole linestrengths for diatomic molecules: Application to the H, CO, HF, and O molecules. <i>Journal of Chemical Physics</i> , 2021 , 155, 214303	3.9	4
239	HELIOS-K 2.0 Opacity Calculator and Open-source Opacity Database for Exoplanetary Atmospheres. <i>Astrophysical Journal, Supplement Series</i> , 2021 , 253, 30	8	26
238	Time-resolved Fourier transform infrared emission spectroscopy of CO $\nu = 1$ and $\nu = 2$ extended bands in the ground X ¹ Σ^+ state produced by formamide glow discharge. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 262, 107521	2.1	3
237	Five carbon- and nitrogen-bearing species in a hot giant planets atmosphere. <i>Nature</i> , 2021 , 592, 205-208	30.4	23
236	ExoMol molecular line lists XLII. Rovibronic molecular line list for the low-lying states of NO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2021 , 504, 5768-5777	4.3	4
235	An improved rovibrational linelist of formaldehyde, H ₂ C ₁₆ O. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 266, 107563	2.1	7
234	Electric-quadrupole and magnetic-dipole contributions to the $\nu_2 + \nu_3$ band of carbon dioxide near 3.3 μm . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 266, 107558	2.1	5
233	Electric quadrupole transitions in carbon dioxide. <i>Journal of Chemical Physics</i> , 2021 , 154, 211104	3.9	3

232	Theoretical rovibronic spectroscopy of the calcium monohydroxide radical (CaOH). <i>Journal of Chemical Physics</i> , 2021 , 154, 234302	3.9	1
231	A method for calculating temperature-dependent photodissociation cross sections and rates. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 16390-16400	3.6	6
230	Modelling the non-local thermodynamic equilibrium spectra of silylene (SiH). <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11990-12004	3.6	2
229	The ExoMolOP database: Cross sections and k-tables for molecules of interest in high-temperature exoplanet atmospheres. <i>Astronomy and Astrophysics</i> , 2021 , 646, A21	5.1	24
228	A spectroscopic model for the low-lying electronic states of NO. <i>Journal of Chemical Physics</i> , 2021 , 154, 074112	3.9	4
227	Artificial Symmetries for Calculating Vibrational Energies of Linear Molecules. <i>Symmetry</i> , 2021 , 13, 548	2.7	1
226	The HITRAN2020 molecular spectroscopic database. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 277, 107949	2.1	96
225	The update of the line positions and intensities in the line list of carbon dioxide for the HITRAN2020 spectroscopic database. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021 , 276, 107896	2.1	2
224	ExoMol line lists [XLI]. High-temperature molecular line lists for the alkali metal hydroxides KOH and NaOH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2021 , 502, 1128-1135	4.3	2
223	Rovibronic spectroscopy of PN from first principles. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22057-22066	3.2	2
222	Estimation of H ₂ O Absorption Line Contributions to Atmospheric Transmission in the Ultraviolet Spectral Region. <i>Atmospheric and Oceanic Optics</i> , 2021 , 34, 547-552	0.8	0
221	Treating linear molecules in calculations of rotation-vibration spectra. <i>Journal of Chemical Physics</i> , 2020 , 153, 154106	3.9	5
220	MARVEL Analysis of the Measured High-resolution Rovibronic Spectra of the Calcium Monohydroxide Radical (CaOH). <i>Astrophysical Journal, Supplement Series</i> , 2020 , 248, 9	8	5
219	Vibrationally resolved electron impact electronic excitation of BeH. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020 , 53, 135202	1.3	
218	ExoMol line lists [XXXVIII]. High-temperature molecular line list of silicon dioxide (SiO ₂). <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 495, 1927-1933	4.3	5
217	Ions in the Thermosphere of Exoplanets: Observable Constraints Revealed by Innovative Laboratory Experiments. <i>Astrophysical Journal</i> , 2020 , 895, 77	4.7	10
216	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	4.3	20
215	A weak spectral signature of water vapour in the atmosphere of HD 179949 b at high spectral resolution in the L band. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 494, 108-119	4.3	10

214	ExoMol line lists [XXXIX]. Ro-vibrational molecular line list for CO ₂ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 496, 5282-5291	4.3	22
213	Empirical Line Lists in the ExoMol Database. <i>Atoms</i> , 2020 , 8, 7	2.1	14
212	The high-temperature rotation-vibration spectrum and rotational clustering of silylene (SiH ₂). <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2020 , 246, 106929	2.1	9
211	Empirical rovibrational energy levels of ammonia up to 7500 cm ⁻¹ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2020 , 251, 107027	2.1	12
210	ExoMol molecular line lists [XXXVII]. Spectra of acetylene. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 493, 1531-1545	4.3	22
209	Observation of electric-quadrupole infrared transitions in water vapor. <i>Physical Review Research</i> , 2020 , 2,	3.9	14
208	Contribution of new water vapor absorption lines to the atmospheric transmission in the transparency window 8-12 μm 2020 ,		1
207	A semi-empirical potential energy surface and line list for H ₂ ¹⁶ O extending into the near-ultraviolet. <i>Atmospheric Chemistry and Physics</i> , 2020 , 20, 10015-10027	6.8	8
206	Detection of electric-quadrupole transitions in water vapour near 5.4 and 2.5 μm. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 12476-12481	3.6	10
205	Analysis of the first overtone bands of isotopologues of CO and SiO in stellar spectra. <i>Astronomy and Astrophysics</i> , 2020 , 633, A52	5.1	7
204	Analysis of the TiO isotopologues in stellar optical spectra. <i>Astronomy and Astrophysics</i> , 2020 , 642, A77	5.1	4
203	Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment. <i>Astrophysical Journal</i> , 2020 , 888, 21	4.7	12
202	Hot Exoplanet Atmospheres Resolved with Transit Spectroscopy (HEARTS). <i>Astronomy and Astrophysics</i> , 2020 , 641, A123	5.1	32
201	ExoMol line lists [XL]. Rovibrational molecular line list for the hydronium ion (H ₃ O ⁺). <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 497, 2340-2351	4.3	3
200	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	2.1	54
199	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	4.3	10
198	The infrared spectrum of PF ₃ and analysis of rotational energy clustering effect. <i>Molecular Physics</i> , 2020 , 118, e1581951	1.7	4
197	ExoMol molecular line lists [XXXIII]. The spectrum of Titanium Oxide. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019 , 488, 2836-2854	4.3	84

196	Water vapour in the atmosphere of the habitable-zone eight-Earth-mass planet K2-18 b. <i>Nature Astronomy</i> , 2019 , 3, 1086-1091	12.1	127
195	A variationally computed room temperature line list for AsH. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3264-3277	3.6	7
194	Spectroscopic line parameters of NO, NO ₂ , and N ₂ O for the HITEMP database. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2019 , 232, 35-53	2.1	32
193	Variationally Computed IR Line List for the Methyl Radical CH. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 4755-4763	2.8	6
192	ExoMol line lists XXXII. The rovibronic spectrum of MgO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019 , 486, 2351-2365	4.3	14
191	The rotation-vibration spectrum of methyl fluoride from first principles. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3496-3505	3.6	9
190	Theoretical rotation-vibration spectroscopy of cis- and trans-diphosphene (PH) and the deuterated species PHD. <i>Journal of Chemical Physics</i> , 2019 , 150, 194308	3.9	5
189	Nonresonant Raman spectra of the methyl radical 12CH ₃ simulated in variational calculations. <i>Journal of Molecular Spectroscopy</i> , 2019 , 362, 77-83	1.3	2
188	Transformation Properties under the Operations of the Molecular Symmetry Groups G ₃₆ and G ₃₆ (EM) of Ethane H ₃ CCH ₃ . <i>Symmetry</i> , 2019 , 11, 862	2.7	1
187	ExoMol line list XXXIV. A rovibrational line list for phosphinidene (PH) in its Σ^+ and Δ electronic states. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019 , 488, 2332-2342	4.3	5
186	ExoMol molecular line lists XXXVI: X ² Σ ⁺ and A ² Σ ⁺ transitions of SH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019 , 490, 1652-1665	4.3	14
185	The ExoMol project: An update. <i>Proceedings of the International Astronomical Union</i> , 2019 , 15, 287-296	0.1	
184	ExoMol molecular line lists XXXV. A rotation-vibration line list for hot ammonia. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019 , 490, 4638-4647	4.3	41
183	Spectroscopy of YO from first principles. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22794-22810	3.6	9
182	Analysis of gaseous ammonia (NH ₃) absorption in the visible spectrum of Jupiter - Update. <i>Icarus</i> , 2019 , 321, 572-582	3.8	9
181	Analysis of the red and green optical absorption spectrum of gas phase ammonia. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018 , 209, 224-231	2.1	8
180	An experimental water line list at 1950 K in the 6250-670 cm ⁻¹ region. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018 , 205, 213-219	2.1	9
179	Anomalous phosphine sensitivity coefficients as probes for a possible variation of the proton-to-electron mass ratio. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018 , 473, 4986-4992	4.3	3

178	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	2.1	35
177	ExoMol molecular line lists DXXVII. Spectra of C ₂ H ₄ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2018 , 478, 3220-3232	4.3	29
176	The ExoMol Atlas of Molecular Opacities. <i>Atoms</i> , 2018 , 6, 26	2.1	36
175	Symmetry Adaptation of the Rotation-Vibration Theory for Linear Molecules. <i>Symmetry</i> , 2018 , 10, 137	2.7	10
174	EXOCROSS: a general program for generating spectra from molecular line lists. <i>Astronomy and Astrophysics</i> , 2018 , 614, A131	5.1	78
173	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	2.1	21
172	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	4.3	10
171	Climbing the Rotational Ladder to Chirality. <i>Physical Review Letters</i> , 2018 , 121, 193201	7.4	10
170	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	4.3	20
169	ExoMol molecular line lists DXXVI: spectra of SH and NS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018 , 478, 270-282	4.3	15
168	A chemical survey of exoplanets with ARIEL. <i>Experimental Astronomy</i> , 2018 , 46, 135-209	1.3	148
167	A Population Study of Gaseous Exoplanets. <i>Astronomical Journal</i> , 2018 , 155, 156	4.9	144
166	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	2.1	21
165	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	1.3	13
164	ExoMol line lists DXXIX. The rotation-vibration spectrum of methyl chloride up to 1200 K. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018 , 479, 3002-3010	4.3	9
163	ExoMol line lists XXVIII: the rovibronic spectrum of AlH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018 , 479, 1401-1411	4.3	25
162	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	4.3	145
161	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	4.3	26

160	Treating linear molecule HCCH in calculations of rotation-vibration spectra. <i>Journal of Chemical Physics</i> , 2018 , 149, 014101	3.9	14
159	Pressure-dependent water absorption cross sections for exoplanets and other atmospheres. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017 , 187, 453-460	2.1	34
158	GPU Accelerated Intensities MPI (GAIN-MPI): A new method of computing Einstein-A coefficients. <i>Computer Physics Communications</i> , 2017 , 214, 216-224	4.2	15
157	Determination of glyphosate in surface water with high organic matter content. <i>Environmental Science and Pollution Research</i> , 2017 , 24, 7880-7888	5.1	13
156	Total internal partition sums for 166 isotopologues of 51 molecules important in planetary atmospheres: Application to HITRAN2016 and beyond. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017 , 203, 70-87	2.1	94
155	High-resolution absorption measurements of NH ₃ at high temperatures: 2100-500 cm ⁻¹ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017 , 189, 60-65	2.1	9
154	Simulating electric field interactions with polar molecules using spectroscopic databases. <i>Scientific Reports</i> , 2017 , 7, 45068	4.9	6
153	Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets. <i>Molecular Astrophysics</i> , 2017 , 8, 1-18	1.7	55
152	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	2.1	21
151	ExoMol molecular line lists XIX: high-accuracy computed hot line lists for H ₂ 18O and H ₂ 17O. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017 , 466, 1363-1371	4.3	36
150	A semi-classical approach to the calculation of highly excited rotational energies for asymmetric-top molecules. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 1847-1856	3.6	1
149	A hybrid line list for CH and hot methane continuum. <i>Astronomy and Astrophysics</i> , 2017 , 605,	5.1	49
148	Molecular line shape parameters for exoplanetary atmospheric applications. <i>Journal of Physics: Conference Series</i> , 2017 , 810, 012010	0.3	4
147	Lightning chemistry on Earth-like exoplanets. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017 , 470, 187-196	4.3	41
146	Absorption spectra of ammonia near 1 μ m. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017 , 203, 392-397	2.1	10
145	Symmetry-Adapted Ro-vibrational Basis Functions for Variational Nuclear Motion Calculations: TROVE Approach. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4368-4381	6.4	45
144	ExoMol line list LXXI. Nitric Oxide (NO). <i>Monthly Notices of the Royal Astronomical Society</i> , 2017 , 470, 882-897	4.3	51
143	Structure-based sampling and self-correcting machine learning for accurate calculations of potential energy surfaces and vibrational levels. <i>Journal of Chemical Physics</i> , 2017 , 146, 244108	3.9	82

142	ExoMol molecular line lists [XXIII]. Spectra of PO and PS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017 , 472, 3648-3658	4-3	25
141	ExoMol molecular line lists [XX]. A comprehensive line list for H3+. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017 , 468, 1717-1725	4-3	25
140	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	4-3	20
139	Ab initio calculations to support accurate modelling of the rovibronic spectroscopy calculations of vanadium monoxide (VO). <i>Molecular Physics</i> , 2016 , 114, 3232-3248	1-7	12
138	Detecting Chirality in Molecules by Linearly Polarized Laser Fields. <i>Physical Review Letters</i> , 2016 , 117, 033001	7-4	34
137	Enhanced sensitivity to a possible variation of the proton-to-electron mass ratio in ammonia. <i>Physical Review A</i> , 2016 , 93,	2-6	9
136	ExoMol molecular line lists [XVII]. The rotation-vibration spectrum of hot SO3. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 462, 4300-4313	4-3	26
135	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	4-3	19
134	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. <i>Journal of Molecular Spectroscopy</i> , 2016 , 327, 73-94	1-3	280
133	ExoMol molecular line lists [XIV]. The rotation-vibration spectrum of hot SO2. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 459, 3890-3899	4-3	47
132	Duo: A general program for calculating spectra of diatomic molecules. <i>Computer Physics Communications</i> , 2016 , 202, 262-275	4-2	98
131	ExoMol molecular line lists [XIII]. The spectrum of CaO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 456, 4524-4532	4-3	33
130	Radiative lifetimes and cooling functions for astrophysically important molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016 , 49, 044002	1-3	33
129	Predicted Landé-factors for open shell diatomic molecules. <i>Journal of Molecular Spectroscopy</i> , 2016 , 330, 57-62	1-3	11
128	ExoMol line lists [XVIII]. The high-temperature spectrum of VO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 463, 771-793	4-3	80
127	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE 12 C 2 MOLECULE. <i>Astrophysical Journal, Supplement Series</i> , 2016 , 224, 44	8	37
126	Communication: Tunnelling splitting in the phosphine molecule. <i>Journal of Chemical Physics</i> , 2016 , 145, 091102	3-9	13
125	A highly accurate ab initio potential energy surface for methane. <i>Journal of Chemical Physics</i> , 2016 , 145, 104305	3-9	32

124	Theab initio calculation of spectra of open shell diatomic molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016 , 49, 102001	1.3	47
123	A near infrared line list for NH ₃ : Analysis of a Kitt Peak spectrum after 35 years. <i>Journal of Molecular Spectroscopy</i> , 2016 , 325, 7-12	1.3	20
122	ExoMol molecular line lists LXVI. The rotation-vibration spectrum of hot H ₂ S. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 460, 4063-4074	4.3	54
121	DETECTION OF AN ATMOSPHERE AROUND THE SUPER-EARTH 55 CANCRI E. <i>Astrophysical Journal</i> , 2016 , 820, 99	4.7	156
120	Radiative cooling of HO and its deuterated isotopologues. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 26268-26274	3.6	5
119	A global ab initio dipole moment surface for methyl chloride. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2016 , 184, 100-110	2.1	13
118	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	1.3	23
117	The dipole moment surface for hydrogen sulfide H ₂ S. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015 , 161, 41-49	2.1	17
116	Accurate ab initio vibrational energies of methyl chloride. <i>Journal of Chemical Physics</i> , 2015 , 142, 244306	3.9	39
115	ExoMol line lists LVIII. A variationally computed line list for hot formaldehyde. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015 , 448, 1704-1714	4.3	42
114	ExoMol molecular line lists LIX. The spectrum of AlO. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015 , 449, 3613-3619	4.3	66
113	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	4.3	17
112	ExoMol line lists LVII. The rotation-vibration spectrum of phosphine up to 1500 K. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015 , 446, 2337-2347	4.3	75
111	The calculated rovibronic spectrum of scandium hydride, ScH. <i>Molecular Physics</i> , 2015 , 113, 1998-2011	1.7	32
110	TAU-REX I: A NEXT GENERATION RETRIEVAL CODE FOR EXOPLANETARY ATMOSPHERES. <i>Astrophysical Journal</i> , 2015 , 802, 107	4.7	161
109	Automatic differentiation method for numerical construction of the rotational-vibrational Hamiltonian as a power series in the curvilinear internal coordinates using the Eckart frame. <i>Journal of Chemical Physics</i> , 2015 , 143, 014105	3.9	57
108	High-resolution absorption measurements of NH ₃ at high temperatures: 500–100 cm ⁻¹ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015 , 167, 126-134	2.1	18
107	A variationally calculated room temperature line-list for H ₂ O ₂ . <i>Journal of Molecular Spectroscopy</i> , 2015 , 318, 84-90	1.3	27

106	A theoretical room-temperature line list for 15NH_3 . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015 , 152, 28-36	2.1	28
105	The status of spectroscopic data for the exoplanet characterisation missions. <i>Experimental Astronomy</i> , 2015 , 40, 563-575	1.3	23
104	Development of a General Approach to the Modeling of Free and Confined Polyatomic Systems. <i>Russian Physics Journal</i> , 2015 , 58, 1040-1043	0.7	4
103	\mathcal{T} -REX. II. RETRIEVAL OF EMISSION SPECTRA. <i>Astrophysical Journal</i> , 2015 , 813, 13	4.7	104
102	A global potential energy surface and dipole moment surface for silane. <i>Journal of Chemical Physics</i> , 2015 , 143, 244317	3.9	26
101	Ro-vibrational averaging of the isotropic hyperfine coupling constant for the methyl radical. <i>Journal of Chemical Physics</i> , 2015 , 143, 244306	3.9	10
100	A hybrid variational-perturbation calculation of the ro-vibrational spectrum of nitric acid. <i>Journal of Chemical Physics</i> , 2015 , 142, 094309	3.9	9
99	Roto-translational states of the interstitial molecular hydrogen in silicon: A theoretical study. <i>Journal of Chemical Physics</i> , 2015 , 143, 164305	3.9	3
98	ExoMol molecular line lists IXI. The spectrum of nitric acid. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015 , 452, 1702-1706	4.3	16
97	ExoMol molecular line lists IXII. Line lists for eight isotopologues of CS. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015 , 454, 1931-1939	4.3	20
96	The EChO science case. <i>Experimental Astronomy</i> , 2015 , 40, 329-391	1.3	26
95	MARVEL analysis of the measured high-resolution spectra of 14NH_3 . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015 , 161, 117-130	2.1	60
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