Andrey Yachmenev

List of Publications by Year
in descending order

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55	2,416	304368	205818
papers	citations	22 h-index	48 g-index

55	55	55	1523
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	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. Journal of Molecular Spectroscopy, 2016, 327, 73-94.	0.4	364
3	A Variationally Computed T = 300 K Line List for NH₃. Journal of Physical Chemistry A, 2009, 113, 11845-11855.	1.1	159
4	The 2020 edition of the GEISA spectroscopic database. Journal of Molecular Spectroscopy, 2021, 380, 111510.	0.4	74
5	On the use of quartic force fields in variational calculations. Chemical Physics Letters, 2013, 574, 1-12.	1.2	66
6	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
7	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
8	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
9	Detecting Chirality in Molecules by Linearly Polarized Laser Fields. Physical Review Letters, 2016, 117, 033001.	2.9	52
10	A new â€œspectroscopicâ€•potential energy surface for formaldehyde in its ground electronic state. Journal of Chemical Physics, 2011, 134, 244307.	1.2	48
11	ExoMol molecular line lists â€“ XXVII. Spectra of C2H4. Monthly Notices of the Royal Astronomical Society, 2018, 478, 3220-3232.	1.6	45
12	Accurate ab initio vibrational energies of methyl chloride. Journal of Chemical Physics, 2015, 142, 244306.	1.2	44
13	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
14	A highly accurate ab initio potential energy surface for methane. Journal of Chemical Physics, 2016, 145, 104305.	1.2	38
15	High-level ab initio potential energy surfaces and vibrational energies of H2CS. Journal of Chemical Physics, 2011, 135, 074302.	1.2	35
16	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
17	Field-Induced Diastereomers for Chiral Separation. Physical Review Letters, 2019, 123, 243202.	2.9	33
18	An ab initio calculation of the vibrational energies and transition moments of HSOH. Journal of Molecular Spectroscopy, 2009, 257, 57-65.	0.4	32

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19	A global potential energy surface and dipole moment surface for silane. Journal of Chemical Physics, 2015, 143, 244317.	1.2	30
20	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
21	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
22	Theoretical rotation-vibration spectrum of thioformaldehyde. Journal of Chemical Physics, 2013, 139, 204308.	1.2	22
23	RichMol: A general variational approach for rovibrational molecular dynamics in external electric fields. Journal of Chemical Physics, 2018, 148, 124102.	1.2	22
24	Treating linear molecule HCCH in calculations of rotation-vibration spectra. Journal of Chemical Physics, 2018, 149, 014101.	1.2	18
25	Climbing the Rotational Ladder to Chirality. Physical Review Letters, 2018, 121, 193201.	2.9	17
26	Observation of electric-quadrupole infrared transitions in water vapor. Physical Review Research, 2020, 2, .	1.3	17
27	A global ab initio dipole moment surface for methyl chloride. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 184, 100-110.	1.1	15
28	Variationally Computed IR Line List for the Methyl Radical CH₃. Journal of Physical Chemistry A, 2019, 123, 4755-4763.	1.1	14
29	Communication: General variational approach to nuclear-quadrupole coupling in rovibrational spectra of polyatomic molecules. Journal of Chemical Physics, 2017, 147, 141101.	1.2	13
30	Ro-vibrational averaging of the isotropic hyperfine coupling constant for the methyl radical. Journal of Chemical Physics, 2015, 143, 244306.	1.2	12
31	ExoMol line lists â€“ XXIX. The rotation-vibration spectrum of methyl chloride up to 1200â€‰K. Monthly Notices of the Royal Astronomical Society, 2018, 479, 3002-3010.	1.6	12
32	Detection of electric-quadrupole transitions in water vapour near 5.4 and 2.5 Î¼m. Physical Chemistry Chemical Physics, 2020, 22, 12476-12481.	1.3	12
33	Laser-induced dynamics of molecules with strong nuclear quadrupole coupling. Journal of Chemical Physics, 2019, 151, 244118.	1.2	11
34	Detecting handedness of spatially oriented molecules by Coulomb explosion imaging. Journal of Chemical Physics, 2021, 154, 071101.	1.2	11
35	Electric-quadrupole and magnetic-dipole contributions to the Î½2+Î½3 band of carbon dioxide near 3.3â€Âµm. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 266, 107558.	1.1	11
36	A theoretical-spectroscopy, ab initio-based study of the electronic ground state of 121SbH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2010, 111, 2279-2290.	1.1	10

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37	Coherent Control of the Rotation Axis of Molecular Superrotors. Journal of Physical Chemistry Letters, 2018, 9, 4206-4209.	2.1	10
38	The rotationâ€“vibration spectrum of methyl fluoride from first principles. Physical Chemistry Chemical Physics, 2019, 21, 3496-3505.	1.3	10
39	Theoretical rotationâ€“torsion spectra of HSOH. Physical Chemistry Chemical Physics, 2010, 12, 8387.	1.3	9
40	Electric quadrupole transitions in carbon dioxide. Journal of Chemical Physics, 2021, 154, 211104.	1.2	9
41	Calculation of electric quadrupole linestrengths for diatomic molecules: Application to the H2, CO, HF, and O2 molecules. Journal of Chemical Physics, 2021, 155, 214303.	1.2	8
42	Picosecond pulse-shaping for strong three-dimensional field-free alignment of generic asymmetric-top molecules. Nature Communications, 2022, 13, 1431.	5.8	8
43	Simulating electric field interactions with polar molecules using spectroscopic databases. Scientific Reports, 2017, 7, 45068.	1.6	7
44	A Hyperfine-resolved Rotationâ€“Vibration Line List of Ammonia (NH₃). Astrophysical Journal, 2019, 870, 24.	1.6	6
45	The Effect of Nuclear-Quadrupole Coupling in the Laser-Induced Alignment of Molecules. Journal of Physical Chemistry A, 2020, 124, 2225-2230.	1.1	6
46	A composite â€˜density fitting + numerical integrationâ€™ approximation for electron-repulsion integrals. Molecular Physics, 2013, 111, 1129-1142.	0.8	5
47	The infrared spectrum of PF₃and analysis of rotational energy clustering effect. Molecular Physics, 2020, 118, e1581951.	0.8	5
48	The nuclear-spin-forbidden rovibrational transitions of water from first principles. Journal of Chemical Physics, 2022, 156, .	1.2	5
49	Laser-induced alignment of weakly bound molecular aggregates. Physical Review A, 2018, 98, .	1.0	4
50	Structure, force fields, and vibrational spectra of cerium tetrahalides. Journal of Structural Chemistry, 2008, 49, 613-620.	0.3	3
51	Controlling rotation in the molecular frame with an optical centrifuge. Physical Review Research, 2021, 3, .	1.3	3
52	A semi-classical approach to the calculation of highly excited rotational energies for asymmetric-top molecules. Physical Chemistry Chemical Physics, 2017, 19, 1847-1856.	1.3	2
53	Nonresonant Raman spectra of the methyl radical 12CH3 simulated in variational calculations. Journal of Molecular Spectroscopy, 2019, 362, 77-83.	0.4	2
54	Active learning of potential-energy surfaces of weakly bound complexes with regression-tree ensembles. Journal of Chemical Physics, 2021, 155, 144109.	1.2	2

#	Article	IF	Citations
55	Ab initio study of rovibronic energies of the CH 2 + molecular ion. Optics and Spectroscopy (English) Tj ETQq1 1 0.784314 rgBT /Over	0.2	1