Alberto Requena

List of Publications by Year
in descending order

139 papers	2,190 citations	201674 27 h-index	330143 37 g-index
149 all docs	149 docs citations	149 times ranked	1837 citing authors

#	Article	IF	Citations
1	Ab Initio Partition Functions and Thermodynamic Quantities for the Molecular Hydrogen Isotopologues. Journal of Physical Chemistry A, 2021, 125, 9226-9241.	2.5	3
2	Quantum description of linearly coupled harmonic oscillator systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 025101.	1.5	3
3	On the Role of Entropy in the Stabilization of Î±-Helices. Journal of Chemical Information and Modeling, 2020, 60, 6523-6531.	5.4	8
4	Tuning the Optical Properties of Novel Antitumoral Drugs Based on Cyclometalated Iridium(III) Complexes. Journal of Physical Chemistry A, 2019, 123, 8644-8649.	2.5	6
5	Energetic Self-Folding Mechanism in Î±-Helices. Journal of Physical Chemistry B, 2019, 123, 8186-8194.	2.6	4
6	Quantum solutions of identical linearly coupled harmonic oscillators using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 055101.	1.5	3
7	Intraresidual Correlated Motions in Peptide Chains. Journal of Chemical Information and Modeling, 2019, 59, 4524-4527.	5.4	2
8	Antibodies as Carrier Molecules: Encapsulating Anti-Inflammatory Drugs inside Herceptine. Journal of Physical Chemistry B, 2018, 122, 2064-2072.	2.6	8
9	A new fluorescence turn-on chemosensor for nanomolar detection of Al³⁺ constructed from a pyridineâ€“pyrazole system. New Journal of Chemistry, 2018, 42, 2933-2941.	2.8	29
10	Structure, Spectra, and DFT Simulation of Nickel Benzazolate Complexes with Tris(2-aminoethyl)amine Ligand. Inorganic Chemistry, 2017, 56, 3663-3673.	4.0	13
11	DFT Simulation of Structural and Optical Properties of 9-Aminoacridine Half-Sandwich Ru(II), Rh(III), and Ir(III) Antitumoral Complexes and Their Interaction with DNA. Journal of Chemical Theory and Computation, 2017, 13, 3898-3910.	5.3	21
12	A Pyreneâ€Pyrazoleâ€Based Rotamer Senses Hg2+on the Nanomolar Scale. ChemistrySelect, 2017, 2, 2512-2519.	1.5	12
13	Understanding the connection between conformational changes of peptides and equilibrium thermal fluctuations. Physical Chemistry Chemical Physics, 2017, 19, 3459-3463.	2.8	2
14	Quantum treatment of HÃ©nonâ€“Heiles systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 025101.	1.5	3
15	Quantum solution of coupled harmonic oscillator systems beyond normal coordinates. Journal of Mathematical Chemistry, 2017, 55, 1964-1984.	1.5	6
16	Relaxation pathways of the OD stretch fundamental of HOD in liquid H2O. Journal of Chemical Physics, 2016, 145, 244502.	3.0	5
17	A rotating spiral structure in the innermost regions around IRC+10216. Journal of Physics: Conference Series, 2016, 728, 022005.	0.4	0
18	HIGH-RESOLUTION ROTATIONAL SPECTRUM, DUNHAM COEFFICIENTS, AND POTENTIAL ENERGY FUNCTION OF NaCl. Astrophysical Journal, 2016, 825, 150.	4.5	5

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19	Conformational Changes of Trialanine in Water Induced by Vibrational Relaxation of the Amide I Mode. Journal of Physical Chemistry B, 2016, 120, 348-357.	2.6	9
20	HINTS OF A ROTATING SPIRAL STRUCTURE IN THE INNERMOST REGIONS AROUND IRC +10216. Astrophysical Journal, 2016, 818, 192.	4.5	24
21	Mutagenic effects induced by the attack of NO2 radical to the guanine-cytosine base pair. Frontiers in Chemistry, 2015, 3, 13.	3.6	7
22	Si-BEARING MOLECULES TOWARD IRC+10216: ALMA UNVEILS THE MOLECULAR ENVELOPE OF CWLeo. Astrophysical Journal Letters, 2015, 805, L13.	8.3	40
23	Assessing the Importance of Proton Transfer Reactions in DNA. Accounts of Chemical Research, 2014, 47, 2467-2474.	15.6	98
24	Structure and Spectroscopic Properties of Nickel Benzazolate Complexes with Hydrotris(pyrazolyl)borate Ligand. Inorganic Chemistry, 2014, 53, 5502-5514.	4.0	8
25	Theoretical Study of the Temperature Dependence of the Vibrational Relaxation of the H₂O Bend Fundamental in Liquid Water and the Subsequent Distortion of the Hydrogen Bond Network. Journal of Physical Chemistry B, 2014, 118, 9427-9437.	2.6	13
26	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. Journal of Molecular Modeling, 2014, 20, 2401.	1.8	24
27	Rovibrational energies, partition functions and equilibrium fractionation of the CO2 isotopologues. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 147, 233-251.	2.3	12
28	Instantaneous normal mode analysis of the vibrational relaxation of the amide I mode of alanine dipeptide in water. Journal of Chemical Physics, 2013, 138, 205102.	3.0	6
29	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. Journal of Chemical Theory and Computation, 2013, 9, 4947-4958.	5.3	62
30	Conformational changes of Î²-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6527.	2.8	21
31	Impact of DFT functionals on the predicted magnesiumâ€“DNA interaction: an ONIOM study. Highlights in Theoretical Chemistry, 2013, , 271-279.	0.0	0
32	Molecular dynamics with quantum transitions study of the vibrational relaxation of the HOD bend fundamental in liquid D2O. Journal of Chemical Physics, 2012, 136, 234507.	3.0	9
33	Hybrid Quantum/Classical Simulations of the Vibrational Relaxation of the Amide I Mode of N-Methylacetamide in D₂O Solution. Journal of Physical Chemistry B, 2012, 116, 2969-2980.	2.6	20
34	Antioxidant Properties of Î²-Carotene Isomers and Their Role in Photosystems: Insights from Ab Initio Simulations. Journal of Physical Chemistry A, 2012, 116, 3498-3506.	2.5	30
35	Using the Screened Coulomb Potential To Illustrate the Variational Method. Journal of Chemical Education, 2012, 89, 1152-1158.	2.3	8
36	Impact of DFT functionals on the predicted magnesiumâ€“DNA interaction: an ONIOM study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	23

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37	Theoretical vibrational terms and rotational constants for the 15N substituted isotopologues of N2O calculated using normal hyperspherical coordinates. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 26-46.	2.3	3
38	A spectroscopic potential energy surface for FCN. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1155-1169.	2.3	4
39	Atomistic Molecular Dynamics Simulations of the Interactions of Oleic and 2-Hydroxyoleic Acids with Phosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2011, 115, 11727-11738.	2.6	21
40	Combined effect of stacking and solvation on the spontaneous mutation in DNA. Physical Chemistry Chemical Physics, 2011, 13, 14584.	2.8	52
41	Host-pathogen interaction of root-knot nematode Meloidogyne incognita on pepper in the southeast of Spain. European Journal of Plant Pathology, 2011, 131, 511-518.	1.7	3
42	Vibrational dynamics of polyatomic molecules in solution: assignment, time evolution and mixing of instantaneous normal modes. Theoretical Chemistry Accounts, 2011, 128, 769-782.	1.4	19
43	A method for analyzing the vibrational energy flow in biomolecules in solution. Journal of Chemical Physics, 2011, 135, 204106.	3.0	16
44	Theoretical study of the low-lying excited states of -carotene isomers by a multireference configuration interaction method. Chemical Physics, 2010, 373, 98-103.	1.9	32
45	Instantaneous normal modes, resonances, and decay channels in the vibrational relaxation of the amide I mode of N-methylacetamide-D in liquid deuterated water. Journal of Chemical Physics, 2010, 132, 224501.	3.0	33
46	Molecular Dynamics Simulations and Instantaneous Normal-Mode Analysis of the Vibrational Relaxation of the Câ^'H Stretching Modes ofN-methylacetamide-din Liquid Deuterated Water. Journal of Physical Chemistry A, 2010, 114, 11450-11461.	2.5	16
47	A Theoretical Study of the Reaction of Î²-Carotene with the Nitrogen Dioxide Radical in Solution. Journal of Physical Chemistry B, 2010, 114, 4366-4372.	2.6	41
48	Theoretical Study of the Tautomerism in the One-Electron Oxidized Guanineâ^'Cytosine Base Pair. Journal of Physical Chemistry B, 2010, 114, 13439-13445.	2.6	32
49	Could the addition of hp-hMG and GnRH antagonists modulate the response in IVF-ICSI cycles?. Human Fertility, 2010, 13, 41-49.	1.7	10
50	Hybrid quantum/classical simulation of the vibrational relaxation of the bend fundamental in liquid water. Journal of Chemical Physics, 2009, 131, 204505.	3.0	15
51	Aerosol Lidar Intercomparison in the Framework of SPALINETâ€"The Spanish Lidar Network: Methodology and Results. IEEE Transactions on Geoscience and Remote Sensing, 2009, 47, 3547-3559.	6.3	30
52	Efficient parabolic evaluation of coupling terms in hybrid quantum/classical simulations. Chemical Physics, 2009, 358, 57-60.	1.9	3
53	Double proton transfer mechanism in the adenineâ€"uracil base pair and spontaneous mutation in RNA duplex. Chemical Physics Letters, 2009, 484, 64-68.	2.6	34
54	Intermolecular Proton Transfer in Microhydrated Guanineâ^'Cytosine Base Pairs: a New Mechanism for Spontaneous Mutation in DNA. Journal of Physical Chemistry A, 2009, 113, 10549-10556.	2.5	77

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55	Effects of Hydration on the Proton Transfer Mechanism in the Adenineâ˜Thymine Base Pair. Journal of Physical Chemistry A, 2009, 113, 7892-7898.	2.5	71
56	Density Functional Theory Study of the Stability and Vibrational Spectra of the Î²-Carotene Isomers. Journal of Physical Chemistry A, 2009, 113, 9899-9907.	2.5	24
57	Vibrational Bound States of the He2Ne+ Cation. Journal of Physical Chemistry A, 2009, 113, 14896-14903.	2.5	1
58	On the interaction of a beam of polar molecules with a static and a resonant RF field as a source of molecular interferences. European Physical Journal D, 2008, 49, 297-303.	1.3	6
59	The Rotating Morseâ€“Pekeris Oscillator Revisited. Journal of Chemical Education, 2008, 85, 1675.	2.3	2
60	An analytical perturbation treatment of the rotating Morse oscillator. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 105102.	1.5	4
61	A Density Functional Theory Study of the Structure and Vibrational Spectra of Î²-Carotene, Capsanthin, and Capsorubin. Journal of Physical Chemistry A, 2008, 112, 4815-4825.	2.5	34
62	Full quantum vibrational simulation of the relaxation of the cyanide ion in water using the Ehrenfest method with quantum corrections. Journal of Chemical Physics, 2008, 129, 154501.	3.0	20
63	The Ehrenfest method with quantum corrections to simulate the relaxation of molecules in solution: Equilibrium and dynamics. Journal of Chemical Physics, 2007, 126, 014503.	3.0	40
64	Optimal internal coordinates, vibrational spectrum, and effective Hamiltonian for ozone. Journal of Chemical Physics, 2007, 126, 244305.	3.0	11
65	A modified Ehrenfest method that achieves Boltzmann quantum state populations. Chemical Physics Letters, 2006, 417, 53-57.	2.6	44
66	On the use of optimal internal vibrational coordinates for symmetrical bent triatomic molecules. Journal of Chemical Physics, 2005, 122, 224319.	3.0	15
67	Surface hopping simulation of the vibrational relaxation of I2 in liquid xenon using the collective probabilities algorithm. Journal of Chemical Physics, 2004, 121, 10611-10622.	3.0	16
68	Theoretical calculations of vibrational frequencies and rotational constants of the N2O isotopomers. Journal of Molecular Spectroscopy, 2003, 217, 43-58.	1.2	9
69	Collective probabilities algorithm for surface hopping calculations. Journal of Chemical Physics, 2003, 119, 6489-6499.	3.0	9
70	Molecular dynamics simulation of the I2(X)â‹¯Ar isomers population in a free-jet expansion: Thermodynamics versus kinetic control. Journal of Chemical Physics, 2002, 116, 1944-1953.	3.0	30
71	A theoretical study of the vibrational spectrum of the CS2 molecule. Journal of Chemical Physics, 2002, 116, 7495-7508.	3.0	13
72	Size evolution of the vibrational predissociation process in Br2Â·Â·Â·Nen clusters: Simulation and kinetic study. Faraday Discussions, 2001, 118, 257-268.	3.2	9

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73	Variational Calculations of Rovibrational Energies for CO2. Journal of Molecular Spectroscopy, 2001, 205, 62-72.	1.2	24
74	Optimal generalized internal vibrational coordinates and potential energy surface for the ground electronic state of SO2. Journal of Chemical Physics, 2001, 115, 139-148.	3.0	35
75	Excited vibrational states and potential energy function for OCS determined using generalized internal coordinates. Journal of Chemical Physics, 2000, 113, 5695-5704.	3.0	17
76	Time evolution of reactants, intermediates, and products in the vibrational predissociation of Br2â‹¯Ne: A theoretical study. Journal of Chemical Physics, 2000, 113, 10130-10142.	3.0	24
77	Experimental and theoretical study of the photofragmentation process: Ar3++hÎ½â†'Ar2++Ar. Journal of Chemical Physics, 2000, 113, 2175-2181.	3.0	8
78	Mixed quantum classical steps: a DVR hopping method. PhysChemComm, 2000, 3, 29-35.	0.8	0
79	Hybrid quantum/classical simulation and kinetic study of the vibrational predissociation of Cl2â‹¯Nen (n=2,â€Š3). Journal of Chemical Physics, 1999, 111, 4577-4588.	3.0	27
80	Competition between electronic and vibrational predissociation in Arâ€"I2(B): a molecular dynamics with quantum transitions study. Chemical Physics, 1999, 240, 229-239.	1.9	30
81	Global potential energy surfaces for the CO2 and CS2 molecules. Chemical Physics Letters, 1999, 313, 670-678.	2.6	13
82	Determination of a Potential Energy Surface for CO2Using Generalized Internal Vibrational Coordinates. Journal of Molecular Spectroscopy, 1999, 195, 137-146.	1.2	23
83	Determination of highly excited rovibrational states for N2O using generalized internal coordinates. Journal of Chemical Physics, 1999, 110, 6339-6352.	3.0	26
84	Optimal generalized internal vibrational coordinates for symmetrical linear triatomic molecules. Chemical Physics Letters, 1998, 298, 36-42.	2.6	10
85	Vibrational predissociation of the I2â‹¯Ne2 cluster: A molecular dynamics with quantum transitions study. Journal of Chemical Physics, 1998, 109, 6320-6328.	3.0	37
86	Optimization of vibrational coordinates. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1681.	1.7	32
87	Application of trajectory surface hopping to vibrational predissociation. Chemical Physics Letters, 1997, 280, 185-188.	2.6	25
88	Variational calculations of vibrational states of N2O using hyperspherical normal coordinates. Journal of Chemical Physics, 1996, 105, 6099-6110.	3.0	11
89	Hyperspherical Kinematic Vibrational Coordinates for Linear Triatomic Molecules. The Journal of Physical Chemistry, 1995, 99, 11051-11060.	2.9	14
90	A vibrational Hamiltonian model for triatomic molecules based on the Kratzer and Poschl Teller potentials. International Journal of Quantum Chemistry, 1994, 52, 165-175.	2.0	4

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91	Excited state dynamics in HgAr2: statistical analysis of vibrational state distribution. Faraday Discussions, 1994, 97, 131-142.	3.2	5
92	Curvilinear Jacobi and Radau normal coordinates for linear triatomic molecules. Application to CO2. Chemical Physics, 1993, 175, 255-264.	1.9	21
93	Generalized hyperspherical coordinates for molecular vibrations. The Journal of Physical Chemistry, 1993, 97, 5831-5835.	2.9	13
94	A theoretical study of the HgAr2(3P1â†1S0) vibronic spectrum. Journal of Chemical Physics, 1993, 98, 1007-1017.	3.0	40
95	Vibrational levels of water by the self-consistent-field method using Radau coordinates. The Journal of Physical Chemistry, 1992, 96, 4341-4346.	2.9	10
96	Use of rotated Jacobi coordinates to calculate vibrational levels of hydrogen cyanide. The Journal of Physical Chemistry, 1992, 96, 9691-9696.	2.9	13
97	Vibrational self-consistent-field approximation for triatomic molecules using hyperspherical modes with application to H2O. International Journal of Quantum Chemistry, 1992, 42, 475-488.	2.0	6
98	The adiabatic multi-step separation method for vibrational states: application to SO2. Computational and Theoretical Chemistry, 1992, 254, 91-98.	1.5	0
99	Self-consistent-field calculation of vibrational bound states for triatomic molecules using transformed Jacobi coordinates. The Journal of Physical Chemistry, 1991, 95, 2292-2297.	2.9	17
100	Variational calculation of vibrational energies of triatomic molecules usingSCFoptimized modes. International Journal of Quantum Chemistry, 1991, 40, 685-694.	2.0	14
101	Energy eigenvalues for Lennard-Jones potentials using the hypervirial perturbative method. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 2771-2781.	1.5	11
102	Twoâ€¢center matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1990, 93, 3408-3412.	3.0	15
103	Rotationalâ€“vibrational matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1989, 90, 5536-5540.	3.0	14
104	Improved analytic potential models for bent AB2 molecules. Journal of Molecular Spectroscopy, 1989, 136, 185-196.	1.2	12
105	Analytical perturbation treatment of vibrational stretch-bend couplings. Journal of Quantitative Spectroscopy and Radiative Transfer, 1989, 42, 149-155.	2.3	1
106	Perturbative virtualSCF CItreatment for energy levels of coupled oscillator systems. International Journal of Quantum Chemistry, 1989, 36, 49-60.	2.0	2
107	SCF calculations of excited vibrational energy levels for normal modes. Computational and Theoretical Chemistry, 1988, 166, 339-344.	1.5	0
108	Perturbative multi-step adiabatic treatment for energy levels of multidimensional coupled systems. Computational and Theoretical Chemistry, 1988, 166, 345-350.	1.5	0

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109	Variational HEG calculation of vibration rotation transition moments for diatomic molecules.. Computational and Theoretical Chemistry, 1988, 166, 351-356.	1.5	0
110	Perturbed Morse expansion for triatomic molecules. Computational and Theoretical Chemistry, 1988, 166, 357-362.	1.5	1
111	Analytical expressions for vibrational matrix elements of Morse oscillators. Physical Review A, 1988, 38, 4205-4212.	2.5	9
112	Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation. Molecular Physics, 1987, 61, 1513-1518.	1.7	1
113	HypervirialSCFtreatment for vibrational energy levels of triatomic molecules. International Journal of Quantum Chemistry, 1987, 32, 511-516.	2.0	2
114	Charge distribution analysis on Arâ€”H2 system. Computational and Theoretical Chemistry, 1986, 136, 99-110.	1.5	5
115	Hypervirial treatment of centrifugal distortion of 2Î energy levels. Journal of Quantitative Spectroscopy and Radiative Transfer, 1986, 35, 29-37.	2.3	0
116	Rotational predissociation of the Ar-H2 van der Waals molecule. Journal of Quantitative Spectroscopy and Radiative Transfer, 1986, 35, 127-130.	2.3	2
117	About the overestimation of the basis set superposition error on interaction energy calculations for van der Waals systems. Journal of Chemical Physics, 1986, 84, 5077-5080.	3.0	29
118	Rovibrational energy levels and expectation values for perturbed Kratzer oscillators. Journal of Chemical Physics, 1986, 85, 3939-3944.	3.0	18
119	Matrix elements for rotating Morse oscillators. Physical Review A, 1986, 34, 4380-4386.	2.5	13
120	Hypervirial calculation of perturbedâ€”Morse-oscillator potentials for diatomic molecules. Journal of Quantitative Spectroscopy and Radiative Transfer, 1985, 34, 233-242.	2.3	3
121	Calculation of the absolute infrared frequencies and intensities of a diatomic molecule or of local diatomic groups. Computers & Chemistry, 1985, 9, 115-120.	1.2	1
122	Ab initiocalculations of intermolecular potentials. The ground state of the Arï£¿H2van der Waals molecule. Journal of Computational Chemistry, 1985, 6, 39-45.	3.3	14
123	Perturbed morse oscillator in diatomic molecules: an hypervirial treatment. Computational and Theoretical Chemistry, 1985, 120, 157-162.	1.5	1
124	Perturbative treatment of anharmonic diatomic oscillators in the generator coordinate description. Computational and Theoretical Chemistry, 1985, 120, 41-45.	1.5	0
125	Predissociation in van der Waals molecules. Computational and Theoretical Chemistry, 1985, 120, 47-62.	1.5	0
126	Microcomputer-based question bank for training and assessment in biochemistry. Biochemical Education, 1984, 12, 108-111.	0.1	3

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127	Vibrational-rotational levels of diatomicRKRpotentials. International Journal of Quantum Chemistry, 1984, 25, 677-686.	2.0	1
128	Self-consistent field vibrational energies for a system of coupled oscillators using the hypervirial and the Hellmann-Feynman theorems. Journal of Quantitative Spectroscopy and Radiative Transfer, 1983, 29, 471-475.	2.3	5
129	Energy levels for a system of coupled oscillators. Computational and Theoretical Chemistry, 1983, 93, 221-226.	1.5	0
130	Approximated Eigenenergy for doubly perturbed oscillators. Computational and Theoretical Chemistry, 1983, 93, 227-230.	1.5	1
131	Hypervirial calculations of Morse oscillator matrix elements. Journal of Chemical Physics, 1983, 78, 4792-4793.	3.0	17
132	Perturbation for a rigid rotator in an electric field. International Journal of Quantum Chemistry, 1982, 22, 1263-1270.	2.0	9
133	On the stabilization angle of the complex rotation method. Chemical Physics Letters, 1981, 78, 13-15.	2.6	9
134	Vibrational and rotational predissociation of triatomic van der Waals molecules. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1981, 63, 46-49.	0.2	3
135	Energy levels for perturbed Morse oscillators. International Journal of Quantum Chemistry, 1980, 17, 931-942.	2.0	12
136	Semiclassical model for accidental predissociation in diatomic molecules. Journal of Molecular Spectroscopy, 1980, 82, 364-378.	1.2	10
137	Rotational predissociation of triatomic van der Waals molecules. Journal of Chemical Physics, 1980, 72, 3018-3026.	3.0	39
138	Rotational effects in the vibrational predissociation of Xâ‹…â‹…â‹…H2 van der Waals molecules. Journal of Chemical Physics, 1980, 73, 4347-4352.	3.0	27
139	The wavefunction of the complex coordinate method. Molecular Physics, 1980, 40, 1107-1115.	1.7	44