Michael E Harding

List of Publications by Year
in descending order

56 papers	3,024 citations	236912 25 h-index	161844 54 g-index
58 all docs	58 docs citations	58 times ranked	3067 citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
3	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	3.0	367
4	Parallel Calculation of CCSD and CCSD(T) Analytic First and Second Derivatives. Journal of Chemical Theory and Computation, 2008, 4, 64-74.	5.3	249
5	Quasi-Particle Self-Consistent GW for Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2528-2541.	5.3	114
6	Theoretical investigation of electronic excitation energy transfer in bichromophoric assemblies. Journal of Chemical Physics, 2008, 128, 074505.	3.0	84
7	Quantitative prediction of gas-phase F19 nuclear magnetic shielding constants. Journal of Chemical Physics, 2008, 128, 244111.	3.0	79
8	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.	3.0	72
9	Coupled-cluster reference values for the GW27 and GW100 test sets for the assessment of GW methods. Molecular Physics, 2015, 113, 1952-1960.	1.7	70
10	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.	5.1	49
11	The hyperfine structure in the rotational spectrum of water: Lamb-dip technique and quantum-chemical calculations. Chemical Physics Letters, 2009, 473, 21-25.	2.6	46
12	Dissociation Energy of the HOOO Radical. Journal of Physical Chemistry A, 2009, 113, 11238-11241.	2.5	46
13	Electron Affinities, Well Depths, and Vibrational Spectroscopy of cis- and trans-HOCO. Journal of the American Chemical Society, 2011, 133, 19606-19609.	13.7	45
14	Frequency-comb spectroscopy on pure quantum states of a single molecular ion. Science, 2020, 367, 1458-1461.	12.6	45
15	Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513.	3.0	44
16	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
17	High-Accuracy Extrapolated ab Initio Thermochemistry of the Propargyl Radical and the Singlet C₃H₂ Carbenes. Journal of Physical Chemistry A, 2009, 113, 12447-12453.	2.5	39
18	Parallel Calculation of CCSDT and Mk-MRCCSDT Energies. Journal of Chemical Theory and Computation, 2010, 6, 2339-2347.	5.3	39

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19	Intrinsic fluorescence properties of rhodamine cations in gas-phase: triplet lifetimes and dispersed fluorescence spectra. Physical Chemistry Chemical Physics, 2013, 15, 8162.	2.8	37
20	The empirical equilibrium structure of diacetylene. Journal of Molecular Spectroscopy, 2008, 251, 220-223.	1.2	36
21	On the geometry of the HO3 radical. Chemical Physics, 2008, 346, 53-55.	1.9	32
22	Millimeter- and submillimeter-wave spectroscopy of disulfur dioxide, OSSO. Journal of Molecular Spectroscopy, 2015, 307, 33-39.	1.2	32
23	Optimized auxiliary basis sets for density fitted post-Hartreeâ€“Fock calculations of lanthanide containing molecules. Molecular Physics, 2018, 116, 1523-1538.	1.7	32
24	Coupled-cluster calculations of C2H2Si and CNHSi structural isomers. Journal of Chemical Physics, 2009, 130, 214303.	3.0	30
25	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
26	Betheâ€“Salpeter correlation energies of atoms and molecules. Journal of Chemical Physics, 2018, 149, 144106.	3.0	24
27	Why Benchmark-Quality Computations Are Needed To Reproduce 1-Adamantyl Cation NMR Chemical Shifts Accurately. Journal of Physical Chemistry A, 2011, 115, 2340-2344.	2.5	23
28	High-Resolution Spectroscopy of C₃ around 3 Î¼m. Journal of Physical Chemistry A, 2013, 117, 3332-3339.	2.5	23
29	Rotational spectra and hyperfine structure of isotopic species of deuterated cyanoacetylene, DC3N. Chemical Physics, 2008, 346, 132-138.	1.9	22
30	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.	2.5	21
31	Tunneling in a Simple Bond Scission: The Surprising Barrier in the H Loss from HCOOH⁺. Journal of Physical Chemistry A, 2010, 114, 10016-10023.	2.5	20
32	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.	5.3	20
33	Differential Manyâ€Body Cooperativity in Electronic Spectra of Oligonuclear Transitionâ€Metal Complexes. ChemPhysChem, 2016, 17, 37-45.	2.1	19
34	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.	1.7	17
35	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.	3.0	16
36	High-resolution OPO spectroscopy of Si2C3 at 5Î¼m: Observation of hot band transitions associated with Î½3. Journal of Molecular Spectroscopy, 2011, 270, 75-78.	1.2	15

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37	Benchmarking the Lithiumâ€“Thiophene Complex. ChemPhysChem, 2013, 14, 708-715.	2.1	14
38	Characterization of Nonanuclear Europium and Gadolinium Complexes by Gas-Phase Luminescence Spectroscopy. Journal of Physical Chemistry Letters, 2014, 5, 1727-1731.	4.6	14
39	High-Accuracy Extrapolated Ab Initio Thermochemistry of Vinyl Chloride. Journal of Physical Chemistry A, 2007, 111, 13623-13628.	2.5	13
40	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.	2.5	13
41	High-Accuracy Extrapolated Ab Initio Thermochemistry of the Vinyl, Allyl, and Vinoxy Radicals. Journal of Physical Chemistry A, 2012, 116, 7668-7676.	2.5	12
42	A highly flexible molecule: The peculiar case of ethynyl isothiocyanate HCCNCS. Journal of Chemical Physics, 2018, 149, 104304.	3.0	12
43	Hyperfine-Resolved Near-Infrared Spectra of H₂¹⁷O. Journal of Physical Chemistry A, 2021, 125, 7884-7890.	2.5	11
44	Gas-Phase Photoluminescence Characterization of Stoichiometrically Pure Nonanuclear Lanthanoid Hydroxo Complexes Comprising Europium or Gadolinium. Inorganic Chemistry, 2016, 55, 3316-3323.	4.0	10
45	Understanding UVâ€“Vis Spectra of Halogenated Tetraazaperopyrenes (TAPPs): A Computational Study. Journal of Physical Chemistry A, 2019, 123, 3160-3169.	2.5	9
46	The bromine nuclear quadrupole moment revisited. Molecular Physics, 2013, 111, 1382-1389.	1.7	7
47	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.	2.8	7
48	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.	2.5	5
49	Equilibrium molecular structures of vinyl carbon chains: Vinyl acetylene, vinyl diacetylene, and vinyl cyanide. Journal of Molecular Spectroscopy, 2018, 350, 10-17.	1.2	5
50	High-accuracy extrapolated ab initio thermochemistry of the NCN radical. Chemical Physics Letters, 2018, 706, 613-616.	2.6	4
51	Determination of accurate rest frequencies and hyperfine structure parameters of cyanobutadiyne, HC5N. Journal of Molecular Spectroscopy, 2020, 371, 111303.	1.2	3
52	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></mml:mrow></mml:msub></mml:mrow></mml:math> (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></mml:mrow></mml:msub></mml:mrow></mml:math> (304â€“cmâ»1) fundamentals. Journal of Molecular Spectroscopy, 2021, 379, 111469.	1.2	3
53	The Heâ€“H3+ complex. II. Infrared predissociation spectrum and energy term diagram. Journal of Chemical Physics, 2022, 156, 144308.	3.0	3
54	The Heâ€“H3+ complex. I. Vibration-rotation-tunneling states and transition probabilities. Journal of Chemical Physics, 2022, 156, 144307.	3.0	2

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55	Infrared action spectroscopy of fundamental nitrilium ions: Protonated vinyl- and ethyl cyanide. Journal of Molecular Spectroscopy, 2022, 386, 111615.	1.2	1
56	Systematic construction of complementary auxiliary basis sets from and for atomic natural orbitals. Molecular Physics, 2013, 111, 2585-2593.	1.7	0