Miguel Carvajal

List of Publications by Year
in descending order

68 papers	1,341 citations	279798 23 h-index	377865 34 g-index
68 all docs	68 docs citations	68 times ranked	685 citing authors

#	Article	IF	Citations
1	Vibrational energies for NH3 based on high level ab initio potential energy surfaces. Journal of Chemical Physics, 2002, 117, 11265-11276.	3.0	68
2	SU(2) approximation to the coupling of Morse oscillators. Chemical Physics Letters, 1999, 308, 91-98.	2.6	63
3	An extended SU(2) model for coupled Morse oscillators. Chemical Physics, 2000, 260, 105-123.	1.9	63
4	Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378.	1.7	55
5	Rotational spectrum of¹³C₂-methyl formate (HCOO¹³CH₃) and detection of the two¹³C-methyl formate in Orion. Astronomy and Astrophysics, 2009, 500, 1109-1118.	5.1	55
6	Potential parameters of PH3 obtained by simultaneous fitting of ab initio data and experimental vibrational band origins. Chemical Physics, 2003, 290, 59-67.	1.9	51
7	Ab initio dipole moment and theoretical rovibrational intensities in the electronic ground state of PH3. Journal of Molecular Spectroscopy, 2006, 239, 71-87.	1.2	47
8	ROTATIONAL SPECTRUM AND TENTATIVE DETECTION OF DCOOCH₃-METHYL FORMATE IN ORION. Astrophysical Journal, 2010, 714, 1120-1132.	4.5	46
9	Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317.	3.0	43
10	Microwave and submillimeter spectroscopy and first ISM detection of¹⁸O-methyl formate. Astronomy and Astrophysics, 2012, 538, A119.	5.1	43
11	Detection of vibrationally excited methyl formate in W51 e2. Astronomy and Astrophysics, 2008, 489, 589-600.	5.1	41
12	Spectroscopic Description of H2O in the su(2) Vibron Model Approximation. Journal of Molecular Spectroscopy, 2002, 214, 52-68.	1.2	40
13	Reinvestigation of the ground and first torsional state of methylformate. Journal of Molecular Spectroscopy, 2007, 246, 158-166.	1.2	40
14	Rotationâ€“Vibration Motion of Pyramidal XY3 Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to NH3. Advances in Quantum Chemistry, 2005, 48, 209-238.	0.8	37
15	Equivalent rotations associated with the permutation inversion group revisited: symmetry projection of the rovibrational functions of methane. Molecular Physics, 2011, 109, 797-812.	1.7	31
16	¹³ C-METHYL FORMATE: OBSERVATIONS OF A SAMPLE OF HIGH-MASS STAR-FORMING REGIONS INCLUDING ORION-KL AND SPECTROSCOPIC CHARACTERIZATION. Astrophysical Journal, Supplement Series, 2014, 215, 25.	7.7	31
17	Simulation of the Raman spectra of CO2: Bridging the gap between algebraic models and experimental spectra. Journal of Chemical Physics, 2014, 141, 054306.	3.0	31
18	Analytic evaluation of Franck-Condon integrals for anharmonic vibrational wave functions. Physical Review A, 1999, 59, 3462-3470.	2.5	28

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19	Vibrational energies of PH3 calculated variationally at the complete basis set limit. Journal of Chemical Physics, 2008, 129, 044309.	3.0	28
20	A novel connection between algebraic spectroscopic parameters and force constants in the description of vibrational excitations of linear triatomic molecules. Journal of Molecular Spectroscopy, 2009, 253, 1-15.	1.2	28
21	The complexity of Orion: an ALMA view. Astronomy and Astrophysics, 2017, 604, L2.	5.1	28
22	GLOBAL ASSIGNMENT AND EXTENSION OF MILLIMETER- AND SUBMILLIMETER-WAVE SPECTRAL DATABASE OF ¹³ C ₁ -METHYL FORMATE (H ¹³ COOCH ₃) IN THE GROUND AND FIRST EXCITED STATES. Astrophysical Journal, Supplement Series, 2010, 190, 315-321.	7.7	26
23	Theoretical spectroscopic characterization at low temperatures of detectable sulfur-organic compounds: Ethyl mercaptan and dimethyl sulfide. Journal of Chemical Physics, 2014, 140, 124302.	3.0	23
24	The microwave and submillimeterwave spectrum of 13C1-methyl formate in its ground torsional state (H13COOCH3). Journal of Molecular Structure, 2006, 795, 4-8.	3.6	21
25	PH3 revisited: Theoretical transition moments for the vibrational transitions below. Journal of Molecular Spectroscopy, 2008, 252, 121-128.	1.2	21
26	CCSD(T) Study of Dimethyl-Ether Infrared and Raman Spectra. Journal of Physical Chemistry A, 2011, 115, 13573-13580.	2.5	18
27	THz spectroscopy and first ISM detection of excited torsional states of¹³C-methyl formate. Astronomy and Astrophysics, 2014, 568, A58.	5.1	18
28	Calculation of Transition State Energies in the HCNâ€“HNC Isomerization with an Algebraic Model. Journal of Physical Chemistry A, 2019, 123, 9544-9551.	2.5	17
29	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF ETHYL MERCAPTAN AND DIMETHYL SULFIDE ISOTOPOLOGUES: A ROUTE TOWARD THEIR ASTROPHYSICAL DETECTION. Astrophysical Journal, 2014, 796, 50.	4.5	16
30	The potential energy surface of CO₂ from an algebraic approach. International Journal of Quantum Chemistry, 2012, 112, 3498-3507.	2.0	15
31	A study of the Raman spectrum of CO2 using an algebraic approach. Chemical Physics Letters, 2012, 554, 208-213.	2.6	14
32	Excited state quantum phase transitions in the bending spectra of molecules. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 261, 107436.	2.3	14
33	Ab initio potential energy surface, electric-dipole moment, polarizability tensor, and theoretical rovibrational spectra in the electronic ground state of. Chemical Physics, 2008, 346, 146-159.	1.9	13
34	Highly correlated ab initio study of the far infrared spectra of methyl acetate. Journal of Chemical Physics, 2013, 138, 044319.	3.0	13
35	Impact of nonconvergence and various approximations of the partition function on the molecular column densities in the interstellar medium. Astronomy and Astrophysics, 2019, 627, A65.	5.1	13
36	Configuration localized wave functions: General formalism and applications to vibrational spectroscopy of diatomic molecules. Physical Review A, 2000, 61, .	2.5	12

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37	The broadband rotational spectrum of fully deuterated acetaldehyde (CD3CDO) in a CW supersonic expansion. Journal of Molecular Spectroscopy, 2017, 342, 17-24.	1.2	12
38	THz extended spectrum of the monodeuterated methyl formate (DCOOCH₃). Astronomy and Astrophysics, 2015, 576, A39.	5.1	11
39	High-resolution infrared and microwave study of10BF2OH and11BF2OH: the 5, 6l, 71, 8l, 91and 8191vibrationally excited states. Molecular Physics, 2004, 102, 1641-1652.	1.7	10
40	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.	2.3	10
41	Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate. Journal of Chemical Physics, 2014, 141, 104303.	3.0	10
42	Toward a Global Analysis Method Based on Anharmonic Ladder Operators: Application to Hydrogen Sulfide (H₂³²S). Journal of Physical Chemistry A, 2015, 119, 12823-12838.	2.5	10
43	An approach to global rovibrational analysis based on anharmonic ladder operators: Application to Hydrogen Selenide. Chemical Physics, 2012, 392, 63-70.	1.9	9
44	An algebraic alternative for the accurate simulation of CO 2 Raman spectra. Journal of Raman Spectroscopy, 2020, 51, 569-583.	2.5	9
45	Isocyanic acid (HNCO) in the hot molecular core G331.512-0.103: observations and chemical modelling. Monthly Notices of the Royal Astronomical Society, 2021, 504, 4428-4444.	4.4	9
46	Configuration localized Morse wave functions: Application to vibrational transitions in anharmonic diatomic molecules. Physical Review A, 1999, 59, 1852-1858.	2.5	8
47	Rotational spectrum, structure and internal rotation in CH3CCl3. Journal of Molecular Spectroscopy, 2008, 247, 160-166.	1.2	8
48	Highly correlated ab initio study of the low frequency modes of propane and various monosubstituted isotopologues containing D and 13C. Physical Chemistry Chemical Physics, 2013, 15, 10258.	2.8	8
49	Comparison between phase space structures in coupled Morse systems and in various su(2) approximations. Chaos, 2001, 11, 464-473.	2.5	7
50	Raman and infrared spectra of dimethyl ether 13C-isotopologue (CH3O13CH3) from a CCSD(T) potential energy surface. Journal of Molecular Spectroscopy, 2012, 279, 3-11.	1.2	7
51	CCSD(T) Study of CD₃â€“Oâ€“CD₃ and CH₃â€“Oâ€“CD₃ Far-Infrared Spectra. Journal of Physical Chemistry A, 2012, 116, 6901-6910.	2.5	7
52	New Spectral Characterization of Dimethyl Ether Isotopologues CH₃OCH₃ and ¹³CH₃OCH₃ in the THz Region. Astrophysical Journal, Supplement Series, 2019, 241, 13.	7.7	7
53	Comprehensive vibrational analysis of CO2 based on a polyad-preserving model. European Physical Journal D, 2017, 71, 1.	1.3	6
54	Probing the methyl torsional barriers of the doubly substituted methyl-ethyl Criegee intermediate by FTMW spectroscopy. Journal of Molecular Spectroscopy, 2018, 353, 23-27.	1.2	6

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55	Competitive Gas Phase Reactions for the Production of Isomers C₂O₂H₄. Spectroscopic Constants of Methyl Formate. Journal of Physical Chemistry A, 2019, 123, 9658-9668.	2.5	6
56	Quantum fidelity susceptibility in excited state quantum phase transitions: application to the bending spectra of nonrigid molecules. SciPost Physics, 2022, 12, .	4.9	6
57	Vibrational energies of monodeuterated dimethyl ether based on high level ab initio potential energy surfaces. Chemical Physics Letters, 2014, 592, 200-205.	2.6	5
58	Ab initio spectroscopic characterization of the radical CH3OCH2 at low temperatures. Journal of Chemical Physics, 2019, 150, 194102.	3.0	5
59	Anharmonicity-induced excited-state quantum phase transition in the symmetric phase of the two-dimensional limit of the vibron model. Physical Review A, 2022, 105, .	2.5	5
60	Symmetry projection of the rovibrational functions of methane. , 2010, , .		3
61	The SiÂ+ÂSO2 collision and an extended network of neutralâ€“neutral reactions between silicon and sulphur bearing species. Monthly Notices of the Royal Astronomical Society, 2022, 515, 369-377.	4.4	2
62	Spectroscopy and Dynamics of Medium-Sized Molecules and Clusters: Theory, Experiment, and Applications. Journal of Physical Chemistry A, 2016, 120, 475-476.	2.5	1
63	Theoretical spectroscopic study of acetyl (CH3CO), vinoxy (CH2CHO), and 1-methylvinoxy (CH3COCH2) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	1
64	Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra. , 2006, , 171-183.		1
65	Algebraic vibrational description of the symmetric isotopologues of CO2: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si220.svg"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>13</mml:mn></mml:mrow></mml:msup><mml:msup><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mrow><mml:mn>16</mml:mn></mml:mrow></mml:msup></mml:mrow></m <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si221.svg"><mml:mrow><mml:	1.9	1
66	Novel results from an algebraic approach to molecular bending dynamics. Journal of Physics: Conference Series, 2011, 284, 012049.	0.4	0
67	An algebraic approach applied to the determination of the polarizability in CO₂. Journal of Physics: Conference Series, 2014, 512, 012009.	0.4	0
68	Theoretical spectroscopic study of acetyl (CH3CO), vinoxy (CH2CHO), and 1-methylvinoxy (CH3COCH2) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	0