Robert J Le Roy

List of Publications by Year
in descending order

51 papers	2,972 citations	201575 27 h-index	168321 53 g-index
53 all docs	53 docs citations	53 times ranked	1285 citing authors

#	Article	IF	Citations
1	Suppression of Parahydrogen Superfluidity in a Doped Nanoscale Bose Fluid Mixture. Physical Review Letters, 2019, 123, 093001.	2.9	2
2	Equation of state and first principles prediction of the vibrational matrix shift of solid parahydrogen. Journal of Chemical Physics, 2019, 151, 244501.	1.2	6
3	A new empirical potential energy function for Ar₂. Molecular Physics, 2018, 116, 1598-1623.	0.8	10
4	Constructing high-accuracy intermolecular potential energy surface with multi-dimension Morse/Long-Range model. Molecular Physics, 2018, 116, 843-853.	0.8	11
5	LEVEL: A computer program for solving the radial SchrÃ¶dinger equation for bound and quasibound levels. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 186, 167-178.	1.1	454
6	betaFIT: A computer program to fit pointwise potentials to selected analytic functions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 186, 210-220.	1.1	25
7	dPotFit: A computer program to fit diatomic molecule spectral data to potential energy functions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 186, 179-196.	1.1	39
8	Full empirical potential curves for the X 1Î£+ and A 1Î states of CH+ from a direct-potential-fit analysis. Journal of Chemical Physics, 2016, 144, 024311.	1.2	28
9	Raman Vibrational Shifts of Small Clusters of Hydrogen Isotopologues. Journal of Physical Chemistry A, 2015, 119, 12551-12561.	1.1	20
10	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
11	Dissociation energies and potential energy functions for the ground Xâ€‰1Î£+ and â€œavoided-crossingâ€•Aâ€‰1Î£+ states of NaH. Journal of Chemical Physics, 2015, 142, 044305.	1.2	16
12	First-principles prediction of the Raman shifts in parahydrogen clusters. Journal of Chemical Physics, 2014, 141, 014310.	1.2	15
13	Microwave and infrared spectra of COâ€“(pH2)2, COâ€“(oD2)2, and mixed COâ€“pH2â€“He trimers. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	4
14	Accurate Analytic Potential and Bornâ€“Oppenheimer Breakdown Functions for MgH and MgD from a Direct-Potential-Fit Data Analysis. Journal of Physical Chemistry A, 2013, 117, 13373-13387.	1.1	34
15	Direct-potential-fit analysis for the system of Br2. Journal of Molecular Spectroscopy, 2013, 283, 32-43.	0.4	13
16	Long-range damping functions improve the short-range behaviour of â€˜MLRâ€™ potential energy functions. Molecular Physics, 2011, 109, 435-446.	0.8	62
17	A DPF data analysis yields accurate analytic potentials for Li2a3Î£u+ and Li213Î£g+ that incorporate 3-state mixing near the 13Î£g+ state asymptote. Journal of Molecular Spectroscopy, 2011, 268, 199-210.	0.4	31
18	Theoretical study of the microwave spectrum of isotopologues of OCSâ€“(He)2. Canadian Journal of Chemistry, 2010, 88, 1146-1154.	0.6	5

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19	Accurate analytic potentials for Li2(Xâ€‰Î£1g+) and Li2(Aâ€‰Î£1u+) from 2 to 90 Ã…, and the radiative lifetime of Li(2p). Journal of Chemical Physics, 2009, 131, 204309.	1.2	102
20	Ground State Potential Energy Curve and Dissociation Energy of MgH. Journal of Physical Chemistry A, 2007, 111, 12495-12505.	1.1	78
21	Spectroscopy and Potential Energy Surfaces of Vander Waals Molecules. Advances in Chemical Physics, 2007, , 353-420.	0.3	128
22	A new potential function form incorporating extended long-range behaviour: application to ground-state Ca2. Molecular Physics, 2007, 105, 663-677.	0.8	111
23	Calculation of absolute scattering phase shifts. Molecular Physics, 2006, 104, 147-150.	0.8	6
24	An accurate analytic potential function for ground-state N2 from a direct-potential-fit analysis of spectroscopic data. Journal of Chemical Physics, 2006, 125, 164310.	1.2	201
25	Resolution of a convergence problem in direct-potential-fit data analyses: Applications to GaH(X1Î£+) and ArH+(X1Î£+). Journal of Molecular Spectroscopy, 2006, 238, 260-263.	0.4	9
26	Direct-potential-fit analysis of new infrared and UV/visible AÎ£+1-XÎ£+1 emission spectra of AgH and AgD. Journal of Chemical Physics, 2005, 123, 204304.	1.2	43
27	Potential energy, Î› doubling and Bornâ€“Oppenheimer breakdown functions for the Bâ€Š1Îu â€œbarrierâ€•state of Li2. Journal of Chemical Physics, 2003, 119, 7398-7416.	1.2	61
28	Representing Bornâ€“Oppenheimer breakdown radial correction functions for diatomic molecules. Computational and Theoretical Chemistry, 2002, 591, 175-187.	1.5	59
29	Improved Parameterization for Combined Isotopomer Analysis of Diatomic Spectra and Its Application to HF and DF. Journal of Molecular Spectroscopy, 1999, 194, 189-196.	0.4	124
30	FTIR Emission Spectra, Molecular Constants, and Potential Curve of Ground State GeO. Journal of Molecular Spectroscopy, 1999, 194, 197-202.	0.4	71
31	How do quantum effects change conclusions about heterogeneous cluster behavior based on classical mechanics simulations?. Journal of Chemical Physics, 1998, 108, 8626-8639.	1.2	6
32	Linewidths and shifts of very low temperature CO in He: A challenge for theory or experiment?. Journal of Chemical Physics, 1996, 105, 4005-4014.	1.2	43
33	Nearâ€dissociation expansions and dissociation energies for Mg+â€“(rare gas) bimers. Journal of Chemical Physics, 1994, 101, 10217-10228.	1.2	66
34	An efficient new method for calculating eigenvalues and spectra of van der Waals complexes. Journal of Chemical Physics, 1993, 99, 360-376.	1.2	18
35	Calculated rovibrational energy levels and infrared spectrum of He-C2H2. Molecular Physics, 1992, 77, 111-134.	0.8	22
36	Direct determination of longâ€range inverseâ€power potential coefficients from spectroscopic data. Journal of Chemical Physics, 1991, 94, 3479-3495.	1.2	15

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37	Monte Carlo simulations of structural properties and infrared spectra of SF6â€“(Ar)n clusters. Journal of Chemical Physics, 1988, 88, 2898-2912.	1.2	105
38	The secular equation/perturbation theory method for calculating spectra of van der Waals complexes. Journal of Chemical Physics, 1985, 83, 1197-1203.	1.2	25
39	Orbiting resonance model for recombination of physisorbed atoms. Journal of Chemical Physics, 1984, 81, 4149-4159.	1.2	11
40	A twoâ€isotope higherâ€order RKRâ€type inversion procedure. Journal of Chemical Physics, 1984, 81, 3996-4001.	1.2	25
41	Functional form for representing all vibrational eigenenergies of a diatomic molecule state. IV. Application to the Br2B(3Î+0u) state. Journal of Chemical Physics, 1984, 81, 66-72.	1.2	13
42	Predissociation of HDâ€“Ar van der Waals molecules by internal rotation. Journal of Chemical Physics, 1983, 78, 4040-4043.	1.2	41
43	Efficient calculation of highâ€order semiclassical scattering phase shifts. Journal of Chemical Physics, 1982, 77, 3527-3532.	1.2	7
44	On the application, breakdown, and nearâ€dissociation behavior of the higherâ€order JWKB quantization condition. Journal of Chemical Physics, 1978, 68, 3139-3148.	1.2	36
45	Energies and widths of quasibound levels (orbiting resonances) for spherical potentials. Journal of Chemical Physics, 1978, 69, 3622-3631.	1.2	130
46	Intermolecular potentials and isotope effects for molecular hydrogenâ€“inert gas complexes. Journal of Chemical Physics, 1975, 63, 338-344.	1.2	63
47	Long-Range Potential Coefficients From RKR Turning Points: C₆ and C₈ for B(3Î_{Ou}⁺)-State Cl₂, Br₂, and I₂. Canadian Journal of Physics, 1974, 52, 246-256.	0.4	114
48	Anisotropic intermolecular potentials from an analysis of spectra of H2â€and D2â€inert gas complexes. Journal of Chemical Physics, 1974, 61, 4750-4769.	1.2	196
49	Comment on the uv resonance spectrum and groundâ€state dissociation energy of I2. Journal of Chemical Physics, 1974, 61, 438-438.	1.2	5
50	Improved Spectroscopic Dissociation Energy for Groundâ€State Ar2. Journal of Chemical Physics, 1972, 57, 573-574.	1.2	53
51	Shape Resonances and Rotationally Predissociating Levels: The Atomic Collision Timeâ€Delay Functions and Quasibound Level Properties of H2(X 1Î£g+). Journal of Chemical Physics, 1971, 54, 5114-5126.	1.2	161