

# Vladimir Spirko

## List of Publications by Year in descending order

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164  
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117571  
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133188  
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165  
docs citations

165  
times ranked

2403  
citing authors

#	ARTICLE	IF	CITATIONS
1	The stability of covalent dative bond significantly increases with increasing solvent polarity. <i>Nature Communications</i> , 2022, 13, 2107.	5.8	13
2	Relating Binding Energy and Scattering Length of Weakly Bound Dimers of Strontium. <i>Annalen Der Physik</i> , 2021, 533, 2000588.	0.9	1
3	Radial molecular property functions of the $\langle \text{mmi:math} \text{ xmlns:mmi="http://www.w3.org/1998/Math/MathML"} \text{ altimg="si5.svg" } \rangle \langle \text{mmi:mrow} \langle \text{mmi:msup} \langle \text{mmi:mi} \text{ A } \rangle \text{ /mmi:mi } \rangle \text{ /mmi:mn } \rangle \text{ 2 } \langle \text{mmi:mn} \rangle \text{ /mmi:msup } \langle \text{mmi:msup} \rangle \text{ mmil:style } \text{ mathvariant="normal" } \rangle \langle \text{mmi:mi} \rangle \text{ f } \langle \text{mmi:msup} \rangle \langle \text{mmi:mo} \rangle + \langle \text{mmi:mo} \rangle \text{ /mmi:msup } \rangle \text{ /mmi:mnrow } \langle \text{mmi:math} \rangle \text{ state of hydroxyl. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 266, 107530. }$		
4	Real-space imaging of anisotropic charge of $\text{f}$ -hole by means of Kelvin probe force microscopy. <i>Science</i> , 2021, 374, 863-867.	6.0	71
5	Dissociative recombination of $\text{N}_2\text{H}^+$ ions with electrons in the temperature range of 80–350 K. <i>Journal of Chemical Physics</i> , 2020, 152, 024301.	1.2	4
6	Morphing radial molecular property functions of hydroxyl. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2020, 254, 107211.	1.1	6
7	Universal behavior of diatomic halo states and the mass sensitivity of their properties. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2019, 52, 025102.	0.6	4
8	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.	1.6	3
9	Morphing ab initio potential energy curve of beryllium monohydride. <i>Journal of Molecular Spectroscopy</i> , 2016, 330, 89-95.	0.4	3
10	EFFECTIVE HYPERFINE-STRUCTURE FUNCTIONS OF AMMONIA. <i>Astrophysical Journal</i> , 2016, 824, 147.	1.6	2
11	Enhanced sensitivity to a possible variation of the proton-to-electron mass ratio in ammonia. <i>Physical Review A</i> , 2016, 93, .	1.0	9
12	Accurate prediction of $\text{H}_{3}\text{O}^+$ and $\text{D}_{3}\text{O}^+$ sensitivity coefficients to probe a variable proton-to-electron mass ratio. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 454, 2292-2298.	1.6	10
13	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
14	Potential microwave probes of the proton-to-electron mass ratio at very high redshifts. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 439, 1136-1139.	1.6	4
15	The role of molecular quadrupole transitions in the depopulation of metastable helium. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 446, 2738-2743.	1.6	5
16	Localised quantum states of atomic and molecular particles physisorbed on carbon-based nanoparticles. <i>Journal of Chemical Physics</i> , 2014, 141, 114702.	1.2	1
17	Highly Sensitive Ammonia Probes of a Variable Proton-to-Electron Mass Ratio. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 919-923.	2.1	7
18	Effective potential energy curves of the ground electronic state of $\text{CH}^+$ . <i>Journal of Chemical Physics</i> , 2013, 138, 024315.	1.2	19

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19	Radiative association of He\$_{2}^{+}\$: the role of quartet states. Monthly Notices of the Royal Astronomical Society, 2013, 435, 1541-1546.	1.6	8
20	Relation between properties of long-range diatomic bound states. Physical Review A, 2013, 87, .	1.0	10
21	Radiative association of He <sup>+&lt;/sup&gt;<sub>2</sub>&gt; revisited. Astronomy and Astrophysics, 2013, 553, A42.</sup>	2.1	13
22	Radiative association of LiHe+. Chemical Physics Letters, 2012, 531, 59-63.	1.2	21
23	Vibrational Energies of LiH2+and LiD2+in the $\tilde{\chi}_1^1$ +Electronic State. Journal of Physical Chemistry A, 2011, 115, 11313-11320.	1.1	6
24	Vibrational dynamics of adsorbed CO2: Separability of the CO2 asymmetric stretching mode. Collection of Czechoslovak Chemical Communications, 2011, 76, 669-682.	1.0	1
25	Potential energy curve of N2 revisited. Collection of Czechoslovak Chemical Communications, 2011, 76, 327-341.	1.0	2
26	<i>Ab initio</i> vibrational dynamics of molecular hydrogen on graphene: An effective interaction potential. Journal of Chemical Physics, 2010, 132, 194708.	1.2	12
27	On the Elusive Twelfth Vibrational State of Beryllium Dimer. Science, 2009, 326, 1382-1384.	6.0	94
28	The structure and vibrational dynamics of the pyrrole dimer. Physical Chemistry Chemical Physics, 2009, 11, 3885.	1.3	13
29	The ab initio assigning of the vibrational probing modes of tryptophan: linear shifting of approximate anharmonic frequencies vs. multiplicative scaling of harmonic frequencies. Physical Chemistry Chemical Physics, 2009, 11, 3921.	1.3	10
30	Potential energy function of $\text{Al}\text{Al}$ -Graphene. Journal of Molecular Spectroscopy, 2008, 248, 77-80.	1.4	1
31	Assigning the NH Stretches of the Guanine Tautomers Using Adiabatic Separation: CCSD(T) Benchmark Calculations. Journal of Physical Chemistry A, 2008, 112, 1854-1856.	1.1	11
32	Dependence of the $\text{Al}\text{Al}$ -Graphene Conformation on Molecular Charge Determined from Ab Initio Computations and NMR Spectra. Journal of Physical Chemistry B, 2008, 112, 1796-1805.	1.2	22
33	Quasiplanarity of the Peptide Bond. Journal of Physical Chemistry A, 2008, 112, 693-699.	1.1	15
34	Probing the Flexibility of Internal Rotation in Silylated Phenols with the NMR Scalar Spin-Spin Coupling Constants. Journal of Physical Chemistry A, 2008, 112, 5167-5174.	1.1	6
35	Computed lifetimes of metastable states of the NO2+ dication. Journal of Chemical Physics, 2008, 128, 144301.	1.2	15
36	Energies and Electric Dipole Moments of the Bound Vibrational States of HN2+ and DN2+. Collection of Czechoslovak Chemical Communications, 2008, 73, 873-897.	1.0	10

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37	Tuning ab initio data to scattering length: The $\alpha\hat{\ell}+3$ state of KRb. <i>Journal of Chemical Physics</i> , 2007, 127, 121101.	1.2	10
38	Radiative transition probabilities of CO <sup>2+</sup> . <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2654-2664.	1.0	6
39	Theoretical study of the ground and excited states of 7-methyl guanine and 9-methyl guanine: comparison with experiment. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3059-3065.	1.3	30
40	Theoretical study of photoacidity of HCN: the effect of complexation with water. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4866-4873.	1.3	10
41	Bound and low-lying quasi-bound rotation-vibration levels of the ground electronic state of. <i>Chemical Physics</i> , 2006, 330, 190-203.	0.9	29
42	Potential energy curve of Be <sub>2</sub> in its ground electronic state. <i>Journal of Molecular Spectroscopy</i> , 2006, 235, 268-270.	0.4	31
43	A theoretical study of FeNC in the 6 $\tilde{\ell}$ electronic ground state. <i>Journal of Molecular Spectroscopy</i> , 2006, 236, 234-247.	0.4	35
44	Theoretical Investigations into the Blue-Shifting Hydrogen Bond in Benzene Complexes. <i>ChemPhysChem</i> , 2006, 7, 640-643.	1.0	27
45	Vibrational predissociation of H <sub>5</sub> <sup>+</sup> . <i>Journal of Chemical Physics</i> , 2006, 124, 244303.	1.2	12
46	Theoretical study of the CS <sub>2</sub> <sup>+</sup> dication. <i>Journal of Chemical Physics</i> , 2006, 125, 164308.	1.2	11
47	Computed lifetimes of metastable states of CO <sub>2</sub> <sup>+</sup> . <i>Journal of Chemical Physics</i> , 2006, 124, 214303.	1.2	34
48	Potential Energy Curve of N <sub>2</sub> in Its Ground Electronic State. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 731-739.	1.0	4
49	A Complete Set of NMR Chemical Shifts and Spin-Spin Coupling Constants for L-Alanyl-L-alanine Zwitterion and Analysis of Its Conformational Behavior. <i>Journal of the American Chemical Society</i> , 2005, 127, 17079-17089.	6.6	38
50	Sugar Pucker Modulates the Cross-Correlated Relaxation Rates across the Glycosidic Bond in DNA. <i>Journal of the American Chemical Society</i> , 2005, 127, 14663-14667.	6.6	24
51	Calculation of the photodetachment cross sections of the HCN $\tilde{\ell}$ and HNC $\tilde{\ell}$ dipole-bound anions as described by a one-electron Drude model. <i>Journal of Chemical Physics</i> , 2004, 121, 1824-1829.	1.2	8
52	New rotation-vibration band and potential energy function of NeH <sup>+</sup> in the ground electronic state. <i>Journal of Molecular Structure</i> , 2004, 695-696, 5-11.	1.8	11
53	First local minimum of the formic acid dimer exhibits simultaneously red-shifted O-H-O and improper blue-shifted C-H-O hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 37-41.	1.3	384
54	The Infrared Spectrum of CN in Its Ground Electronic State. <i>Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 73-89.	1.0	22

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55	Vibrational linestrengths for the ground and first excited electronic states of HeH <sub>2</sub> +. Theoretical Chemistry Accounts, 2003, 110, 170-175.		0.5	10
56	Bound and continuum vibrational states of the bifluoride anion. Chemical Physics Letters, 2003, 376, 595-605.		1.2	4
57	Transforming from internal coordinates to Cartesian displacements in the Eckart frame: a Taylor series expansion approach. Journal of Molecular Spectroscopy, 2003, 217, 142-145.		0.4	11
58	Why is the N1-H stretch vibration frequency of guanine shifted upon dimerization to the red and the amino N-H stretch vibration frequency to the blue?. Physical Chemistry Chemical Physics, 2003, 5, 1290-1294.		1.3	44
59	Radiative association of HeH <sub>2</sub> +. Journal of Chemical Physics, 2003, 118, 10547-10560.		1.2	34
60	Bound and quasi-bound states of the Li-FH van der Waals molecule: The effects of the potential energy surface and of the basis set superposition error. Computational and Theoretical Chemistry, 2002, 591, 151-174.		1.5	10
61	Dimensionality of proton transfer in the intramolecular hydrogen bond of formimidol. Chemical Physics Letters, 2002, 355, 319-326.		1.2	10
62	Improper, Blue-Shifting Hydrogen Bond between Fluorobenzene and Fluoroform. Journal of Physical Chemistry A, 2001, 105, 5560-5566.		1.1	138
63	Inversion splittings of SiH <sub>3</sub> <sup>-</sup> . An ab initio study. Computational and Theoretical Chemistry, 2001, 547, 139-143.		1.5	1
64	Multidimensional WKB approximation and the lifetime calculation. Physical Review A, 2001, 64, .		1.0	9
65	Can ordinary single-reference coupled-cluster methods describe potential energy surfaces with nearly spectroscopic accuracy? The renormalized coupled-cluster study of the vibrational spectrum of HF. Journal of Chemical Physics, 2001, 115, 5796-5804.		1.2	53
66	Lifetimes and dissociation pathways of the quasi-bound states of the Na-FH van der Waals molecule. Journal of Molecular Structure, 2000, 555, 43-60.		1.8	6
67	Bound and quasibound states of the Na-FH van der Waals molecule. Journal of Chemical Physics, 2000, 112, 189-202.		1.2	23
68	Double Tunneling: An Overlooked Quantum Effect in Anionic Molecular Clusters. Physical Review Letters, 2000, 84, 1140-1143.		2.9	5
69	Adiabatic energies and perturbative non-adiabatic corrections for Coulombic three-particle systems in the hyperspherical harmonics formalism. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 429-441.		0.6	2
70	Brillouin-Wigner perturbation methods for coupled oscillators. Physical Review A, 1999, 61, .		1.0	7
71	Coupled-cluster methods with internal and semi-internal triply excited clusters: Vibrational spectrum of the HF molecule. Journal of Chemical Physics, 1999, 111, 6679-6692.		1.2	86
72	Ab InitioCalculated Rotation-Vibration Line Strengths for the ( $v_{HH} = 0 \rightarrow 1$ ) Transition of HeH <sub>2</sub> +. Journal of Molecular Spectroscopy, 1998, 187, 206-209.		0.4	5

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73	Vibrational dependence of the dipole moment and radiative transition probabilities in the X1 Sigma + state of HF: a linear-response coupled-cluster study. <i>Molecular Physics</i> , 1998, 94, 55-64.	0.8	13
74	Expectation Values of Quasibound States: Nuclear Quadrupole Coupling Constants of BH in the X1 $\tilde{\Sigma}^+$ and B1 $\tilde{\Sigma}^+$ States. <i>Collection of Czechoslovak Chemical Communications</i> , 1998, 63, 1309-1320.	1.0	0
75	Zero Kinetic Energy (ZEKE) Photoelectron Spectroscopic Study of Thioanisole and Its van der Waals Complexes with Argon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8631-8638.	1.1	26
76	The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH $\tilde{\alpha}$ and OH $\tilde{\alpha}$ $\cdot$ H <sub>2</sub> O. <i>Chemical Physics</i> , 1997, 214, 91-101.	0.9	19
77	Ab initio Calculated Rotation-Vibration Linestrengths for HeH <sub>2</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1997, 182, 364-370.	0.4	18
78	Symmetry Analysis of the Vibrational Dynamics of the H <sub>3</sub> D <sub>2</sub> <sup>+</sup> and H <sub>2</sub> D <sub>3</sub> <sup>+</sup> Complexes. <i>Journal of Molecular Spectroscopy</i> , 1997, 183, 212-217.	0.4	3
79	Vibrational Dynamics of H <sub>5</sub> <sup>+</sup> and Its Deuterated Isotopomers. <i>Journal of Molecular Spectroscopy</i> , 1997, 183, 218-223.	0.4	7
80	Calculation of Rotation-Vibration Energy Levels in Ground State C <sub>3</sub> by a Born-Oppenheimer-Type Separation of the Vibrational Motions. <i>Journal of Molecular Spectroscopy</i> , 1997, 183, 129-138.	0.4	18
81	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlated ab initio quantum chemical calculations and anharmonic analysis of the aniline inversion motion. <i>Journal of Chemical Physics</i> , 1996, 105, 11042-11050.	1.2	115
82	Method for calculating analytical solutions of the Schrödinger equation: Anharmonic oscillators and generalized Morse oscillators. <i>Physical Review A</i> , 1996, 53, 2009-2020.	1.0	27
83	Effective characteristic polynomials and two-point Padé approximants as summation techniques for the strongly divergent perturbation expansions of the ground state energies of anharmonic oscillators. <i>Physical Review E</i> , 1996, 53, 2925-2939.	0.8	36
84	Molecular quadrupole moment functions of HF and N <sub>2</sub> . I. Ab initio linear-response coupled-cluster results. <i>Journal of Chemical Physics</i> , 1996, 104, 4699-4715.	1.2	79
85	Molecular quadrupole moment functions of HF and N <sub>2</sub> . II. Rovibrational effects. <i>Journal of Chemical Physics</i> , 1996, 104, 4716-4727.	1.2	20
86	Molecular quadrupole moment function of ammonia. <i>Journal of Chemical Physics</i> , 1996, 105, 11068-11074.	1.2	18
87	Calculation and Prediction of the Spectrum of Diatomic Molecules by the Generalized Reduced Potential Curve (GRPC) Method. <i>Journal of Molecular Spectroscopy</i> , 1995, 169, 555-582.	0.4	16
88	Ab Initio Predicted Rotation-Vibration Energy Levels of HeH <sub>2</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1995, 172, 265-274.	0.4	29
89	Formation of HeH <sup>+</sup> by radiative association of He <sup>+</sup> + H. An advanced ab initio study. <i>Chemical Physics Letters</i> , 1995, 236, 177-183.	1.2	35
90	Ab initio determination of the rate coefficient for radiative association of. <i>Chemical Physics</i> , 1995, 193, 287-296.	0.9	37

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91	Nonadiabatic corrections for coupled Morse oscillators using Hutson and Howard perturbation theory. <i>Journal of Chemical Physics</i> , 1995, 102, 8916-8921.	1.2	14
92	Nonadiabatic corrections for coupled oscillators using Rayleigh-Schrödinger perturbation theory of very high orders. <i>Journal of Chemical Physics</i> , 1995, 102, 8906-8915.	1.2	24
93	Ab initio calculations of anharmonic vibrational transition intensities of trans-2,3-dideuteriooxirane. <i>Journal of Chemical Physics</i> , 1995, 103, 10110-10115.	1.2	23
94	Ab initio study of the phenol-water cation radical. <i>Journal of Chemical Physics</i> , 1994, 101, 990-997.	1.2	74
95	The vibrational and temperature dependence of the magnetic properties of the oxonium ion ( $\text{H}_3\text{O}^+$ ). <i>Chemical Physics</i> , 1994, 184, 1-11.	0.9	26
96	Extended ab Initio Study of the Vibrational Dynamics of H+5 and D+5 Including All Vibrational Modes. <i>Journal of Molecular Spectroscopy</i> , 1994, 164, 500-509.	0.4	23
97	Ab initio calculations on Ar-NO+: Structure and vibrational frequencies. <i>Journal of Chemical Physics</i> , 1994, 100, 5403-5410.	1.2	30
98	Ab Initio Study of Linestrengths of Vibration-Rotation Transitions of Ammonia and Methyl Cations. <i>Journal of Molecular Spectroscopy</i> , 1993, 158, 433-444.	0.4	10
99	Vibrational Dynamics of H+5: Ab Initio Calculation of the Low-Lying Vibrational States. <i>Journal of Molecular Spectroscopy</i> , 1993, 159, 521-533.	0.4	12
100	The Temperature Dependence and Isotope Shift of Nitrogen Shielding in Ammonia. <i>Journal of Molecular Spectroscopy</i> , 1993, 160, 311-314.	0.4	6
101	On the use of divergent series in vibrational spectroscopy. Two-and three-dimensional oscillators. <i>Journal of Chemical Physics</i> , 1993, 99, 7331-7336.	1.2	38
102	Frequency-dependent polarizabilities and first hyperpolarizabilities of H <sub>2</sub> O. <i>Journal of Chemical Physics</i> , 1993, 98, 7159-7164.	1.2	103
103	Dipole hyperpolarizability surfaces of ammonia. <i>Journal of Chemical Physics</i> , 1993, 99, 9815-9819.	1.2	13
104	Theoretical <sup>17</sup> O nuclear quadrupole coupling surface for the hydroxonium ion. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 2811-2814.	1.7	2
105	The vibrational dependence of the magnetic hyperfine interaction constants of ammonia. <i>Journal of Molecular Spectroscopy</i> , 1992, 152, 342-354.	0.4	20
106	Ab initio potential energy function and geometry of the state of ammonia. <i>Journal of Molecular Spectroscopy</i> , 1992, 152, 199-204.	0.4	2
107	Potential energy function and rotation-vibration energy levels of NH <sub>3</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1992, 153, 276-284.	0.4	17
108	Inversion/out-of-plane bending rovibrational energy levels of partially deuterated SiH <sub>3</sub> , CH <sub>3</sub> , CH <sub>3</sub> <sup>+</sup> , and NH <sub>3</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1992, 153, 285-287.	0.4	6

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109	Rotation-vibration energies of FHF <sup>-</sup> and ClHCl <sup>-</sup> from high-level correlated calculations of potential energy surfaces. <i>Chemical Physics</i> , 1991, 151, 45-58.	0.9	19
110	Anharmonic potential function, geometry, and energy levels of SiH <sub>3</sub> . <i>Journal of Molecular Spectroscopy</i> , 1991, 147, 478-487.	0.4	8
111	Inversion-vibration energies of CH <sub>3</sub> <sup>-</sup> and adiabatic electron affinity of CH <sub>3</sub> . <i>Journal of Molecular Spectroscopy</i> , 1991, 147, 526-540.	0.4	11
112	Potential energy function and rotation-vibration energy levels of CH <sub>3</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1991, 149, 235-241.	0.4	16
113	Theoretical calculations of the nuclear quadrupole coupling in the spectra of D <sub>3</sub> <sup>+</sup> , H <sub>2</sub> D <sup>+</sup> , and HD <sub>2</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1991, 150, 137-163.	0.4	6
114	An ab initio investigation of the potential energy function and rotation-vibration energies of H <sub>2</sub> O <sup>-</sup> Na <sup>+</sup> . <i>Chemical Physics Letters</i> , 1991, 185, 265-269.	1.2	7
115	The magnetizability and g-factor surfaces of ammonia. <i>Chemical Physics</i> , 1991, 153, 189-200.	0.9	35
116	Ab initio calculations of vibrational spectra of nonrigid molecules. <i>The Journal of Physical Chemistry</i> , 1990, 94, 5493-5496.	2.9	13
117	Ab initio calculations of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X 1Σ <sup>+</sup> and A 1Σ <sup>+</sup> states of all isotopic species of LiH. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 283-295.	1.0	18
118	Theoretical description of nuclear quadrupole coupling in light diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 357-372.	1.0	12
119	Dipole polarizability surfaces of ammonia. <i>Chemical Physics</i> , 1990, 144, 343-351.	0.9	9
120	Variational calculations on the Ag vibrational states, the automerization, and the predicted Raman spectrum of cyclobutadiene. <i>Journal of Chemical Physics</i> , 1990, 92, 6069-6076.	1.2	10
121	Theoretical <sup>14</sup> N nuclear quadrupole coupling surface for ammonia. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1990, 86, 1991-1994.	1.7	7
122	Propargylene: A C <sub>3</sub> H <sub>2</sub> isomer with unusual bonding. <i>Journal of Chemical Physics</i> , 1989, 91, 4763-4773.	1.2	76
123	Extended measurements of the 1½ band of CD <sub>3</sub> and the determination of the vibrational potential function for methyl. <i>Journal of Chemical Physics</i> , 1989, 90, 2125-2133.	1.2	43
124	Vibrational dynamics of hydrogen bonds: The system OH <sup>-</sup> -H <sub>2</sub> O. <i>Journal of Molecular Spectroscopy</i> , 1989, 136, 340-355.	0.4	16
125	Vibrational spectrum of FHF <sup>-</sup> from high-level correlated calculations of potential energy surfaces. <i>Chemical Physics Letters</i> , 1989, 161, 519-527.	1.2	13
126	Ab initio calculation of deuteron quadrupole coupling constants for low-lying rovibrational levels of HD in its X 1Π <sup>g+</sup> and B 1Π <sup>u+</sup> states. <i>Chemical Physics Letters</i> , 1989, 157, 337-342.	1.2	19

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127	Anharmonic potential function and effective geometries for the NH <sub>3</sub> molecule. <i>Journal of Molecular Spectroscopy</i> , 1989, 133, 331-344.	0.4	106
128	Electric dipole moment function of ammonia. <i>Journal of Molecular Spectroscopy</i> , 1989, 136, 317-332.	0.4	23
129	Ab initio calculations on the energy of activation and tunneling in the automerization of cyclobutadiene. <i>Journal of Chemical Physics</i> , 1988, 89, 3008-3015.	1.2	69
130	The $v_2=1$ invensional dependence of the rotational g-tensors in <sup>14</sup> NH <sub>3</sub> , <sup>15</sup> NH <sub>3</sub> , and <sup>15</sup> ND <sub>3</sub> . <i>Molecular Physics</i> , 1988, 64, 1233-1249.	0.8	21
131	A new Morse-oscillator based Hamiltonian for H <sub>3</sub> <sup>+</sup> : Explicit expressions for some vibrational matrix elements. <i>Journal of Molecular Spectroscopy</i> , 1987, 124, 430-436.	0.4	9
132	Prediction of the $n^{1/2}$ invensional energy levels of the phosphine, arsine, and stibine molecules. <i>Journal of Molecular Spectroscopy</i> , 1986, 119, 426-432.	0.4	11
133	The $\hat{l}''k = \hat{A}\pm 2$ and $\hat{l}''k = \hat{A}\pm 3$ forbidden transitions in the vibrational-rotational spectra of symmetric top molecules NH <sub>3</sub> and H <sub>3</sub> O <sup>+</sup> . <i>Journal of Molecular Structure</i> , 1986, 141, 361-366.	1.8	10
134	A new Morse-oscillator based Hamiltonian for H <sub>3</sub> <sup>+</sup> : Extension to H <sub>2</sub> D <sup>+</sup> and D <sub>2</sub> H <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1986, 115, 269-293.	0.4	24
135	An ab initio investigation of the potential function of PH <sub>3</sub> . <i>Journal of Molecular Spectroscopy</i> , 1986, 118, 88-95.	0.4	6
136	A new Morse-oscillator based Hamiltonian for H <sub>3</sub> <sup>+</sup> : Calculation of line strengths. <i>Journal of Molecular Spectroscopy</i> , 1986, 118, 208-231.	0.4	32
137	The development of a new Morse-oscillator based rotation-vibration Hamiltonian for H <sub>3</sub> <sup>+</sup> . <i>Journal of Molecular Spectroscopy</i> , 1985, 112, 183-202.	0.4	84
138	A preliminary determination of the equilibrium geometry and inversion potential in H <sub>3</sub> O <sup>+</sup> from experiment. <i>Journal of Molecular Spectroscopy</i> , 1984, 107, 208-211.	0.4	39
139	An <i>ab initio</i> investigation of the potential function and rotation-vibration energies of NH <sub>3</sub> . <i>Canadian Journal of Physics</i> , 1984, 62, 1801-1805.	0.4	28
140	Vibrational anharmonicity and the inversion potential function of NH <sub>3</sub> . <i>Journal of Molecular Spectroscopy</i> , 1983, 101, 30-47.	0.4	179
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158	Vibration-inversion-rotation spectra of ammonia. A vibration-inversion-rotation Hamiltonian for NH <sub>3</sub> . <i>Journal of Molecular Spectroscopy</i> , 1973, 48, 17-37.	0.4	100
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