Michael E Harding

List of Publications by Year
in descending order

56 papers	3,024 citations	270111 25 h-index	182931 54 g-index
58 all docs	58 docs citations	58 times ranked	3436 citing authors

#	Article	IF	Citations
1	Infrared action spectroscopy of fundamental nitrilium ions: Protonated vinyl- and ethyl cyanide. Journal of Molecular Spectroscopy, 2022, 386, 111615.	0.4	1
2	The Heâ€“H3+ complex. I. Vibration-rotation-tunneling states and transition probabilities. Journal of Chemical Physics, 2022, 156, 144307.	1.2	2
3	The Heâ€“H3+ complex. II. Infrared predissociation spectrum and energy term diagram. Journal of Chemical Physics, 2022, 156, 144308.	1.2	3
4	High-resolution infrared study of vinyl acetylene: The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si195.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>Î½</mml:mi></mml:mrow><mml:mrow><mml:mn>13</mml:mn> (214â€“cmâ^1) and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si196.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>Î½</mml:mi></mml:mrow><mml:mrow><mml:mn>18</mml:mn> (304â€“cmâ^1) fundamentals. Journal of Molecular Spectroscopy, 2021, 379, 111469.	0.4	3
5	Hyperfine-Resolved Near-Infrared Spectra of H₂¹⁷O. Journal of Physical Chemistry A, 2021, 125, 7884-7890.	1.1	11
6	Descendant of the X-ogen carrier and a â€˜mass of 69â€™: infrared action spectroscopic detection of HC₃O⁺ and HC₃S⁺. Molecular Physics, 2020, 118, e1776409.	0.8	17
7	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	1.2	28
8	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
9	Determination of accurate rest frequencies and hyperfine structure parameters of cyanobutadiyne, HC5N. Journal of Molecular Spectroscopy, 2020, 371, 111303.	0.4	3
10	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	1.2	375
11	Frequency-comb spectroscopy on pure quantum states of a single molecular ion. Science, 2020, 367, 1458-1461.	6.0	45
12	Understanding UVâ€“Vis Spectra of Halogenated Tetraazaperopyrenes (TAPPs): A Computational Study. Journal of Physical Chemistry A, 2019, 123, 3160-3169.	1.1	9
13	Optimized auxiliary basis sets for density fitted post-Hartreeâ€“Fock calculations of lanthanide containing molecules. Molecular Physics, 2018, 116, 1523-1538.	0.8	32
14	Vibronic Coupling Analysis of the Ligand-Centered Phosphorescence of Gas-Phase Gd(III) and Lu(III) 9-Oxophenalen-1-one Complexes. Journal of Physical Chemistry A, 2018, 122, 2461-2467.	1.1	5
15	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	1.2	44
16	Betheâ€“Salpeter correlation energies of atoms and molecules. Journal of Chemical Physics, 2018, 149, 144106.	1.2	24
17	A highly flexible molecule: The peculiar case of ethynyl isothiocyanate HCCNCS. Journal of Chemical Physics, 2018, 149, 104304.	1.2	12
18	High-accuracy extrapolated ab initio thermochemistry of the NCN radical. Chemical Physics Letters, 2018, 706, 613-616.	1.2	4

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19	Equilibrium molecular structures of vinyl carbon chains: Vinyl acetylene, vinyl diacetylene, and vinyl cyanide. Journal of Molecular Spectroscopy, 2018, 350, 10-17.	0.4	5
20	Correlation of the structural information obtained for europium-chelate ensembles from gas-phase photoluminescence and ion-mobility spectroscopy with density-functional computations and ligand-field theory. Physical Chemistry Chemical Physics, 2017, 19, 6105-6112.	1.3	7
21	Differential Manyâ€Body Cooperativity in Electronic Spectra of Oligonuclear Transitionâ€Metal Complexes. ChemPhysChem, 2016, 17, 37-45.	1.0	19
22	Quasi-Particle Self-Consistent GW for Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2528-2541.	2.3	114
23	Gas-Phase Photoluminescence Characterization of Stoichiometrically Pure Nonanuclear Lanthanoid Hydroxo Complexes Comprising Europium or Gadolinium. Inorganic Chemistry, 2016, 55, 3316-3323.	1.9	10
24	The hyperfine structure in the rotational spectra of D217O and HD17O: Confirmation of the absolute nuclear magnetic shielding scale for oxygen. Journal of Chemical Physics, 2015, 142, 124308.	1.2	16
25	Coupled-cluster reference values for the GW27 and GW100 test sets for the assessment of GW methods. Molecular Physics, 2015, 113, 1952-1960.	0.8	70
26	Millimeter- and submillimeter-wave spectroscopy of disulfur dioxide, OSSO. Journal of Molecular Spectroscopy, 2015, 307, 33-39.	0.4	32
27	Substitutional Photoluminescence Modulation in Adducts of a Europium Chelate with a Range of Alkali Metal Cations: A Gas-Phase Study. Journal of Physical Chemistry A, 2014, 118, 94-102.	1.1	13
28	Characterization of Nonanuclear Europium and Gadolinium Complexes by Gas-Phase Luminescence Spectroscopy. Journal of Physical Chemistry Letters, 2014, 5, 1727-1731.	2.1	14
29	Effect of Proton Substitution by Alkali Ions on the Fluorescence Emission of Rhodamine B Cations in the Gas Phase. Journal of Physical Chemistry A, 2014, 118, 3787-3794.	1.1	21
30	Systematic construction of complementary auxiliary basis sets from and for atomic natural orbitals. Molecular Physics, 2013, 111, 2585-2593.	0.8	0
31	Intrinsic fluorescence properties of rhodamine cations in gas-phase: triplet lifetimes and dispersed fluorescence spectra. Physical Chemistry Chemical Physics, 2013, 15, 8162.	1.3	37
32	High-Resolution Spectroscopy of C₃ around 3 Î¼m. Journal of Physical Chemistry A, 2013, 117, 3332-3339.	1.1	23
33	The bromine nuclear quadrupole moment revisited. Molecular Physics, 2013, 111, 1382-1389.	0.8	7
34	Benchmarking the Lithiumâ€“Thiophene Complex. ChemPhysChem, 2013, 14, 708-715.	1.0	14
35	High-Accuracy Extrapolated Ab Initio Thermochemistry of the Vinyl, Allyl, and Vinoxy Radicals. Journal of Physical Chemistry A, 2012, 116, 7668-7676.	1.1	12
36	Why Benchmark-Quality Computations Are Needed To Reproduce 1-Adamantyl Cation NMR Chemical Shifts Accurately. Journal of Physical Chemistry A, 2011, 115, 2340-2344.	1.1	23

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37	Vibrational Energy Levels via Finite-Basis Calculations Using a Quasi-Analytic Form of the Kinetic Energy. Journal of Chemical Theory and Computation, 2011, 7, 1428-1442.	2.3	20
38	Electron Affinities, Well Depths, and Vibrational Spectroscopy of cis- and trans-HOCO. Journal of the American Chemical Society, 2011, 133, 19606-19609.	6.6	45
39	High-resolution OPO spectroscopy of Si2C3 at 5Î¼m: Observation of hot band transitions associated with Î½3. Journal of Molecular Spectroscopy, 2011, 270, 75-78.	0.4	15
40	Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513.	1.2	44
41	Parallel Calculation of CCSDT and Mk-MRCCSDT Energies. Journal of Chemical Theory and Computation, 2010, 6, 2339-2347.	2.3	39
42	Tunneling in a Simple Bond Scission: The Surprising Barrier in the H Loss from HCOOH⁺. Journal of Physical Chemistry A, 2010, 114, 10016-10023.	1.1	20
43	Coupled-cluster calculations of C2H2Si and CNHSi structural isomers. Journal of Chemical Physics, 2009, 130, 214303.	1.2	30
44	The hyperfine structure in the rotational spectrum of water: Lamb-dip technique and quantum-chemical calculations. Chemical Physics Letters, 2009, 473, 21-25.	1.2	46
45	Dissociation Energy of the HOOO Radical. Journal of Physical Chemistry A, 2009, 113, 11238-11241.	1.1	46
46	High-Accuracy Extrapolated ab Initio Thermochemistry of the Propargyl Radical and the Singlet C₃H₂ Carbenes. Journal of Physical Chemistry A, 2009, 113, 12447-12453.	1.1	39
47	A new experimental absolute nuclear magnetic shielding scale for oxygen based on the rotational hyperfine structure of H2O17. Journal of Chemical Physics, 2009, 131, 234304.	1.2	72
48	Hyperfine structure in theJ= 1â€“0 transitions of DCO⁺, DNC, and HN¹³C: astronomical observations and quantum-chemical calculations. Astronomy and Astrophysics, 2009, 507, 347-354.	2.1	49
49	Rotational spectra and hyperfine structure of isotopic species of deuterated cyanoacetylene, DC3N. Chemical Physics, 2008, 346, 132-138.	0.9	22
50	The empirical equilibrium structure of diacetylene. Journal of Molecular Spectroscopy, 2008, 251, 220-223.	0.4	36
51	On the geometry of the HO3 radical. Chemical Physics, 2008, 346, 53-55.	0.9	32
52	Parallel Calculation of CCSD and CCSD(T) Analytic First and Second Derivatives. Journal of Chemical Theory and Computation, 2008, 4, 64-74.	2.3	249
53	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	1.2	367
54	Theoretical investigation of electronic excitation energy transfer in bichromophoric assemblies. Journal of Chemical Physics, 2008, 128, 074505.	1.2	84

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55	Quantitative prediction of gas-phase F19 nuclear magnetic shielding constants. Journal of Chemical Physics, 2008, 128, 244111.	1.2	79
56	High-Accuracy Extrapolated Ab Initio Thermochemistry of Vinyl Chloride. Journal of Physical Chemistry A, 2007, 111, 13623-13628.	1.1	13